

Finite element error estimates for a phase field model associated to binary alloys

Den Naturwissenschaftlichen Fakultäten
der Friedrich-Alexander-Universität Erlangen-Nürnberg
zur
Erlangung des Doktorgrades

vorgelegt von
Baasansuren Jadamba
aus Bulgan

Als Dissertation genehmigt von der Naturwissen-
schaftlichen Fakultäten der Universität Erlangen-Nürnberg

Tag der mündlichen Prüfung: 21.07.2004

Vorsitzender der

Promotionskommission: Prof. Dr. L. Dahlenburg

Erstberichterstatter: Prof. Dr. P. Knabner

Zweitberichterstatter: PD Dr. W. Merz

Acknowledgments

First and foremost, I wish to express my deepest appreciations to my advisor Prof. Dr. P. Knabner for his enthusiasm, able supervision and support. I am very grateful to him for giving me an opportunity to work at the Institute for Applied Mathematics and to do this work. I sincerely thank him for giving me a topic, which not only has an appealing real world application but also a challenging mathematical structure.

During the preparation of this work, the one who had a great impact on the present work and me is Dr. Ch. Eck. I have no words to describe the help, encouragement, support he kindly extended. His vast knowledge over the subject, guided to remove many misconceptions and helped me to broaden my understanding in the field. The hours of long discussions with him are highly appreciated. I would also like to thank PD. Dr. W. Merz for his kind suggestions on the work and being supportive throughout my stay at the institute.

I am glad to acknowledge the support I received from all members of the institute and thankful to them for creating a pleasant working environment at the institute. My special thanks to Herr P. Mirsch.

It is a pleasure for me to dedicate this work to my parents who have always been source of encouragement for me. Finally, I also wish to thank Akhtar for his love and support.

Contents

1	Introduction	3
1.1	Modeling of solidification	3
1.2	Works on phase field models	5
1.3	Overview of this work	6
2	A phase field model	9
2.1	Phase transitions in alloys	9
2.2	A model for binary alloys	11
2.3	Dendritic structures and anisotropy of the surface tension	14
3	Error estimates for the solution of a fully discrete scheme	19
3.1	Preliminaries	21
3.2	Energy estimates for the phase field model	26
3.3	Spectrum estimates	35
3.4	Fully discrete finite element method	40
3.5	Error estimates	47
4	Numerical experiments for the discretization error	69
4.1	Approximate error and experiments	69
4.2	Nonlinear least squares problem	70
4.3	Linear least squares problem	73
4.4	Data and numerical scheme	73
4.5	Tests for an anisotropic model	77
5	Adaptive simulation of dendritic crystals	81
5.1	The problem	81
5.2	Numerical results	85
A	Appendix	91
A.1	Formal asymptotic expansions	91
	Bibliography	99

Zusammenfassung**103****Lebenslauf****105**

Chapter 1

Introduction

1.1 Modeling of solidification

Solidification phenomena play an important role for a variety of processes. An important application arises, for example, in the casting of metals and alloys. The quality of the casting products depends on certain properties of the material and microstructures forming during the solidification. Therefore it is important to study the microstructures in order to influence and improve the quality of the products. Solidification is a phase transition process which can be modeled by Stefan type approaches with surface tension and kinetic effects. The interface between liquid and solid phases is described in such models as a surface of zero thickness, therefore the models are called sharp interface models. The models involve equations for thermodynamic variables (temperature and composition) in each phase and impose certain conditions on the moving interface. Sharp interface models are well studied and documented in the literature. The numerical solution procedures for these models involve an explicit tracking of the interface which leads to complicated numerical algorithms due to the complex geometries of the interface.

In recent years, the so-called phase field models were introduced as an alternative approach for the modeling of phase transition processes. The essential difference between phase field and sharp interface models is the introduction of an order parameter in the former which henceforth will be referred to as the *phase field*.

In the phase field approaches, one considers a diffuse transition layer between solid and liquid phases instead of a sharp interface. The phase field, usually denoted by $\varphi = \varphi(x, t)$, is a function of space and time and its value determines the phase at the point $x \in \Omega = \Omega_L \cup \Omega_S$ at time t (cf. Figure 1.1). The function is supposed to take constant values in pure solid and pure liquid phases. The intermediate values correspond to the

position of the diffuse interface (cf. Figure 1.2). Phase field models contain

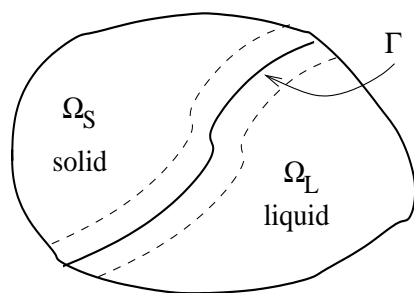


Figure 1.1: Interface

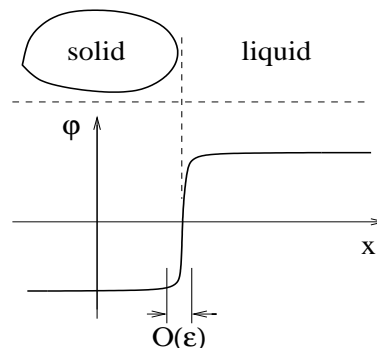


Figure 1.2: Profile of φ

a small parameter ε representing the thickness of the transition layer. By making this parameter sufficiently small one may approximate classical sharp interface models. Relations between phase field and sharp interface models have been considered by many authors. The convergence of the phase field model to the sharp interface model in the limit of the interface thickness parameter to zero has been established for various models.

There are several advantages of the phase field approach in the modeling of growth phenomena. One major advantage is that it provides a simple and elegant description of various realistic situations. Besides this, the phase field formulation is convenient for many numerical solution procedures since there is no necessity for any explicit tracking of the moving interface and the solution is quite simple to obtain.

Considering the solidification process one may have a situation which involves only a pure material and its melt. In this case the process can be modeled by a system of partial differential equations involving temperature T and phase field φ . These models are often referred to as *models for pure material*.

On the other hand, if a material consisting of several substances (an alloy) is under consideration, then in addition to temperature T and phase field φ , the concentrations of the alloy components need to be taken into account. As a consequence of this one additionally has diffusion equations for the concentration of the alloy components c_i , $i = 1, 2, \dots, n - 1$ with n being the number of components of the alloy. These models are termed as *models for alloys*. We will consider a phase field model for binary alloys.

For pure material as well as for alloy problems one has a coupled nonlinear system of parabolic partial differential equations whose solution can only be found numerically except for very simple cases. One of the challenges of

numerical methods for phase field models lies on the parameter ε which is very small for recovering physically realistic cases. Therefore, the grid size in numerical simulations (using for example, finite element methods) should at least be of order ε , a requirement which eventually leads to a large number of degrees of freedom and hence demands a big amount of computational work. Due to this reason it is advantageous to use a grid which is fine in the vicinity of the interface and coarse away from the interface. Accuracy of the numerical methods in dependence of the parameter ε is also of major interest.

1.2 Works on phase field models

In this section, we make a brief review of what has been done in the past years regarding phase field models. The review is in no way complete since there has been an enormous amount of work done in the field, especially in the last few years. A phase field model for solidification in *pure material* was introduced by Caginalp [7] as a new approach to phase transition problems. The author performed a mathematical analysis of the model, established relations between various models and studied their asymptotic limits to sharp interface models in his later works [8, 9] as well. The convergence of phase field models to sharp interface models was investigated by Caginalp and Chen [14].

A numerical analysis of an anisotropic phase field model has been presented by Caginalp and Lin [11], and Lin [36]. Caginalp and Socolovsky [15] have presented numerical studies of various problems modeled by the phase field approach such as crystal growth and motion by mean curvature. Kobayashi [34] proposed a different type of phase field model and presented numerical simulations of dendritic crystal growth by introducing an anisotropy of the surface tension. Fabbri and Voller [25] have made qualitative comparisons between the models of Caginalp and Kobayashi and their sharp interface limits using numerical simulations in one dimension.

In recent years quite a number of works regarding numerical methods, computational efficiency, model parameters, simulation of dendritic growth by introducing anisotropy into phase field models, quality of solutions and stability issues of various models have been done. We mention here works of Braun, McFadden and Coriell [5], and Karma and Rappel [30]. Wang and Sekerka [44] have investigated dendrite tip shapes and tip velocities in pure melt. Adaptive computations of dendritic microstructures using phase field models have been done by Provatas, Goldenfeld and Dantzig [39]. Feng and Prohl [27] have derived finite element error estimates for a model for pure material and investigated the dependence of error constants on the

interface thickness parameter ε in their work. They have proved that the error constants depend in low polynomial order on ε^{-1} under reasonable requirements on space and time mesh sizes.

Recently, Caginalp and Xie [12] have introduced phase field models for phase transitions in *binary alloys*. The mathematical model, asymptotic analysis, convergence to the sharp interface models were also covered in their work [13]. Wheeler, Boettinger and McFadden [46] have proposed an *isothermal* model of phase transitions in binary alloys and presented numerical simulations in one and two dimensions. Warren and Boettinger [45] have computed two dimensional dendritic structures by using an anisotropic isothermal phase field model. More recently, a similar isothermal phase field model has been considered by Kessler et al. [31]. An analysis of the model and numerical results with an adaptive mesh strategy have also been presented in this work. Error estimates for a finite element method for the above model were done by Kessler and Scheid [32], and the issue of existence of solutions has been raised by Rappaz and Scheid [40].

1.3 Overview of this work

In this work, we consider a phase field model for binary alloys consisting of the equations for phase field φ , temperature T and concentration c of a component of the alloy. Our aim is to present a detailed study of a numerical scheme both from theoretical and computational point of view. We derive error estimates for a fully discrete finite element method for the model. The dependence of the errors on the parameter ε is here of particular importance.

We also investigate the dependence of the error on ε numerically and present results supporting the theoretical predictions. Finally, we consider some aspects of simulation of dendritic growth in two and three dimensions by introducing anisotropy into the model.

The work is organized into five chapters. We begin by studying the physical background of a model for binary alloys and the derivation of the model equations by using a free energy functional. We also discuss anisotropy of the surface tension and derive a phase field model that we later use for the simulation of dendritic structures. Chapter 3, which is divided into several sections and subsections, deals with error estimates. Each section of this chapter contains results of their own significance which collectively lead to the main error estimates presented in Section 3.5. In Section 3.1 we introduce some function spaces and norms. The section also contains some embedding and interpolation theorems which we use. In Section 3.2 we derive some energy estimates for the solution of the problem in different norms. Section 3.3 of this chapter is devoted to the spectrum estimate for the problem. A fully

discrete scheme for the model is introduced and analyzed in Section 3.4. We also derive some stability estimates for the discrete solution and a discrete version of the spectrum estimate in this section. With the above preparations, the actual error estimates are derived in Section 3.5.

Chapter 4 contains numerical experiments that analyze the dependence of the error on the parameter ε . We also deal with the least square problems arising from the identification of parameters in error functionals. Test results in two and three dimensions are presented here and the connection to the theoretical results of the previous chapter is discussed.

In Chapter 5 we simulate dendritic structures by using the anisotropic phase field model for alloys introduced in Chapter 2. The numerical scheme and some computational aspects are addressed in this chapter. Finally, we present results of the simulations of dendritic growth in two and three dimensions.

Appendix A.1 contains a formal asymptotic expansions of the phase field system. Inner (near to the interface between solid and liquid) and outer (far from the interface) expansions are considered here and some conditions on the coefficient functions of the inner expansions are derived. The appendix serves as a basis for the spectrum estimates considered in Section 3.3.

Chapter 2

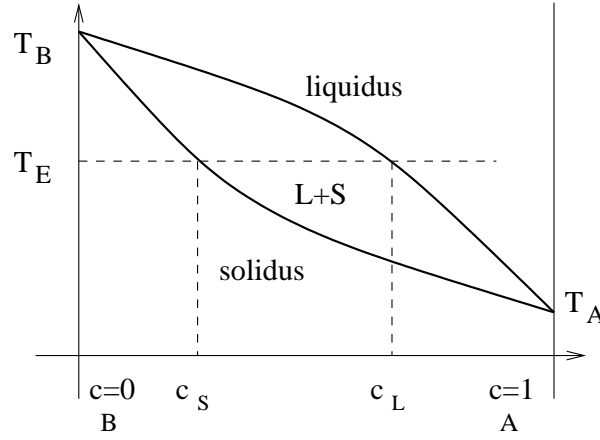
A phase field model

This chapter is concerned with the derivation of a phase field model for binary alloys. Before presenting the main model we discuss some physical background of the underlying process and formulate a related sharp interface model.

2.1 Phase transitions in alloys

Let us consider phase transformations occurring in a binary alloy that exists in solid and liquid phases. The equilibrium melting temperature describing the phase transition depends on the composition of the alloy in this case. The relation between the temperature and the concentration of a component of the alloy is described by a (c, T) phase diagram. A simple example of a phase diagram is shown in Figure 2.1. The solid and liquid phases are separated by two curves, the liquidus and solidus lines, merging at the melting points $(0, T_B)$ and $(1, T_A)$ of the pure materials A and B . At temperature T_E which lies between T_A and T_B we have different concentration values at the solidus and liquidus line. The concentration has a jump from c_S to c_L at the phase boundary. At the temperatures greater than T_B or less than T_A , we have stable liquid and solid phases, respectively. The diagram corresponds to the situation that the solute is rejected into the liquid as the material freezes.

The classical approach for modeling phase transformations are sharp interface models. A typical example is the modified Stefan model with surface tension and kinetics where a material is in liquid and solid phases in some region which we represent by $\Omega \in \mathbb{R}^N$. The two phases are separated by an interface $\Gamma(t)$. Denote by $T(x, t)$ the temperature and by $c(x, t)$ the concentration of the component A of the alloy. The two phase alloy model [13] is

Figure 2.1: A (c, T) phase diagram

then formulated as

$$C_V T_t = \nabla \cdot (K \nabla T) \quad \text{in } \Omega \setminus \Gamma(t) \quad (2.1a)$$

$$[T]_{-}^{+} = 0 \quad \text{on } \Gamma(t) \quad (2.1b)$$

$$\ell v = [K \nabla T \cdot n]_{-}^{+} \quad \text{on } \Gamma(t) \quad (2.1c)$$

$$c_t = D^{\pm} \Delta c \quad \text{in } \Omega \setminus \Gamma(t) \quad (2.1d)$$

$$-v[c]_{-}^{+} = [D \nabla c \cdot n]_{-}^{+} \quad \text{on } \Gamma(t) \quad (2.1e)$$

$$T - T_B = -\frac{\sigma}{[s]_E} (\kappa + \alpha v) + \frac{1}{2} (m_L c_+ + m_S c_-) \quad \text{on } \Gamma(t) \quad (2.1f)$$

$$m_L c_+ = m_S c_-, \quad (2.1g)$$

where C_V is the specific heat per unit volume, K the thermal conductivity, ℓ the latent heat per unit volume, v the normal velocity of the interface and n is the unit normal vector to the interface. The jump between solid ($-$) and liquid ($+$) phases is denoted by $[\cdot]_{-}^{+}$. The subscript t is used for the derivatives with respect to time. Moreover, D^{\pm} are the diffusivities of the solute in the liquid and solid phases and T_B is the melting temperature of the pure B material. The entropy difference in equilibrium between liquid and solid phases is denoted by $[s]_E$ and the sum of the principal curvatures at a point on $\Gamma(t)$ is denoted by κ . The surface tension σ and the relaxation scaling α are present in the interface condition (2.1f). The Gibbs-Thompson effects (the term with $\sigma\kappa$) and kinetic undercoolings (the term with $\sigma\alpha v$) are reflected by this condition. The limits of c from the liquid and solid sides are denoted by c_+ and c_- , respectively. Finally, the values m_L, m_S are the slopes of the liquidus and solidus lines on the (c, T) phase diagram.

The sharp interface problem can be formulated as follows: Find (T, c, Γ) satisfying (2.1) subjected to some initial and boundary conditions.

2.2 A model for binary alloys

A phase field model for binary alloys can be derived by means of a free energy functional which depends on temperature T , concentration c and an order parameter (or phase field) φ . The order parameter φ is a smooth function taking value 1 in liquid and -1 in solid.

We consider a free energy functional with parameters ξ and a

$$\mathcal{F}(\varphi, T, c) = \int_{\Omega} \left\{ \frac{\xi^2}{2} |\nabla \varphi|^2 + \frac{1}{a} F(\varphi) + P(\varphi, T, c) \right\} dx \quad (2.2)$$

and with a double well potential

$$F(\varphi) = \frac{1}{4}(\varphi^2 - 1)^2$$

and the bulk free energy density $P(\varphi, T, c)$. The bulk free energy is typically given by an interpolation between the free energies of the two phases, for example,

$$P(\varphi, T, c) = \zeta(\varphi)P_L(T, c) + (1 - \zeta(\varphi))P_S(T, c)$$

with a function ζ satisfying $\zeta(1) = 1$ and $\zeta(-1) = 0$. The parameter ξ is the length scale associated to the microscopic interaction strength and a is related with the depth of the double well potential. We use a bulk free energy chosen as in [13], e.g.

$$\begin{aligned} P(\varphi, T, c) = & -\frac{[s]_A}{2}(T - T_A)\varphi c - \frac{[s]_B}{2}(T - T_B)\varphi(1 - c) \\ & - Vc(1 - c) + RT[c \ln c + (1 - c) \ln(1 - c)] - C_V T \ln T. \end{aligned}$$

The constants T_A, T_B are equilibrium melting points, and $[s]_A, [s]_B$ are entropy differences between the two phases of the pure materials A and B . The term $Vc(1 - c)$ arises from the differences in bonding energies and the terms involving logarithms with the gas constant R correspond to the free energy of mixing (temperature times entropy of mixing). Specific heat per unit volume is denoted by C_V .

The double well potential $F(\varphi)$ reflects the association of lower free energies in pure phases (at $\varphi = \pm 1$, pure liquid or solid). The term $\frac{1}{2}\xi^2|\nabla\varphi|^2$ introduces a surface free energy to the model and provides smooth transitions between phases. We will reconsider this term for an application of the phase field model in the next section.

In context of statistical mechanics the correct function φ which occurs in equilibrium is that minimizing the free energy. In a dynamic approximation, the equation for the phase field φ is derived by relaxation

$$\tau\varphi_t = -\frac{\delta\mathcal{F}}{\delta\varphi} \quad (2.3)$$

where $\frac{\delta\mathcal{F}}{\delta\varphi}$ is the Fréchet derivative of \mathcal{F} with respect to φ defined by

$$\left(\frac{\delta\mathcal{F}}{\delta\varphi}, \psi\right) = \lim_{s \rightarrow 0} \frac{1}{s} (\mathcal{F}(\varphi + s\psi, T, c) - \mathcal{F}(\varphi, T, c)).$$

With the definition of macroscopic parameters

$$\varepsilon = \xi a^{1/2}, \quad \sigma = \frac{2\sqrt{2}}{3}\xi a^{-1/2}, \quad \alpha = \frac{\tau}{\xi^2} \quad (2.4)$$

we can write the phase field equation in the following form:

$$\alpha\varepsilon^2\varphi_t = \varepsilon^2\Delta\varphi + \varphi(1 - \varphi^2) + \frac{\sqrt{2}\varepsilon}{3\sigma} ([s]_A(T - T_A)c + [s]_B(T - T_B)(1 - c))$$

where ε corresponds to the interface thickness and σ to the surface tension. Furthermore, we use the notations

$$f(\varphi) := F'(\varphi) = \varphi^3 - \varphi \quad (2.5a)$$

$$q(T, c) := -\frac{\sqrt{2}}{3\sigma} ([s]_A(T - T_A)c + [s]_B(T - T_B)(1 - c)) \quad (2.5b)$$

to write the phase field equation as follows:

$$\alpha\varepsilon\varphi_t - \varepsilon\Delta\varphi + \frac{1}{\varepsilon}f(\varphi) + q(T, c) = 0.$$

An equation for the temperature is derived from the density of the internal energy u . The relation

$$u = P - T\frac{\partial P}{\partial T}$$

(with $C_V = 1$) gives us

$$u = T + Vc(1 - c) + L(c)\varphi$$

where

$$L(c) = \frac{[s]_A}{2}T_Ac + \frac{[s]_B}{2}T_B(1 - c)$$

is half of the latent heat. With the simplifications $V = 0$ (that is true for ideal mixtures) and $T_A[s]_A = T_B[s]_B$ which makes the latent heat independent of the concentration, we get by

$$u_t = \nabla \cdot (K \nabla T)$$

the equation

$$T_t + L\varphi_t = \nabla \cdot (K \nabla T)$$

with K being the heat conductivity.

The equation for the concentration c can be derived by

$$c_t = \nabla \cdot \left(\tilde{D}c(1-c) \nabla \left(\frac{1}{T} \frac{\partial P}{\partial c} \right) \right)$$

with $\tilde{D}c(1-c)$ being a term reflecting the scenario that mobility vanishes in two pure materials and attains its peak at equal concentrations of the two materials of the alloy. Setting

$$\begin{aligned} D &= \tilde{D}R \\ M(c) &= \frac{1}{R} \frac{[s]_B - [s]_A}{2} c(1-c) \end{aligned}$$

we get

$$c_t = \nabla \cdot (D \nabla c) + \nabla \cdot (DM(c) \nabla \varphi).$$

The solute diffusivity D may depend on the phase field φ and can be taken as

$$D(\varphi) = \frac{1}{2}(d_L - d_S)(1 + \varphi) + d_S \quad (2.6)$$

with d_L, d_S being the solute diffusivities of liquid and solid material. Usually d_S is much smaller than d_L .

Now, we have a phase field system for (φ, T, c)

$$\alpha \varepsilon \varphi_t - \varepsilon \Delta \varphi + \frac{1}{\varepsilon} f(\varphi) + q(T, c) = 0 \quad (2.7a)$$

$$T_t - \nabla \cdot (K \nabla T) + L\varphi_t = 0 \quad (2.7b)$$

$$c_t - \nabla \cdot (D \nabla c) - \nabla \cdot (DM(c) \nabla \varphi) = 0 \quad (2.7c)$$

in $(0, \mathcal{T}] \times \Omega$ considered with the boundary conditions

$$\nabla \varphi \cdot n = 0 \quad (2.8a)$$

$$K \nabla T \cdot n = 0 \quad (2.8b)$$

$$(D \nabla c + DM(c) \nabla \varphi) \cdot n = 0 \quad (2.8c)$$

on $\partial\Omega$, and initial conditions

$$\varphi(0, x) = \varphi_0(x), \quad T(0, x) = T_0(x), \quad c(0, x) = c_0(x) \text{ in } \Omega. \quad (2.9)$$

The interface can be approximately specified as $\Gamma(t) = \{x : \varphi(x, t) = 0\}$.

We mention here that a phase field model for the case of a pure material can be derived similar way as for the case with binary alloys. Namely, by setting $c = 0$ (or $c = 1$) in the free energy functional for binary alloys and repeating the same procedure of derivation.

An example of the model for pure material is

$$\alpha\varepsilon\varphi_t - \varepsilon\Delta\varphi + \frac{1}{\varepsilon}f(\varphi) - \frac{\sqrt{2}}{3\sigma}[s]_E(T - T_M) = 0 \quad (2.10)$$

$$T_t - \nabla \cdot (K\nabla T) + L\varphi_t = 0 \quad (2.11)$$

considered in $\Omega \times (0, \mathcal{T}]$ with the boundary conditions

$$\nabla\varphi \cdot n = 0, \quad K\nabla T \cdot n = 0 \quad \text{on } \partial\Omega$$

and initial functions $\varphi(x, 0) = \varphi_0(x)$, $T(x, 0) = T_0(x)$.

The free energy functional \mathcal{F} corresponding to the above model is given by

$$\mathcal{F}(\varphi, T) = \int_{\Omega} \left\{ \frac{\xi^2}{2} |\nabla\phi|^2 + \frac{1}{4a}(\varphi^2 - 1)^2 - \frac{[s]_E}{2}(T - T_M)\varphi \right\}$$

where all the parameters are the same as in the binary alloy case.

2.3 Dendritic structures and anisotropy of the surface tension

An interesting application of the phase field models is dendritic growth. Dendritic microstructures during solidification arise due to the instability of the solid-liquid interface.

Consider the growth of an equiaxed crystal in a melt. The melt should be undercooled to provide solidification of the crystal. During the growth of the solid in the undercooled melt latent heat is released at the solid liquid interface and flows to the liquid by thermal diffusion. Therefore, the temperature gradient at the interface is negative and this leads to the instability of the interface. The tip of a small perturbation appeared at the interface is surrounded by colder liquid making the temperature gradient steeper. This allows faster transport of the released latent heat away from the tip. Therefore, the tip grows faster than the rest of the interface. Secondary or tertiary arms may develop in the same fashion.

In the case of alloys the growth is governed by both solute and thermal diffusion. The solute rejected from the solidifying material causes solute pile-up ahead of the interface. The rejected solute is carried away by diffusion and the tip of the perturbation tends to grow more rapidly than the other parts of the interface. The temperature and concentration profiles of an equiaxed dendrite is shown in Figure 2.2. The patterns formed are usually symmetric

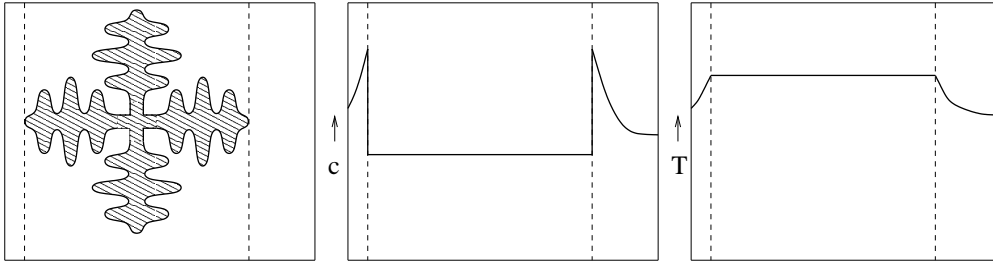


Figure 2.2: Concentration and temperature fields for equiaxed dendrites

due to the crystal structure of the solid material. The growth follows along some preferred directions determined by the crystal orientations of the material. In phase field models the crystal structure can be described by an orientation dependent density of the surface free energy. The interface instability is controlled by the surface tension and the surface tension is related with the parameter ξ in the free energy. Therefore, by making ξ orientation dependent we can include anisotropic surface tension in the model.

In the following, we discuss one possibility of introducing anisotropy for the model described in Section 2.2. The term $\frac{1}{2}\xi^2|\nabla\varphi|^2$ in the free energy functional (cf. (2.2)) is modified to

$$\frac{1}{2}\xi^2\eta^2(\nabla\varphi)|\nabla\varphi|^2$$

with an anisotropy function η . The phase field equation is derived as usual by relaxation as in (2.3) and the scaling of the parameter τ will be the same as in (2.4). As a result of the modification we obtain an anisotropic phase field equation and the equations for temperature and the concentration in the system remain unchanged. We only consider the term

$$\left(\frac{\delta}{\delta\varphi} \left(\int_{\Omega} \frac{1}{2}\eta^2(\nabla\varphi)|\nabla\varphi|^2 dx \right), \psi \right).$$

We have

$$\begin{aligned} & \left(\frac{\delta}{\delta\varphi} \int_{\Omega} \frac{1}{2} \eta^2(\nabla\varphi) |\nabla\varphi|^2 dx, \psi \right) \\ &= \lim_{s \rightarrow 0} \frac{1}{s} \int_{\Omega} \frac{1}{2} \left\{ \eta^2(\nabla\varphi + s\nabla\psi) |\nabla\varphi + s\nabla\psi|^2 - \eta^2(\nabla\varphi) |\nabla\varphi|^2 \right\} dx \\ &= (\eta(\nabla\varphi) |\nabla\varphi|^2 D^1\eta(\nabla\varphi), \nabla\psi) + (\eta^2(\nabla\varphi) \nabla\varphi, \nabla\psi) \end{aligned}$$

where

$$\nabla\varphi = \left(\frac{\partial\varphi}{\partial x}, \frac{\partial\varphi}{\partial y}, \frac{\partial\varphi}{\partial z} \right)^{\top}$$

and

$$D^1\eta(\nabla\varphi) = \left(\frac{\partial\eta}{\partial(\partial\varphi/\partial x)}, \frac{\partial\eta}{\partial(\partial\varphi/\partial y)}, \frac{\partial\eta}{\partial(\partial\varphi/\partial z)} \right)^{\top}.$$

The notations in two dimensions are analogous to the above and the phase field equation is now written as

$$\begin{aligned} \alpha\varepsilon\varphi_t - \varepsilon\nabla \cdot (\eta^2(\nabla\varphi) \nabla\varphi + \eta(\nabla\varphi) |\nabla\varphi|^2 D^1\eta(\nabla\varphi)) \\ + \frac{1}{\varepsilon} f(\varphi) + q(T, c) = 0. \end{aligned} \quad (2.12)$$

The equation combined with (2.7b)–(2.7c) alongwith appropriate boundary and initial conditions can be used for simulating dendritic structures. The boundary conditions for φ can be chosen as

$$(\eta^2(\nabla\varphi) \nabla\varphi + \eta(\nabla\varphi) |\nabla\varphi|^2 D^1\eta(\nabla\varphi)) \cdot n = 0.$$

For the specific form of the function $\eta = \eta(\nabla\varphi)$ there are different possibilities. Four fold anisotropy can be specified as chosen in [30]:

$$\begin{aligned} \eta(\vec{n}) &= 1 - 3\delta_4 + 4\delta_4(n_x^4 + n_y^4 + n_z^4) \\ &= 1 - 3\delta_4 + 4\delta_4(\cos^4\theta + \sin^4\theta(1 - 2\sin^2\varphi\cos^2\varphi)) \end{aligned}$$

where θ, φ are the spherical angles of the unit interface normal $\vec{n} = (n_x, n_y, n_z)^{\top}$ of the solid-liquid interface and δ_4 is the strength of the anisotropy. We have

$$\eta(\nabla\varphi) = 1 - 3\delta_4 + 4\delta_4 \frac{(\partial\varphi/\partial x)^4 + (\partial\varphi/\partial y)^4 + (\partial\varphi/\partial z)^4}{|\nabla\varphi|^4}$$

with the unit normal of the interface represented by $\frac{\nabla\varphi}{|\nabla\varphi|}$. With homogeneous Neumann boundary condition the weak form of the anisotropic equation is written as

$$\alpha\varepsilon(\varphi_t, \psi) + \varepsilon(\eta^2(\nabla\varphi) \nabla\varphi + \mathbf{s}(\nabla\varphi), \nabla\psi) + \frac{1}{\varepsilon}(f(\varphi), \psi) + (q(T, c), \psi) = 0 \quad (2.13)$$

where $\mathbf{s} = (s_1, s_2, s_3)^\top$ with

$$s_1 = 16\delta_4 \eta(\nabla\varphi) \frac{\partial\varphi}{\partial x} \frac{(\partial\varphi/\partial x)^2 |\nabla\varphi|^2 - [(\partial\varphi/\partial x)^4 + (\partial\varphi/\partial y)^4 + (\partial\varphi/\partial z)^4]}{|\nabla\varphi|^4} \quad (2.14)$$

and analogous expressions for s_2 and s_3 .

In two dimensions the form of η (for four fold anisotropy) can be chosen as

$$\begin{aligned} \eta &= 1 - 3\delta_4 + 4\delta_4 (n_x^4 + n_y^4) \\ &= 1 - 3\delta_4 + 4\delta_4 (\sin^4 \theta + \cos^4 \theta) \end{aligned} \quad (2.15)$$

where θ is now the angle between the normal $\vec{n} = (n_x, n_y)$ of the interface and a certain fixed direction (e.g. the x -axis).

Analogously, we have

$$\eta = 1 - 3\delta_4 + 4\delta_4 \frac{(\partial\varphi/\partial x)^4 + (\partial\varphi/\partial y)^4}{|\nabla\varphi|^4} \quad (2.16)$$

and the same weak anisotropic equation. We may also use $\eta = \eta(\theta(\nabla\varphi)) = 1 + \delta_m \cos(m(\theta(\nabla\varphi) - \theta_0))$ with a reference direction θ_0 (0 for the x -axis), this is equivalent to (2.15) for $m = 4$. This form was employed in [34] for the simulation of dendritic crystals. We use the form for the simulation of six fold dendritic structures. Results of the simulations are discussed in Chapter 5.

Chapter 3

Error estimates for the solution of a fully discrete scheme

The present chapter is devoted to the derivation of some new error estimates for the fully discrete finite element method for a phase field model representing binary alloys. In order to obtain the desired estimates we first propose an alternative formulation for the model, incorporating some simplifications:

$$\alpha\varepsilon\varphi_t - \varepsilon\Delta\varphi + \frac{1}{\varepsilon}f(\varphi) - q(T, \mu) = 0 \quad (3.1a)$$

$$T_t - \nabla \cdot (K\nabla T) + L\varphi_t = 0 \quad (3.1b)$$

$$\mu_t - \nabla \cdot (D\nabla\mu) + M\varphi_t = 0 \quad (3.1c)$$

in $\Omega_{\mathcal{T}} := (0, \mathcal{T}] \times \Omega$ with the initial and boundary conditions

$$\nabla\varphi \cdot n = K\nabla T \cdot n = D\nabla\mu \cdot n = 0 \quad \text{on } \partial\Omega \quad (3.2a)$$

$$\varphi(0, x) = \varphi_0, \quad T(0, x) = T_0, \quad \mu(0, x) = \mu_0 \quad \text{in } \Omega. \quad (3.2b)$$

The connection between this formulation and (2.7)–(2.9) is the assumption that $M(c) = M$ is constant and a linearized chemical potential $\mu = c + M\varphi$. Then (2.7c) gives us the equation (3.1c).

In the system (3.1)–(3.2), $\Omega \subset \mathbb{R}^N$ ($N = 2, 3$) represents a bounded domain with a smooth boundary $\partial\Omega$ and $\mathcal{T} > 0$ is a fixed constant. The function $f(\varphi)$ is the derivative of the double well potential

$$F(\varphi) = \frac{1}{4}(\varphi^2 - 1)^2,$$

that is, $f(\varphi) = \varphi^3 - \varphi$.

Moreover, M is positive and $K(x, t), D(x, t) \in \mathbb{R}^{N \times N}$ are positive definite. We assume that the function q has the form $q(T, \mu) = q_0T + q_1\mu$ with

positive q_0, q_1 and the assumption can be justified by the use of some suitable linearizations. Our primary goal is to consider a fully discrete finite element method for the model (3.1)–(3.2). It is known that the phase field models approximate sharp interface problems when ε becomes small. This implies that in numerical methods one has to use small mesh and time step sizes which should be related to the interface thickness parameter ε . It is clear that the space mesh size should be at least as small as ε so that the grid captures the thin interface.

In the past years, many authors have developed and analyzed numerical approximations of phase field models. For example, Caginalp and Lin [11] and Lin [36] have proposed finite difference schemes for a phase field model and obtained error estimates for the scheme. Chen and Hoffmann [17] proposed a fully discrete finite element method and obtained optimal order error estimates. All the above error estimates have been derived considering a *fixed* ε . The obtained error bounds contain the factor $\exp\left(\frac{T}{\varepsilon^2}\right)$. This is not useful when ε is small.

Recently, Feng and Prohl [27] have derived error estimates for a phase field model with the error constants depending on low polynomial orders of ε^{-1} . They derived error estimates for a fully discrete finite element method under reasonable constraints on the time and space mesh sizes. A spectrum estimate by Chen [16] plays an important role in the techniques used in [27]. We mention that all the above works deal with phase field models for pure material.

The numerical analysis for various phase field models (representing solidification in binary alloys) have also been considered by several authors recently. For instance, Rappaz and Scheid [40] proved the existence of weak solutions of an isothermal (T constant) phase field model for binary alloys. For the same model Kessler and Scheid [32] proposed a finite element method and achieved optimal error estimates by introducing a generalized vectorial elliptic projector. The error bounds in the work contain $\exp\left(\frac{T}{\varepsilon^2}\right)$ factor.

To our knowledge, error estimates in dependence of the parameter ε have not yet been presented for phase field models representing binary alloys. It is the aim of this work to propose and analyze a fully discrete finite element method for the model (3.1)–(3.2) and derive new error estimates for the method. It is shown that the error constants depend on ε^{-1} in low polynomial order similar to that of [27].

Before presenting the main error estimates, we need to take some preparatory steps. In the following sections we derive energy estimates for the solution of the problem, introduce a fully discrete scheme and derive stability estimates for the discrete solution. With the derivation of the discrete version of the spectrum estimate of Chen [16] we conclude the preparatory steps and proceed with the main propositions where the error bounds for the fully

discrete scheme are given.

3.1 Preliminaries

In this section we collect some useful definitions, elementary inequalities and properties of the spaces we use. We start the section with the definitions of function spaces and norms.

3.1.1 Function spaces

Let Ω be an open bounded domain in \mathbb{R}^N . The Lebesgue space $L_p(\Omega)$ ($p \geq 1$) consists of functions u defined on Ω whose p -th powers are integrable functions; i.e., $u \in L_p(\Omega)$ if u is measurable and

$$\|u\|_{L_p(\Omega)} = \left(\int_{\Omega} |u|^p dx \right)^{1/p} \quad (3.3)$$

is finite. For $p = \infty$, the norm is defined as

$$\|u\|_{L_\infty(\Omega)} = \text{ess sup}_{\Omega} |u|.$$

The inner product on $L_2(\Omega)$ is denoted as usual by (\cdot, \cdot) , i.e.,

$$(u, v) = \int_{\Omega} uv dx, \quad \text{for } u, v \in L_2(\Omega).$$

For integer k , the Hölder space $C^k(\bar{\Omega})$ consists of functions with continuous partial derivatives up to order k . A function u satisfying

$$|u(x) - u(y)| \leq C|x - y|^\gamma$$

with $0 < \gamma \leq 1$ is said to be Hölder continuous with exponent γ . For noninteger k the Hölder space $C^k(\bar{\Omega})$ consists of functions whose partial derivatives up to order $[k] = \sup\{m \in \mathbb{Z} \mid m \leq k\}$ are Hölder continuous with exponent $k - [k]$.

When all the weak partial derivatives of u of order $\leq m$ (m positive integer) are in $L_p(\Omega)$, we say that u belongs to the Sobolev space $W_p^m(\Omega)$, i.e.,

$$W_p^m(\Omega) = \{u \in L_p(\Omega) : D^\alpha u \in L_p(\Omega) \forall \alpha \text{ with } |\alpha| \leq m\}.$$

Here $\alpha = (\alpha_1, \dots, \alpha_N)$, ($|\alpha| = \alpha_1 + \dots + \alpha_N$, $\alpha_i \geq 0$, integer) is a multi-index, and

$$D^\alpha u(\mathbf{x}) = \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \cdots \frac{\partial^{\alpha_N}}{\partial x_N^{\alpha_N}} u(\mathbf{x}).$$

The norms are defined, for $1 \leq p < \infty$, by

$$\|u\|_{W_p^m(\Omega)} = \left(\int_{\Omega} \sum_{|\alpha| \leq m} |D^\alpha u|^p dx \right)^{1/p} = \left(\sum_{|\alpha| \leq m} \|D^\alpha u\|_{L_p(\Omega)}^p \right)^{1/p} \quad (3.4)$$

and for $p = \infty$ by

$$\|u\|_{W_\infty^m(\Omega)} = \max_{|\alpha| \leq m} \|D^\alpha u\|_{L_\infty(\Omega)}.$$

We often use Hilbert spaces $H^m(\Omega) = W_2^m(\Omega)$.

The space $H_0^1(\Omega)$ consists of functions $v \in H^1(\Omega)$ such that $v = 0$ on $\partial\Omega$. By $H^{-1}(\Omega)$ we denote the dual space of $H_0^1(\Omega)$, it is defined as the space of all continuous linear functionals on $H_0^1(\Omega)$. The norm on the dual space $H^{-1}(\Omega)$ is defined by

$$\|u\|_{H^{-1}(\Omega)} = \sup_{0 \neq v \in H_0^1(\Omega)} \frac{|(u, v)|}{\|v\|_{H_0^1(\Omega)}}.$$

Let us now define some spaces of time dependent functions. Denote by J the time interval $(0, \mathcal{T})$. The space $L_p(J \times \Omega)$ consists of all measurable functions with

$$\|u\|_{L_p(J \times \Omega)} = \left(\int_0^{\mathcal{T}} \|u(t)\|_{L_p(\Omega)}^p dt \right)^{1/p} \quad (1 \leq p < \infty)$$

being finite ($1 \leq p < \infty$). For the case $p = \infty$ the norm is defined by

$$\|u\|_{L_\infty(J \times \Omega)} = \text{ess sup}_{0 \leq t \leq \mathcal{T}} \|u(t)\|_{L_\infty(\Omega)}.$$

The Sobolev space $W_p^k(J; W_q^\ell(\Omega))$ consists of functions whose time derivatives up to order k belong to $W_q^\ell(\Omega)$ and $t \rightarrow \|u(t, \cdot)\|_{W_q^\ell(\Omega)}$ is in $L_p(J)$. If $p = 2$ we write $H^k(J; W_q^\ell(\Omega))$, analogously $W_p^k(J; H^\ell(\Omega))$ for $q = 2$. The functions with time derivatives of order up to k in $L_p(J)$ and space derivatives up to order ℓ in $L_p(\Omega)$ belong to $W_p^{k, \ell}(J \times \Omega)$.

In the following we give an example of a norm on Sobolev space of non-integer order. For a real number $s \in (0, 1)$, $1 \leq p \leq \infty$ and a nonnegative integer k define

$$\|u\|_{W_p^{k+s}(\Omega)}^p = \|u\|_{W_p^k(\Omega)}^p + \sum_{|\alpha|=k} \int_{\Omega} \int_{\Omega} \frac{|D^\alpha u(x) - D^\alpha u(\xi)|^p}{|x - \xi|^{N+sp}} dx d\xi$$

Other definitions of non-integer order spaces can be found for example in [38]. We use non-integer order Sobolev spaces $W_s^\beta(\Omega)$ and $W_r^{\alpha, \beta}(J \times \Omega)$ where the superscript α indicates the regularity with respect to time and β indicates the regularity with respect to space.

3.1.2 Elementary inequalities

We mention some elementary inequalities in this subsection. We have

Young's inequality. For $1 < p, q < \infty$ with $\frac{1}{p} + \frac{1}{q} = 1$,

$$ab \leq \epsilon a^p + C(\epsilon)b^q \quad (a, b > 0 \text{ and } \epsilon > 0) \quad (3.5)$$

where $C(\epsilon) = (\epsilon p)^{-q/p} q^{-1}$. For $p = q = 2$, we have

$$ab \leq \epsilon a^2 + \frac{1}{4\epsilon} b^2.$$

Hölder's inequality. Let $1 \leq p, q \leq \infty$ and $\frac{1}{p} + \frac{1}{q} = 1$. Then, if $u \in L_p(\Omega), v \in L_q(\Omega)$, we have

$$\int_{\Omega} |uv| dx \leq \|u\|_{L_p(\Omega)} \|v\|_{L_q(\Omega)}. \quad (3.6)$$

In general, for $1 \leq p_1, \dots, p_m \leq \infty$ with $\frac{1}{p_1} + \dots + \frac{1}{p_m} = 1$, and $u_k \in L_{p_k}(\Omega)$ for $k = 1, \dots, m$,

$$\int_{\Omega} |u_1 \dots u_m| dx \leq \prod_{k=1}^m \|u_k\|_{L_{p_k}(\Omega)}.$$

Minkowski's inequality. Let $1 \leq p \leq \infty$ and $u, v \in L_p(\Omega)$. Then

$$\|u + v\|_{L_p(\Omega)} \leq \|u\|_{L_p(\Omega)} + \|v\|_{L_p(\Omega)}. \quad (3.7)$$

3.1.3 Embeddings and interpolation

Let $\Omega \in \mathbb{R}^N$ be a bounded Lipschitz domain and J be a bounded interval. The results collected in this section can be found in [3, 4, 23, 43]. We have the following embedding theorems.

Theorem 3.1 *Suppose $\alpha \geq \beta \geq 0$ and $r, s \in [1, +\infty)$. Let $u \in W_r^\alpha(\Omega)$. If*

$$\alpha - \frac{N}{r} \geq \beta - \frac{N}{s},$$

then $W_r^\alpha(\Omega)$ is continuously embedded in $W_s^\beta(\Omega)$, i.e. $u \in W_s^\beta(\Omega)$ and there exists a constant C independent of u such that

$$\|u\|_{W_s^\beta(\Omega)} \leq C \|u\|_{W_r^\alpha(\Omega)}. \quad (3.8)$$

If the inequality is true with “ $<$ ” instead of “ \leq ” then the embedding is compact and the embedding also holds for $r, s \in [1, +\infty]$.

Theorem 3.2 *Let $\alpha_1, \alpha_2, \beta_1, \beta_2 \geq 0$, $1 < r \leq s < +\infty$ and*

$$\left(\frac{1}{\alpha_1} + \frac{N}{\alpha_2}\right) \left(\frac{1}{r} - \frac{1}{s}\right) + \max\left\{\frac{\beta_1}{\alpha_1}, \frac{\beta_2}{\alpha_2}\right\} \leq 1.$$

Then the space $W_r^{\alpha_1, \alpha_2}(J \times \Omega)$ is continuously embedded in $W_s^{\beta_1, \beta_2}(J \times \Omega)$.

The theorems are a consequence of more general embedding theorems for Besov spaces [4].

We also have the following interpolation properties of Sobolev spaces.

Theorem 3.3 *Let $\Omega \in \mathbb{R}^N$ be a bounded C^k -smooth domain. Then for indices $r, r_1, r_2 \in (1, +\infty)$, $k_1, k_2 \geq 0$, $\lambda \in (0, 1)$ satisfying $k = \lambda k_1 + (1 - \lambda)k_2$, $\frac{1}{r} = \frac{\lambda}{r_1} + \frac{1 - \lambda}{r_2}$ and any function $u \in W_{r_1}^{k_1}(\Omega) \cap W_{r_2}^{k_2}(\Omega)$ the following holds: $u \in W_r^k(\Omega)$ and*

$$\|u\|_{W_r^k(\Omega)} \leq C \|u\|_{W_{r_1}^{k_1}(\Omega)}^\lambda \|u\|_{W_{r_2}^{k_2}(\Omega)}^{1 - \lambda} \quad (3.9)$$

with a constant C independent of u .

Theorem 3.4 *Let $\Omega \in \mathbb{R}^N$ be a bounded C^ℓ -smooth domain and J be a bounded interval. Then for $r, r_1, r_2, s, s_1, s_2 \in (1, +\infty)$, $k, k_1, k_2, \ell_1, \ell_2 \geq 0$, $\lambda \in (0, 1)$ satisfying $k = \lambda k_1 + (1 - \lambda)k_2$, $\ell = \lambda \ell_1 + (1 - \lambda)\ell_2$, $\frac{1}{r} = \frac{\lambda}{r_1} + \frac{1 - \lambda}{r_2}$, $\frac{1}{s} = \frac{\lambda}{s_1} + \frac{1 - \lambda}{s_2}$, and any function $u \in W_{r_1}^{k_1}(J; W_{s_1}^{\ell_1}(\Omega)) \cap W_{r_2}^{k_2}(J; W_{s_2}^{\ell_2}(\Omega))$ the following holds: $u \in W_r^k(J; W_s^\ell(\Omega))$ and*

$$\|u\|_{W_r^k(J; W_s^\ell(\Omega))} \leq C \|u\|_{W_{r_1}^{k_1}(J; W_{s_1}^{\ell_1}(\Omega))}^\lambda \|u\|_{W_{r_2}^{k_2}(J; W_{s_2}^{\ell_2}(\Omega))}^{1 - \lambda} \quad (3.10)$$

for constant C independent of u .

The above two theorems can be concluded from a result in [3]. We have the following corollary of the theorem.

Corollary 3.1 *Let $J \in \mathbb{R}$ be a bounded interval and $\Omega \in \mathbb{R}^N$ be a bounded C^ℓ -smooth domain. Then for $r \in (1, \infty)$, $k \geq 0$ and $\lambda \in (0, 1)$ every $u \in W_r^{k, \ell}(J \times \Omega)$ is also an element of $W_r^{\lambda k}(J; W^{(1 - \lambda)\ell}(\Omega))$ and*

$$\|u\|_{W_r^{\lambda k}(J; W^{(1 - \lambda)\ell}(\Omega))} \leq C \|u\|_{W_r^{k, \ell}(J \times \Omega)} \quad (3.11)$$

for constant C independent of u .

3.1.4 Regularity of a parabolic problem

Consider a linear parabolic initial boundary value problem on a domain $\Omega \in \mathbb{R}^N$ with boundary Γ and a time interval $J = [0, \mathcal{T}]$.

$$\partial_t u - \nabla \cdot (A \nabla u) = g \quad \text{in } J \times \Omega \quad (3.12a)$$

$$A \nabla u \cdot n + au = b \quad \text{on } J \times \Gamma \quad (3.12b)$$

$$u(0, \cdot) = u_0 \quad \text{in } \Omega. \quad (3.12c)$$

For the above problem the following regularity result is valid.

Theorem 3.5 *Suppose $\Omega \in \mathbb{R}^N$ is a domain with a C^2 -smooth boundary Γ , $r > 1$, $r \neq 3$, A is a bounded elliptic tensor with coefficients from $C^0(J \times \Omega) \cap C^{\frac{\beta}{2}, \beta}(J \times \Gamma) \cap L_{s_1}(J; W_{s_2}^1(\Omega))$ with $\beta > 1 - \frac{1}{r}$ and $s_1, s_2 > r$, $\frac{2}{s_1} + \frac{N}{s_2} < 1$. Suppose $g \in L_r(J \times \Omega)$, $a \in C^{\frac{\beta}{2}, \beta}(J \times \Gamma)$, $b \in W_r^{\frac{1}{2} - \frac{1}{2r}, 1 - \frac{1}{r}}(J \times \Gamma)$ and $u_0 \in W_r^{2 - \frac{2}{r}}(\Omega)$. Let for the case $r > 3$ the compatibility condition*

$$(A \nabla u_0 \cdot n + au_0 - b)|_{t=0} = 0$$

be satisfied. Then the solution u of (3.12) is in space $W_r^{1,2}(J \times \Omega)$ and satisfies the a priori estimate

$$\|u\|_{W_r^{1,2}(\Omega)} \leq C \left(\|g\|_{L_r(J \times \Omega)} + \|b\|_{W_r^{\frac{1}{2} - \frac{1}{2r}, 1 - \frac{1}{r}}(J \times \Gamma)} + \|u_0\|_{W_r^{2 - \frac{2}{r}}(\Omega)} \right) \quad (3.13)$$

with a constant C independent of g, b and u_0 .

The theorem follows from a special case of a result in [43] (see also [23]).

3.1.5 Discrete Gronwall lemma

For the error estimates we need the following lemma:

Lemma 3.1 *Assume that, $w_n, n \geq 0$ satisfies*

$$w_n \leq \alpha_n + \sum_{k=0}^{n-1} \beta_k w_k \quad \text{for } n \geq 0, \quad (3.14)$$

where α_n is nondecreasing and $\beta_k \geq 0$. Then

$$w_n \leq \alpha_n \exp \left(\sum_{k=0}^{n-1} \beta_k \right). \quad (3.15)$$

Proof. The proof is done by induction. For $m = 1$, we have

$$w_1 \leq \alpha_1 + \beta_0 w_0 \leq \alpha_1 + \beta_0 \alpha_0 \leq \alpha_1(1 + \beta_0) \leq \alpha_1 \exp(\beta_0).$$

Assume that (3.15) holds for $m - 1$ ($m \leq n$). Set

$$u_m = \alpha_n + \sum_{k=0}^{m-1} \beta_k w_k.$$

Then, we have $u_m - u_{m-1} = \beta_{m-1} w_{m-1}$. Moreover, using (3.14) and the property of the sequence α_n we obtain

$$\begin{aligned} u_m &= u_{m-1} + \beta_{m-1} w_{m-1} \\ &\leq u_{m-1} + \beta_{m-1} \left(\alpha_{m-1} + \sum_{k=0}^{m-2} \beta_k w_k \right) \\ &\leq u_{m-1} + \beta_{m-1} u_{m-1} \leq (1 + \beta_{m-1}) u_{m-1} \\ &\leq \exp(\beta_{m-1}) u_{m-1}. \end{aligned}$$

Since $u_0 = \alpha_n$ and $w_n \leq u_n$, we get the assertion. \square

3.2 Energy estimates for the phase field model

For the later use, we need energy estimates for the solution (φ, T, μ) of (3.1)–(3.2) in terms of negative powers of ε for given initial values $(\varphi_0, T_0, \mu_0) \in [H^2(\Omega)]^3$. For simplicity of the notations, we use further $\|\cdot\|_{L_p}$ for $\|\cdot\|_{L_p(\Omega)}$ and $\|\cdot\|_{H^m}$ for $\|\cdot\|_{H^m(\Omega)}$.

We define the following energy functional:

$$\mathcal{F}(\varphi, T, \mu) = \int_{\Omega} \left(\frac{1}{2\alpha} |\nabla \varphi|^2 + \frac{1}{\alpha \varepsilon^2} F(\varphi) + \frac{q_0}{2L\alpha\varepsilon} T^2 + \frac{q_1}{2M\alpha\varepsilon} \mu^2 \right) dx. \quad (3.16)$$

We make the following assumption regarding the initial values (φ_0, T_0, μ_0) :

Assumptions

There exist nonnegative constants σ_i , $i = 1, 2, \dots, 6$ independent of ε such that

$$|\varphi_0| \leq 1 \text{ in } \Omega \quad (3.17a)$$

$$\mathcal{F}(\varphi_0, T_0, \mu_0) \leq C\varepsilon^{-2\sigma_1} \quad (3.17b)$$

$$\|\varepsilon \Delta \varphi_0 - \frac{1}{\varepsilon} f(\varphi_0) + q_0 T_0 + q_1 \mu_0\|_{L_2(\Omega)} \leq C\varepsilon^{-\sigma_2} \quad (3.17c)$$

$$\|\nabla T_0\|_{H^\ell(\Omega)} \leq C\varepsilon^{-\sigma_3+\ell}, \quad \ell = 0, 1 \quad (3.17d)$$

$$\|\nabla \mu_0\|_{H^\ell(\Omega)} \leq C\varepsilon^{-\sigma_5+\ell}, \quad \ell = 0, 1 \quad (3.17e)$$

The initial functions φ_0, T_0, μ_0 can be chosen such that (3.17) is satisfied for $\sigma_1 = \sigma_2 = 1/2$, $\sigma_3 = \sigma_5 = 0$ and $\sigma_4 = \sigma_6 = 1/2$. We give some remarks on the selection of the constants σ_i . The function φ_0 can be chosen, for example, as $\tanh(\rho/\sqrt{2})$ with $\rho = r/\varepsilon$, where r is the signed distance of a point from the interface. It is the first order term in the asymptotic expansion of the solution φ in the neighbourhood of the interface (cf. Appendix A.1). Since $F(\varphi_0)$ is nonzero only on the transition region of volume $O(\varepsilon)$ and $\nabla\varphi_0 = O(\varepsilon^{-1})$ in the same region, we can choose $\sigma_1 = 1/2$ in (3.17b). Due to $\Delta\varphi_0 = O(\varepsilon^{-2})$ in the transition region, we can also have $\sigma_2 = 1/2$. We take T_0 as smooth approximation of a continuous function whose gradient has a jump over the interface. In this case we have $\sigma_3 = 0$ and $\sigma_4 = 1/2$ in (3.17d). A similar selection is made for μ_0 , so that $\sigma_5 = 0$ and $\sigma_6 = 1/2$ in (3.17e). We further use the above fixed values of σ_i -s.

We also assume that there exists a family of smooth data functions $\{(\varphi_0, T_0, \mu_0)\}_{0 < \varepsilon < 1}$ and constants $\varepsilon_0 \in (0, 1]$ and $C_0 > 0$ such that for all $\varepsilon \in (0, \varepsilon_0]$ the φ component of the solution of the phase field model (3.1)–(3.2) with the initial data (φ_0, T_0, μ_0) satisfies

$$\|\varphi\|_{L^\infty(0, \mathcal{T}; \Omega)} \leq C_0. \quad (3.18)$$

The diffusion tensors K, D are symmetric, elliptic and bounded: $K_{ij} = K_{ji}$, $D_{ij} = D_{ji}$ for $i, j = 1 \dots, N$, there exist positive constants $0 < K_0 \leq K_1$ and $0 < D_0 \leq D_1$ such that

$$\begin{aligned} K_0 |\xi|^2 &\leq K_{ij} \xi_i \xi_j \leq K_1 |\xi|^2 \\ D_0 |\xi|^2 &\leq D_{ij} \xi_i \xi_j \leq D_1 |\xi|^2 \end{aligned} \quad (3.19)$$

where the sum convention is used. We assume that the coefficients of K, D satisfy

$$K_{ij}, D_{ij} \in W_\infty^1(0, \mathcal{T}; W_\infty^1(\Omega)). \quad (3.20)$$

The following result gives estimates for the solution (φ, T, μ) of (3.1)–(3.2) in various norms.

Lemma 3.2 *Assume that (3.17) holds for (φ_0, T_0, μ_0) and (3.18) is valid. If $0 < t_\ell \leq \mathcal{T}$, then the solution to (3.1)–(3.2) satisfies the following:*

- (i) $\text{ess sup}_{[0, t_\ell]} \left\{ \frac{\varepsilon}{2} \|\nabla\varphi\|_{L_2}^2 + \frac{1}{\varepsilon} \|F(\varphi)\|_{L_1} + \frac{q_0}{2L} \|T\|_{L_2}^2 + \frac{q_1}{2M} \|\mu\|_{L_2}^2 \right\} + \int_0^{t_\ell} \left(\alpha\varepsilon \|\varphi_t(s)\|_{L_2}^2 + \frac{q_0 K_0}{L} \|\nabla T(s)\|_{L_2}^2 + \frac{q_1 D_0}{M} \|\nabla\mu(s)\|_{L_2}^2 \right) ds \leq C,$
- (ii) $K_0 \text{ess sup}_{[0, t_\ell]} \|\nabla T\|_{L_2}^2 + \int_0^{t_\ell} \|T_t(s)\|_{L_2}^2 ds \leq C\varepsilon^{-1},$

- (iii) $D_0 \operatorname{ess\,sup}_{[0,t_\ell]} \|\nabla \mu\|_{L_2}^2 + \int_0^{t_\ell} \|\mu_t(s)\|_{L_2}^2 ds \leq C\varepsilon^{-1},$
- (iv) $\frac{\alpha}{2} \operatorname{ess\,sup}_{[0,t_\ell]} \|\varphi_t\|_{L_2}^2 + \int_0^{t_\ell} \|\nabla \varphi_t(s)\|_{L_2}^2 ds \leq C\varepsilon^{-3},$
- (v) $\int_0^{t_\ell} \|\Delta \varphi(s)\|_{L_2}^2 ds \leq C\varepsilon^{-3},$
- (vi) $\operatorname{ess\,sup}_{[0,t_\ell]} \|\Delta \varphi\|_{L_2}^2 \leq C\varepsilon^{-3},$
- (vii) $\int_0^{t_\ell} \|\varphi_{tt}(s)\|_{H^{-1}}^2 ds \leq C\varepsilon^{-5},$
- (viii) $\operatorname{ess\,sup}_{[0,t_\ell]} \|T_t\|_{L_2}^2 + K_0 \int_0^{t_\ell} \|\nabla T_t(s)\|_{L_2}^2 ds \leq C\varepsilon^{-5},$
- (ix) $\operatorname{ess\,sup}_{[0,t_\ell]} \|\mu_t\|_{L_2}^2 + D_0 \int_0^{t_\ell} \|\nabla \mu_t(s)\|_{L_2}^2 ds \leq C\varepsilon^{-5},$
- (x) $\operatorname{ess\,sup}_{[0,t_\ell]} \sum_{i,j=1}^N \left\| \frac{\partial^2 T}{\partial x_i \partial x_j} \right\|_{L_2}^2 \leq C\varepsilon^{-5},$
- (xi) $\operatorname{ess\,sup}_{[0,t_\ell]} \sum_{i,j=1}^N \left\| \frac{\partial^2 \mu}{\partial x_i \partial x_j} \right\|_{L_2}^2 \leq C\varepsilon^{-5},$
- (xii) $\int_0^{t_\ell} \|T_{tt}(s)\|_{H^{-1}}^2 ds \leq C\varepsilon^{-5},$
- (xiii) $\int_0^{t_\ell} \|\mu_{tt}(s)\|_{H^{-1}}^2 ds \leq C\varepsilon^{-5}.$

Furthermore, if

$$\begin{aligned} \lim_{s \rightarrow 0^+} \|\nabla \varphi_t(s)\|_{L_2} &\leq C\varepsilon^{-\xi_1}, & \lim_{s \rightarrow 0^+} \|\nabla T_t(s)\|_{L_2} &\leq C\varepsilon^{-\xi_2}, \\ \text{and } \lim_{s \rightarrow 0^+} \|\nabla \mu_t(s)\|_{L_2} &\leq C\varepsilon^{-\xi_3} \end{aligned} \tag{3.21}$$

for some $\xi_1, \xi_2, \xi_3 \geq 0$, then

- (xiv) (a) $\alpha \int_0^{t_\ell} \|\varphi_{tt}(s)\|_{L_2}^2 ds + \operatorname{ess\,sup}_{[0,t_\ell]} \|\nabla \varphi_t\|_{L_2}^2 \leq C\varepsilon^{-\max\{5, 2\xi_1\}},$
- (b) $\int_0^{t_\ell} \|\Delta \varphi_t(s)\|_{L_2}^2 ds \leq C\varepsilon^{-\max\{5, 2\xi_1\}}.$

Moreover,

$$(xv) \text{ (a) } K_0 \operatorname{ess\,sup}_{[0, t_\ell]} \|\nabla T_t\|_{L_2}^2 + \int_0^{t_\ell} \|T_{tt}(s)\|_{L_2}^2 ds \leq C\varepsilon^{-\max\{5, 2\xi_1, 2\xi_2\}},$$

$$(b) \int_0^{t_\ell} \sum_{i,j=1}^N \left\| \frac{\partial^2 T_t}{\partial x_i \partial x_j} \right\|_{L_2}^2 ds \leq C\varepsilon^{-\max\{5, 2\xi_1, 2\xi_2\}},$$

$$(xvi) \text{ (a) } D_0 \operatorname{ess\,sup}_{[0, t_\ell]} \|\nabla \mu_t\|_{L_2}^2 + \int_0^{t_\ell} \|\mu_{tt}(s)\|_{L_2}^2 ds \leq C\varepsilon^{-\max\{5, 2\xi_1, 2\xi_3\}},$$

$$(b) \int_0^{t_\ell} \sum_{i,j=1}^N \left\| \frac{\partial^2 \mu_t}{\partial x_i \partial x_j} \right\|_{L_2}^2 ds \leq C\varepsilon^{-\max\{5, 2\xi_1, 2\xi_3\}}.$$

Proof. (i) Multiplying (3.1a) by φ_t and integrating over the domain Ω yields

$$\alpha\varepsilon(\varphi_t, \varphi_t) + \varepsilon(\nabla\varphi, \nabla\varphi_t) + \frac{1}{\varepsilon}(F'(\varphi), \varphi_t) - q_0(T, \varphi_t) - q_1(\mu, \varphi_t) = 0.$$

From equation (3.1b) and the boundedness of K , we obtain

$$\begin{aligned} -q_0(T, \varphi_t) &= \frac{q_0}{L}(K\nabla T, \nabla T) + \frac{q_0}{L}(T, T_t) \\ &\geq \frac{q_0 K_0}{L}\|\nabla T\|_{L_2}^2 + \frac{q_0}{2L}\frac{d}{dt}\|T\|_{L_2}^2. \end{aligned}$$

Since an analogous estimate also holds for $-q_1(\mu, \varphi_t)$, we have

$$\alpha\varepsilon\frac{d}{dt}\mathcal{F}(\varphi, T, \mu) + \alpha\varepsilon\|\varphi_t\|_{L_2}^2 + \frac{q_0 K_0}{L}\|\nabla T\|_{L_2}^2 + \frac{q_1 D_0}{M}\|\nabla \mu\|_{L_2}^2 \leq 0.$$

Now integrating the above identity over $[0, t_\ell]$ and using (3.17b) we obtain (i).

(ii) We multiply (3.1b) by T_t and integrate over Ω . Then using Young's inequality (3.5) for the term $-L(\varphi_t, T_t)$ and the identity

$$(Ku, u_t) = \frac{1}{2}\frac{d}{dt}(Ku, u) - \frac{1}{2}(K_t u, u) \quad (3.22)$$

with $u = \nabla T$ results in

$$\|T_t\|_{L_2}^2 + \frac{d}{dt}(K\nabla T, \nabla T) \leq L^2\|\varphi_t\|_{L_2}^2 + C\|\nabla T\|_{L_2}^2.$$

After integrating over $[0, t_\ell]$ and using (i) and (3.17d) we get the assertion.

(iii) The proof of this part is analogous to that of (ii), that is, we multiply (3.1c) by μ_t , integrate and use (i) and (3.17e) to get the desired inequality.

(iv) We differentiate (3.1a) with respect to t and obtain

$$\alpha\varepsilon\varphi_{tt} - \varepsilon\Delta\varphi_t + \frac{1}{\varepsilon}f'(\varphi)\varphi_t - q_0T_t - q_1\mu_t = 0. \quad (3.23)$$

Now by multiplying the above equation by φ_t and integrating, we get

$$\alpha\varepsilon(\varphi_{tt}, \varphi_t) + \varepsilon(\nabla\varphi_t, \nabla\varphi_t) + \frac{1}{\varepsilon}(f'(\varphi)\varphi_t, \varphi_t) = q_0(T_t, \varphi_t) + q_1(\mu_t, \varphi_t).$$

The above identity and the inequalities

$$\begin{aligned} \frac{1}{\varepsilon}(f'(\varphi)\varphi_t, \varphi_t) &\geq -\frac{1}{\varepsilon}\|\varphi_t\|_{L_2}^2 \\ q_0(T_t, \varphi_t) &\leq \frac{1}{\varepsilon}\|\varphi_t\|_{L_2}^2 + \frac{q_0^2\varepsilon}{4}\|T_t\|_{L_2}^2 \\ q_1(\mu_t, \varphi_t) &\leq \frac{1}{\varepsilon}\|\varphi_t\|_{L_2}^2 + \frac{q_1^2\varepsilon}{4}\|\mu_t\|_{L_2}^2 \end{aligned}$$

gives us

$$\frac{\alpha\varepsilon}{2}\frac{d}{dt}\|\varphi_t\|_{L_2}^2 + \varepsilon\|\nabla\varphi_t\|_{L_2}^2 \leq \frac{3}{\varepsilon}\|\varphi_t\|_{L_2}^2 + \frac{q_0^2\varepsilon}{4}\|T_t\|_{L_2}^2 + \frac{q_1^2\varepsilon}{4}\|\mu_t\|_{L_2}^2.$$

The assertion now follows after integrating the above over $[0, t_\ell]$ and taking into account (i)–(iii) and (3.17c).

(v) We use the test function $-\Delta\varphi$ for (3.1a) to get

$$\alpha\varepsilon(\nabla\varphi_t, \nabla\varphi) + \varepsilon(\Delta\varphi, \Delta\varphi) + \frac{1}{\varepsilon}(f(\varphi), -\Delta\varphi) = q_0(T, -\Delta\varphi) + q_1(\mu, -\Delta\varphi).$$

Then the inequalities

$$\frac{1}{\varepsilon}(f(\varphi), -\Delta\varphi) = \frac{1}{\varepsilon}(f'(\varphi), |\nabla\varphi|^2) \geq -\frac{1}{\varepsilon}\|\nabla\varphi\|_{L_2}^2 \quad (3.24)$$

and

$$\begin{aligned} q_1(\mu, -\Delta\varphi) &= q_1(\nabla\mu, \nabla\varphi) \\ &\leq \frac{1}{\varepsilon}\|\nabla\varphi\|_{L_2}^2 + \frac{q_1^2\varepsilon}{4}\|\nabla\mu\|_{L_2}^2 \end{aligned}$$

alongwith the analogous inequality for $q_0(\nabla T, \nabla\varphi)$, yield

$$\frac{\alpha\varepsilon}{2}\frac{d}{dt}\|\nabla\varphi\|_{L_2}^2 + \varepsilon\|\Delta\varphi\|_{L_2}^2 \leq \frac{3}{\varepsilon}\|\nabla\varphi\|_{L_2}^2 + \frac{q_0^2\varepsilon}{2}\|\nabla T\|_{L_2}^2 + \frac{q_1^2\varepsilon}{4}\|\nabla\mu\|_{L_2}^2.$$

Now the assertion follows from integrating the above inequality over $[0, t_\ell]$ and taking into account (i) and (3.17b).

(vi) We multiply (3.1a) by $-\Delta\varphi$, integrate it over Ω and obtain

$$\varepsilon(\Delta\varphi, \Delta\varphi) = -\frac{1}{\varepsilon}(f'(\varphi)\nabla\varphi, \nabla\varphi) + \alpha\varepsilon(\varphi_t, \Delta\varphi) + q_0(\nabla T, \nabla\varphi) + q_1(\nabla\mu, \nabla\varphi).$$

Now, (3.24) and the repeated use of Young's inequality on the right hand side gives us

$$\varepsilon\|\Delta\varphi\|_{L_2}^2 \leq C(\varepsilon^{-1}\|\nabla\varphi\|_{L_2}^2 + \varepsilon\|\varphi_t\|_{L_2}^2 + \varepsilon\|\nabla T\|_{L_2}^2 + \varepsilon\|\nabla\mu\|_{L_2}^2).$$

Integration and inequalities (i)–(iv) lead to the desired estimate.

(vii) From (3.23) we get

$$\|\varphi_{tt}\|_{H^{-1}} \leq \frac{1}{\alpha}\|\nabla\varphi_t\|_{L_2} + \frac{1}{\alpha\varepsilon^2} \sup_{0 \neq \psi \in H^1} \frac{|(f'(\varphi)\varphi_t, \psi)|}{\|\psi\|_{H^1}} + \frac{q_0}{\alpha\varepsilon}\|T_t\|_{L_2} + \frac{q_1}{\alpha\varepsilon}\|\mu_t\|_{L_2}.$$

Using the uniform boundedness of $f'(\varphi)$ and (i)–(iv) after squaring and the time integration we get the assertion.

(viii) Differentiation of (3.1b) with respect to t gives

$$T_{tt} - \nabla \cdot (K\nabla T_t) - \nabla \cdot (K_t\nabla T) + L\varphi_{tt} = 0. \quad (3.25)$$

Now multiplying the above inequality by T_t and integrating, we get

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|T_t\|_{L_2}^2 + K_0 \|\nabla T_t\|_{L_2}^2 &\leq L \|\varphi_{tt}\|_{H^{-1}} (\|\nabla T_t\|_{L_2} + \|T_t\|_{L_2}) + \\ &\quad \frac{K_0}{4} \|\nabla T_t\|_{L_2}^2 + C \|\nabla T\|_{L_2}^2 \\ &\leq \frac{K_0}{2} \|\nabla T_t\|_{L_2}^2 + C (\|T_t\|_{L_2}^2 + \|\nabla T\|_{L_2}^2 + \|\varphi_{tt}\|_{H^{-1}}^2). \end{aligned}$$

Now the desired inequality is derived from the above by integrating it over $[0, t_\ell]$ and using (i), (ii), (vii), (3.17c) and (3.17d).

(ix) Similarly to (viii), we have

$$\mu_{tt} - \nabla \cdot (D\nabla\mu_t) - \nabla \cdot (D_t\nabla\mu) + M\varphi_{tt} = 0. \quad (3.26)$$

The proof is analogous to the proof of (viii).

(x) From equation (3.1b) we have

$$\sum_{i,j=1}^N K_{ij} \frac{\partial^2 T}{\partial x_i \partial x_j} = T_t + L\varphi_t - \sum_{i,j=1}^N \frac{\partial K_{ij}}{\partial x_j} \frac{\partial T}{\partial x_i}.$$

With the test function v and the assumptions (3.20) on K_{ij} we obtain

$$\left(\sum_{i,j=1}^N K_{ij} \frac{\partial^2 T}{\partial x_i \partial x_j}, v \right) \leq \frac{K_0}{2} \|v\|_{L_2}^2 + C(\|T_t\|_{L_2}^2 + \|\varphi_t\|_{L_2}^2 + \|\nabla T\|_{L_2}^2).$$

We use $v = \frac{\partial^2 T}{\partial x_j \partial x_i}$ and (3.19) in above to get

$$\frac{K_0}{2} \sum_{i=1}^N \left\| \frac{\partial^2 T}{\partial x_i \partial x_j} \right\|_{L_2}^2 \leq C(\|T_t\|_{L_2}^2 + \|\varphi_t\|_{L_2}^2 + \|\nabla T\|_{L_2}^2).$$

Now summing over j from 1 to N , and in view of the assertions (ii), (iv) and (viii) we obtain (x).

(xi) The proof for this part is very similar to that of (x).

(xii) Equation (3.25) gives us

$$\begin{aligned} \|T_{tt}\|_{H^{-1}} &\leq \|\nabla \cdot (K \nabla T_t)\|_{H^{-1}} + \|\nabla \cdot (K_t \nabla T)\|_{H^{-1}} + L \|\varphi_{tt}\|_{H^{-1}} \\ &\leq C(\|\nabla T_t\|_{L_2} + \|\nabla T\|_{L_2}^2 + \|\varphi_{tt}\|_{H^{-1}}). \end{aligned}$$

Squaring the above inequality, integrating the resulting inequality over $[0, t_\ell]$ and then using (i), (vii), (viii) gives the assertion.

(xiii) The assertion is derived similarly as above but this time by using equation (3.26).

(xiv) We multiply (3.23) by φ_{tt} and get

$$\alpha \varepsilon \|\varphi_{tt}\|_{L_2}^2 + \frac{\varepsilon}{2} \frac{d}{dt} \|\nabla \varphi_t\|_{L_2}^2 \leq \frac{1}{\varepsilon} |(f'(\varphi)\varphi_t, \varphi_{tt})| + q_0(T_t, \varphi_{tt}) + q_1(\mu_t, \varphi_{tt}).$$

In view of the following inequalities

$$\begin{aligned} \frac{1}{\varepsilon} |(f'(\varphi)\varphi_t, \varphi_{tt})| &\leq \frac{\alpha \varepsilon}{6} \|\varphi_{tt}\|_{L_2}^2 + \frac{C}{\alpha \varepsilon^3} \|\varphi_t\|_{L_2}^2 \\ q_0(T_t, \varphi_{tt}) &\leq \frac{\alpha \varepsilon}{6} \|\varphi_{tt}\|_{L_2}^2 + \frac{3q_0^2}{2\alpha \varepsilon} \|T_t\|_{L_2}^2 \\ q_1(\mu_t, \varphi_{tt}) &\leq \frac{\alpha \varepsilon}{6} \|\varphi_{tt}\|_{L_2}^2 + \frac{3q_1^2}{2\alpha \varepsilon} \|\mu_t\|_{L_2}^2 \end{aligned}$$

and the assertions in (i)–(iii) and (3.21) we get the part (a) of (xiv). For part (b) we multiply equation (3.23) by $-\Delta \varphi_t$ and use Young's inequality to get

$$\varepsilon \|\Delta \varphi_t\|_{L_2}^2 \leq C(\varepsilon \|\varphi_{tt}\|_{L_2}^2 + \varepsilon^{-3} \|\varphi_t\|_{L_2}^2 + \varepsilon^{-1} \|T_t\|_{L_2}^2 + \varepsilon^{-1} \|\mu_t\|_{L_2}^2).$$

Now, the use of (a) and the same set of inequalities as in the proof of the first part results in the desired inequality.

(xv) (a) Multiplying equation (3.25) by T_{tt} , integrating over Ω and using (3.22) with $u = \nabla T_t$ we get

$$\begin{aligned} \|T_{tt}\|_{L_2}^2 + \frac{d}{dt}(K\nabla T_t, \nabla T_t) &\leq C(\|\varphi_{tt}\|_{L_2}^2 + \|\nabla T\|_{L_2}^2 + \|\nabla T_t\|_{L_2}^2) \\ &\quad + C \sum_{i,j=1}^N \left\| \frac{\partial^2 T}{\partial x_i \partial x_j} \right\|_{L_2}^2 \end{aligned} \quad (3.27)$$

after applying Young's inequality on the right hand side. The assertion follows from the use of (i), (viii), (x), (xiv) and the assumption on $\lim_{s \rightarrow 0^+} \|\nabla T_t(s)\|_{L_2}$ in (3.21) after the time integration. For (b), we write equation (3.25) in the following form:

$$\sum_{i,j=1}^N K_{ij} \frac{\partial^2 T_t}{\partial x_i \partial x_j} = T_{tt} + L\varphi_{tt} - \sum_{i,j=1}^N \left(\frac{\partial K_{ij}}{\partial x_i} \frac{\partial T_t}{\partial x_j} + \frac{\partial K_{ij,t}}{\partial x_i} \frac{\partial T}{\partial x_j} + K_{ij,t} \frac{\partial^2 T}{\partial x_i \partial x_j} \right).$$

Using the test function v and the assumptions (3.20) on K_{ij} we obtain

$$\begin{aligned} \left(\sum_{i,j=1}^N K_{ij} \frac{\partial^2 T_t}{\partial x_i \partial x_j}, v \right) &\leq \frac{K_0}{2} \|v\|_{L_2}^2 + C(\|T_{tt}\|_{L_2}^2 + \|\varphi_{tt}\|_{L_2}^2 + \|\nabla T_t\|_{L_2}^2 \\ &\quad + \|\nabla T\|_{L_2}^2) + C \sum_{i,j=1}^N \left\| \frac{\partial^2 T}{\partial x_i \partial x_j} \right\|_{L_2}^2. \end{aligned}$$

We take $v = \frac{\partial^2 T_t}{\partial x_j \partial x_i}$ and use (3.19). Summing over 1 to N as in the proof of (x), integrating over $[0, t_\ell]$, using the estimates (i), (viii), (x), (xiv) and part (a) gives us the desired estimate.

(xvi) Both parts of assertion (xvi) can be proved analogously to (xv).

We also have the following lemma.

Lemma 3.3 *Let the assumptions of Lemma 3.2 hold and let $N \in \{2, 3\}$. Let the coefficients of K, D be in $C^0(J \times \Omega) \cap C^{\frac{\beta}{2}, \beta}(J \times \Gamma) \cap L_{s_1}(J; W_{s_2}^1(\Omega))$ with $\beta > 1 - \frac{1}{r}$, $5 < r \leq 10$, and $s_1, s_2 > r$ satisfy $\frac{2}{s_1} + \frac{N}{s_2} < 1$. Then the following estimates are valid:*

- (i) $\operatorname{ess\,sup}_J \|T(s)\|_{W_\infty^1(\Omega)}^2 ds \leq C\varepsilon^{-\max\{5, 2\xi_1\}}$,
- (ii) $\operatorname{ess\,sup}_J \|\mu(s)\|_{W_\infty^1(\Omega)}^2 ds \leq C\varepsilon^{-\max\{5, 2\xi_1\}}$

with C independent of ε .

Proof. We consider the linear parabolic problem

$$T_t - \nabla \cdot (K \nabla T) = -L\varphi_t \quad \text{in } J \times \Omega \quad (3.28a)$$

$$K \nabla T \cdot n = 0 \quad \text{on } J \times \partial\Omega \quad (3.28b)$$

$$T(0, \cdot) = T_0 \quad \text{in } \Omega. \quad (3.28c)$$

with a given function φ_t satisfying $\varphi_t \in H^1(J; L_2(\Omega)) \cap L_2(J; H^2(\Omega))$. This condition for φ_t is assured by Lemma 3.2. By applying Theorem 3.4 we obtain $\varphi_t \in H^\lambda(J; H^{2(1-\lambda)}(\Omega))$.

By Theorem 3.1, the space $H^\lambda(J; H^{2(1-\lambda)}(\Omega))$ is continuously embedded in the space $L_r(J \times \Omega)$ for $r \leq 10$, if $\lambda = \frac{2}{5}$. The condition on r results from the requirements for the embeddings $H^\lambda(J) \hookrightarrow L_r(J)$ and $H^{2(1-\lambda)}(\Omega) \hookrightarrow L_r(\Omega)$. For the first embedding we have the condition $\lambda - \frac{1}{2} \geq -\frac{1}{r}$, and by choosing $\lambda = \frac{1}{2} - \frac{1}{r}$ in the condition for the second embedding

$$2(1 - \lambda) - \frac{N}{2} \geq -\frac{N}{r}$$

with $N = 3$ we get $r \leq 10$. Therefore we have $\varphi_t \in L_r(J \times \Omega)$ for $r \leq 10$. The diffusion coefficient K satisfies the required regularity conditions, therefore we can apply Theorem 3.5 to the problem (3.28) and it implies

$$\|T\|_{W_r^{1,2}(J \times \Omega)} \leq C \left(\|\varphi_t\|_{L_r(J \times \Omega)} + \|T_0\|_{W_r^{2-\frac{2}{r}}(\Omega)} \right)$$

where we assumed that the initial function T_0 is sufficiently smooth and belongs to $T_0 \in W_r^{2-\frac{2}{r}}(\Omega)$ for a fixed $5 < r \leq 10$. Now using the embedding and interpolations as mentioned above, we obtain

$$\begin{aligned} \|T\|_{W_r^{1,2}(J \times \Omega)} &\leq C \left(\|\varphi_t\|_{H^\lambda(J; H^{2(1-\lambda)}(\Omega))} + \|T_0\|_{W_r^{2-\frac{2}{r}}(\Omega)} \right) \\ &\leq C \left(\|\varphi_t\|_{H^1(J; L_2(\Omega))}^\lambda \|\varphi_t\|_{L_2(J; H^2(\Omega))}^{1-\lambda} + \|T_0\|_{W_r^{2-\frac{2}{r}}(\Omega)} \right). \end{aligned} \quad (3.29)$$

We choose a suitable initial function T_0 such that $\|T_0\|_{W_r^{2-\frac{2}{r}}(\Omega)} \leq C\varepsilon^{-\frac{5}{2}}$. We can indeed get a better power of ε in the above for r near to 5 (see (3.17) and the remarks there). Using now the energy estimates of Lemma 3.2, we obtain from (3.29)

$$\|T\|_{W_r^{1,2}(J \times \Omega)} \leq C\varepsilon^{-\frac{1}{2} \max\{5, 2\xi_1\}}. \quad (3.30)$$

Furthermore, by Corollary 3.1 we obtain $W_r^{1,2} \hookrightarrow W_r^\lambda(J; W_r^{2(1-\lambda)\ell}(\Omega))$. Now, by Theorem 3.1 we have the embeddings $W_r^\lambda(J) \hookrightarrow L_\infty(J)$ and $W_r^{2(1-\lambda)\ell}(\Omega) \hookrightarrow$

$W_\infty^1(\Omega)$ which are valid for $r > 5$. The requirement $r > 5$ results from the conditions of the above two embeddings, $\lambda - \frac{1}{r} > 0$ and $2(1 - \lambda) - \frac{N}{r} > 1$. Then we have $W_r^{1,2}(J \times \Omega) \hookrightarrow L_\infty(J; W_\infty^1(\Omega))$ and this together with the estimate (3.30) concludes the proof of (i). The assertion (ii) is proved analogously by considering the parabolic problem for μ with diffusion coefficient D and sufficiently smooth initial function μ_0 .

3.3 Spectrum estimates

Now we turn our attention to the spectrum estimate which plays a crucial role in the derivation of error estimates. Consider the equation

$$\alpha\varepsilon\varphi_t - \varepsilon\Delta\varphi + \varepsilon^{-1}f(\varphi) - q_0T - q_1\mu = 0. \quad (3.31)$$

For $q_0 = q_1 = 0$ we get the Allen-Cahn equation. Let φ_ε be the first component of the solution of (3.1)–(3.2). In order to study the stability of the solution at a specific time t , we make the following substitution in (3.31)

$$\varphi = \varphi_\varepsilon + \delta e^{-\lambda t}\psi(x) + O(\delta^2)$$

and pass δ to 0. We obtain the following eigenvalue problem over Ω and $\lambda \in \mathbb{C}$:

$$-\varepsilon\Delta\psi + \varepsilon^{-1}f'(\varphi_\varepsilon(\cdot, t))\psi = \alpha\varepsilon\lambda\psi \quad (3.32)$$

With the notation

$$\mathcal{L} = -\varepsilon\Delta + \varepsilon^{-1}f'(\varphi_\varepsilon(\cdot, t))\mathbf{I}$$

for the Allen-Cahn operator we can write the eigenvalue problem as

$$\mathcal{L}\psi = \lambda\alpha\varepsilon\psi. \quad (3.33)$$

Here, \mathbf{I} is the identity operator. The problem is considered with boundary condition $\nabla\psi \cdot n = 0$ on $\partial\Omega$. We multiply equation (3.33) by $\bar{\psi}$, the complex conjugate of ψ , and integrate over Ω and obtain

$$\int_\Omega (\varepsilon|\nabla\psi|^2 + \varepsilon^{-1}f'(\varphi_\varepsilon(\cdot, t))\psi^2) dx = \lambda\alpha\varepsilon \int_\Omega \psi^2 dx.$$

The above equation implies that

$$\lambda = \frac{\varepsilon\|\nabla\psi\|_{L_2}^2 + \varepsilon^{-1}(f'(\varphi_\varepsilon(\cdot, t))\psi, \psi)}{\alpha\varepsilon\|\psi\|_{L_2}^2} \quad (3.34)$$

Therefore, we deduce from the above equation that λ is real.

The aim is to find a lower bound for λ which should be independent of ε . Chen [16] has obtained a lower bound for λ under certain assumptions. One of the assumptions is that the function f satisfies $f \in C^3(\mathbb{R})$ and

$$\begin{cases} f(\pm 1) = 0, & f'(\pm 1) > 0 \\ \int_{-1}^u f(s) ds = \int_1^u f(s) ds > 0, & \forall u \in (-1, 1). \end{cases} \quad (3.35)$$

Notice that the conditions are satisfied by the function $f(\varphi) = \varphi^3 - \varphi$ which is the choice for our problem.

Let Γ is an $N - 1$ dimensional compact manifold embedded in Ω corresponding to the set of zeros of $\phi_\varepsilon(x) = \varphi_\varepsilon(\cdot, t)$. We need local coordinates defined with respect to Γ .

Denote by $r = r(x)$ the signed distance of x to Γ , positive in the liquid and negative in the solid domain. Let $s = s(x)$ be the projection of x on Γ along the normal of Γ (cf. Figure 3.1). For a smooth Γ , there exists a

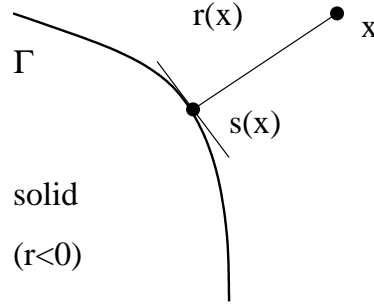


Figure 3.1: Interpretation of the local coordinates (r, s)

constant $d_0 > 0$ such that

$$\Gamma(2d_0) = \{x \in \mathbb{R}^N : |r(x)| < 2d_0\} \subset \Omega$$

and a mapping $\tau : \Gamma(2d_0) \rightarrow (-2d_0, 2d_0) \times \Gamma$ defined by

$$\tau = (r(x), s(x))$$

is a diffeomorphism.

We assume that in $\Gamma(d_0)$, the function $\phi_\varepsilon(x)$ has an expansion

$$\phi_\varepsilon(x) = \theta_0 \left(\frac{r(x)}{\varepsilon} \right) + \varepsilon p_\varepsilon(s(x)) \theta_1 \left(\frac{r(x)}{\varepsilon} \right) + \varepsilon^2 q_\varepsilon(x), \quad \forall x \in \Gamma(d_0) \quad (3.36)$$

with smooth functions $p_\varepsilon(x), q_\varepsilon(x)$ satisfying

$$\sup_{\varepsilon \in (0, 1], x \in \Gamma(d_0)} \left(|p^\varepsilon(x)| + \frac{\varepsilon}{\varepsilon + |r(x)|} |q_\varepsilon(x)| \right) \leq C \quad (3.37)$$

for a positive constant C . The function θ_0 is the lowest order term in the asymptotic expansion in the neighbourhood of Γ . It satisfies (cf. (A1.21), Appendix A.1)

$$-\theta_0'' + f(\theta_0) = 0 \text{ in } \mathbb{R}, \quad \theta_0(0) = 0, \quad \theta_0(\pm\infty) = \pm 1. \quad (3.38)$$

For our selection $f(\varphi) = \varphi^3 - \varphi$ we can compute θ_0 explicitly, i.e.

$$\theta_0(\rho) = \tanh\left(\frac{\rho}{\sqrt{2}}\right)$$

where $\rho = r/\varepsilon$. Function $\theta_1(\rho)$ which belongs to the first order term in the asymptotic expansion satisfies $\theta_1 \in C^1(\mathbb{R}) \cap L_\infty(\mathbb{R})$ and

$$\int_{\mathbb{R}} \theta_1(\theta_0')^2 f''(\theta_0) d\rho = 0$$

(cf. (A1.31) and (A1.32) in Appendix A.1). For the details on the asymptotic expansions we refer to A.1 which contains formal asymptotic expansions of the underlying phase field system.

We also assume that an away from interface condition

$$\inf_{\varepsilon \in (0,1], x \in \Omega \setminus \Gamma(d_0)} f'(\phi_\varepsilon(x)) \geq 0 \quad (3.39)$$

is satisfied. Without any loss of generality, we take $d_0 = 1$.

In the following we collect some results for the Allen-Cahn operator \mathcal{L} . We use the following notations: Let τ^{-1} be the inverse of the mapping $\tau = (r(x), s(x))$ and let

$$J(r, s) = \det \frac{\partial \tau^{-1}(r, s)}{\partial (r, s)}$$

be its Jacobian. Let $z = r/\varepsilon$ be the stretched variable and let $I_\varepsilon = (-1/\varepsilon, 1/\varepsilon)$. In the domain $\Gamma(1)$, functions of variable x and variable (r, s) are identified. We reserve ψ to represent a generic functions of (r, s) and Ψ to represent a

generic function of (z, s) . We shall use the following notations:

$$\begin{aligned}
\langle \Psi, \Phi \rangle &\equiv \int_{I_\varepsilon} \Psi \Phi \, dz, \quad \|\Psi\|^2 = \langle \Psi, \Psi \rangle \\
\langle \Psi, \Phi \rangle_s &\equiv \int_{I_\varepsilon} \Psi \Phi J(\varepsilon z, s) \, dz, \quad \|\Psi\|_s^2 = \langle \Psi, \Psi \rangle_s \\
L^0 \langle \Psi, \Phi \rangle &\equiv \int_{I_\varepsilon} (\Psi_z \Phi_z + f'(\theta_0(z)) \Psi \Phi) \, dz \\
L^s \langle \Psi, \Phi \rangle &\equiv \int_{I_\varepsilon} (\Psi_z \Phi_z + f'(\phi_\varepsilon(\varepsilon z, s)) \Psi \Phi) J(\varepsilon z, s) \, dz \\
(\psi, \phi)_s &\equiv \int_{I_1} \psi \phi J(r, s) \, dr, \quad |\psi|_s^2 = (\psi, \psi)_s \\
L^s(\psi, \phi) &\equiv \int_{I_1} (\varepsilon \psi_r \phi_r + \varepsilon^{-1} f'(\phi_\varepsilon(r, s)) \psi \phi) J(r, s) \, dr.
\end{aligned}$$

We have

$$\|\psi\|_{L^2(\Gamma(1))}^2 = \int_{\Gamma} |\psi|_s^2,$$

and for

$$\Psi(z, s) = \sqrt{\varepsilon} \psi(\varepsilon z, s), \quad \Phi(z, s) = \sqrt{\varepsilon} \phi(\varepsilon z, s), \quad (3.40)$$

we have

$$L^s \langle \Psi, \Phi \rangle = \varepsilon L^s(\psi, \phi), \quad \|\Psi\|_s = |\psi|_s.$$

Assume that the relation (3.40) between ψ and Ψ is always valid. As usual we write $\Psi \perp_s \Phi$ if $\langle \Psi, \Phi \rangle_s = 0$ and $\Psi \perp \Phi$ if $\langle \Psi, \Phi \rangle = 0$.

We define the operator \mathcal{L}_0 by

$$\mathcal{L}_0 = -\frac{d^2}{dz^2} + f'(\theta_0)I$$

in I_ε with Neumann boundary conditions $\frac{d}{dz} = 0$ on ∂I_ε .

Next, we recall two useful lemmas from [16]. We omit the proofs here and refer to the Section 2 of [16] for the details. We have,

Lemma 3.4 ([16, Lemma 2.1])

(1) *The principal eigenvalue λ_1^0 and the corresponding normalized eigenfunction Ψ_1^0 of \mathcal{L}_0 satisfy*

$$\lambda_1^0 \equiv \inf_{\|\Psi\|_s=1} L^0 \langle \Psi, \Psi \rangle = L^0 \langle \Psi_1^0, \Psi_1^0 \rangle = O(e^{-\frac{3m}{2\varepsilon}})$$

where $m = \sqrt{\min\{f'(1), f'(-1)\}}$.

(2) There exists positive constants ε_1 and v_1 such that for all $\varepsilon \in (0, \varepsilon_1]$,

$$\lambda_2^0 \equiv \inf_{\Psi \perp \Psi_1^0, \|\Psi\|=1} L^0 \langle \Psi, \Psi \rangle$$

satisfies

$$\lambda_2^0 \geq v_1.$$

(3) For $\beta = \|\theta_0'\|^{-1}$ we have

$$\|\Psi_1^0 - \beta\theta_0'\|^2 = O(e^{-\frac{3m}{2\varepsilon}}).$$

Consider now the bilinear form $L^s \langle \Psi, \Phi \rangle$, $s \in \Gamma$ and eigenvalues of the corresponding elliptic operator

$$\mathcal{L}_s = -J^{-1} \frac{d}{dz} \left(J \frac{d}{dz} \right) + f'(\phi_\varepsilon(\varepsilon z, s))I$$

on I_ε with homogeneous Neumann boundary conditions. By employing the lower bounds for λ_1^0 and λ_2^0 , Chen [16] has proved the following lemma for the principal eigenvalue of the operator \mathcal{L}_s .

Lemma 3.5 ([16, Lemma 2.2(1)])

The principal eigenvalue $\lambda_1(s)$ and its normalized positive eigenfunction $\Psi_1(z, s)$ of the operator \mathcal{L}_s satisfy

$$\begin{aligned} \lambda_1(s) &\equiv \inf_{\|\Psi\|_s=1} L^s \langle \Psi, \Psi \rangle = L^s \langle \Psi_1, \Psi_1 \rangle = O(\varepsilon^2), \\ \Psi_1(z, s) - \beta\theta_0'(z) &= \Psi_1^R(z, s) \end{aligned} \quad (3.41)$$

where Ψ_1^R satisfies

$$\sup_{s \in \Gamma} (\|\Psi_1^R\|_s + \|(\Psi_1^R)_z\|_s) = O(\varepsilon).$$

The estimate for $\lambda_1(s)$ in the above lemma leads to the following:

Theorem 3.6 ([16, Theorem 2.3]) Assume that (3.36)–(3.39) hold. Then there exists a positive constant C_0 such that for every $\varepsilon \in (0, 1]$ and every $\psi \in H^1(\Omega)$,

$$\int_{\Omega} \varepsilon |\nabla \psi|^2 + \varepsilon^{-1} f'(\phi_\varepsilon) \psi^2 \geq -C_0 \alpha \varepsilon \int_{\Omega} \psi^2. \quad (3.42)$$

Proof. Since $f'(\phi_\varepsilon) \geq 0$ in $\Omega \setminus \Gamma(1)$, we have

$$\begin{aligned}
\int_{\Omega} (\varepsilon |\nabla \psi|^2 + \varepsilon^{-1} f'(\phi_\varepsilon) \psi^2) dx &= \int_{\Omega \setminus \Gamma(1)} (\varepsilon |\nabla \psi|^2 + \varepsilon^{-1} f'(\phi_\varepsilon) \psi^2) dx \\
&\quad + \int_{\Gamma(1)} (\varepsilon |\nabla \psi|^2 + \varepsilon^{-1} f'(\phi_\varepsilon) \psi^2) dx \\
&\geq \int_{\Gamma(1)} (\varepsilon |\nabla \psi|^2 + \varepsilon^{-1} f'(\phi_\varepsilon) \psi^2) dx \\
&= \int_{\Gamma} \int_{I_1} (\varepsilon |\nabla \psi|^2 + \varepsilon^{-1} f'(\phi_\varepsilon) \psi^2) J(r, s) dr ds \\
&= \int_{\Gamma} L^s(\psi, \psi) ds.
\end{aligned}$$

By the relation (3.40) and Lemma 3.5 we have

$$\begin{aligned}
\int_{\Gamma} L^s(\psi, \psi) ds &= \varepsilon^{-1} \int_{\Gamma} L^s \langle \Psi, \Psi \rangle ds \\
&\geq \varepsilon^{-1} \int_{\Gamma} \lambda_1(s) \|\Psi\|_s^2 ds \geq \varepsilon^{-1} (\min_{s \in \Gamma} \lambda_1(s)) \int_{\Gamma} \|\Psi\|_s^2 ds \\
&= \varepsilon^{-1} (\min_{s \in \Gamma} \lambda_1(s)) \int_{\Gamma} |\psi|_s^2 ds = \varepsilon^{-1} (\min_{s \in \Gamma} \lambda_1(s)) \int_{\Gamma(1)} \psi^2 dx \\
&\geq -C_0 \alpha \varepsilon \int_{\Omega} \psi^2 dx
\end{aligned}$$

which implies the assertion of the theorem. \square

3.4 Fully discrete finite element method

In the present section we shall deal with stability estimates and a discrete version of the spectrum estimate. The major aim is to derive an error estimate for a fully discrete scheme where the dependence of the error on ε^{-1} is of polynomial order.

Let \mathcal{T}_h be a quasi-uniform triangulation of Ω and let h be the mesh size of \mathcal{T}_h . Let $J := (0, \mathcal{T}]$ be a time interval. We denote by $V_h \subset H^1(\Omega)$ the finite element subspace of continuous piecewise linear functions associated with the triangulation \mathcal{T}_h . More precisely, we have

$$V_h := \{v_h \in C(\bar{\Omega}) : v_h|_{\mathcal{K}} \in P_1(\mathcal{K}), \forall \mathcal{K} \in \mathcal{T}_h\}.$$

The elliptic projections $P_h^i : H^1(\Omega) \rightarrow V_h$, ($i = I, K, D$) are defined as

follows: For all $t \in J$,

$$(\nabla[\varphi - P_h^I \varphi], \nabla v_h) = 0 \quad \forall v_h \in V_h, \quad (\varphi - P_h^I \varphi, 1) = 0, \quad (3.43a)$$

$$(K \nabla[T - P_h^K T], \nabla v_h) = 0 \quad \forall v_h \in V_h, \quad (T - P_h^K T, 1) = 0, \quad (3.43b)$$

$$(D \nabla[\mu - P_h^D \mu], \nabla v_h) = 0 \quad \forall v_h \in V_h, \quad (\mu - P_h^D \mu, 1) = 0. \quad (3.43c)$$

In the following we summarize some of the well-known approximation properties of elliptic projections. For details the reader is referred to the classical texts by Brenner and Scott [6], Ciarlet [18] and the paper of Feng and Prohl [26]. The diffusion coefficients K and D are symmetric, elliptic, bounded and satisfy condition (3.20). Then the following properties are valid:

$$\|\psi - P_h^i \psi\|_{L_2} + h \|\nabla(\psi - P_h^i \psi)\|_{L_2} \leq Ch^2 \|\psi\|_{H^2}, \quad \forall \psi \in H^2(\Omega), \quad (3.44)$$

$$\|\psi - P_h^i \psi\|_{L_\infty} \leq Ch^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \|\psi\|_{H^2} \quad (N = 2, 3), \quad \forall \psi \in H^2(\Omega), \quad (3.45)$$

$$\|(\psi - P_h^i \psi)_t\|_{L_2(J; L_2(\Omega))} \leq Ch^2 \|\psi_t\|_{L_2(J; H^2(\Omega))}, \quad \forall \psi \in H^1(J; H^2(\Omega)). \quad (3.46)$$

For simplicity of the notation, we use P_h for P_h^I .

We introduce now a fully discrete finite element method for the system (3.1). Let $J_k = \{t_m\}_{m=0}^{M_\ell}$ be the partition of J with time step k , i.e. $t_i - t_{i-1} = k$ for $i = 1, \dots, M_\ell$. The scheme can be formulated as follows:

Find $(\Phi^m, T^m, \mu^m) \in [V_h]^3$, $m = 1, 2, \dots, M_\ell$ such that for all $(u_h, v_h, w_h) \in [V_h]^3$,

$$\begin{aligned} \alpha \varepsilon (d_t \Phi^m, u_h) + \varepsilon (\nabla \Phi^m, \nabla u_h) + \frac{1}{\varepsilon} (f(\Phi^m), u_h) \\ - q_0(T^m, u_h) - q_1(\mu^m, u_h) = 0 \end{aligned} \quad (3.47a)$$

$$(d_t T^m, v_h) + (K^m \nabla T^m, \nabla v_h) + L(d_t \Phi^m, v_h) = 0 \quad (3.47b)$$

$$(d_t \mu^m, w_h) + (D^m \nabla \mu^m, \nabla w_h) + M(d_t \Phi^m, w_h) = 0 \quad (3.47c)$$

where (Φ^m, T^m, μ^m) are approximations of $(\varphi(t_m, \cdot), T(t_m, \cdot), \mu(t_m, \cdot))$, and

$$d_t U^m = \frac{U^m - U^{m-1}}{k}.$$

By K^m, D^m we denote approximations to $K(t_m, \cdot)$ and $D(t_m, \cdot)$. For the derivation of error estimates for the above scheme we need some stability estimates and a discrete version of the spectrum estimate. The following two sections deal with stability and spectrum estimates.

3.4.1 Stability estimates

For the solution $\{(\Phi^m, T^m, \mu^m)\}_{m=1}^{M_\ell}$ of the system (3.47) we have the following lemma.

Lemma 3.6 *Under the assumption $k \leq 2c_0\alpha\varepsilon^2$ with $0 < c_0 < 1/4$, the solution $\{(\Phi^m, T^m, \mu^m)\}_{m=1}^{M_t}$ of (3.47) satisfies the following estimates:*

$$\begin{aligned}
\text{(a)} \quad & \max_{1 \leq m \leq M_t} \left\{ \frac{\varepsilon}{2} \|\nabla \Phi^m\|_{L_2}^2 + \frac{1}{\varepsilon} \|F(\Phi^m)\|_{L_1} + \frac{q_0}{2L} \|T^m\|_{L_2}^2 + \frac{q_1}{2M} \|\mu^m\|_{L_2}^2 \right\} + \\
& k \sum_{m=1}^{M_t} \left\{ (1 - c_0)\alpha\varepsilon \|d_t \Phi^m\|_{L_2}^2 + \frac{\varepsilon k}{2} \|d_t \nabla \Phi^m\|_{L_2}^2 + \frac{k}{4\varepsilon} \|d_t |\Phi^m|^2\|_{L_2}^2 \right. \\
& \left. + \frac{q_0 k}{2L} \|d_t T^m\|_{L_2}^2 + \frac{q_1 k}{2M} \|d_t \mu^m\|_{L_2}^2 + \frac{q_0 K_0}{L} \|\nabla T^m\|_{L_2}^2 + \frac{q_1 D_0}{M} \|\nabla \mu^m\|_{L_2}^2 \right\} \\
& \leq C \tag{3.48}
\end{aligned}$$

and

$$\begin{aligned}
\text{(b)} \quad & \max_{2 \leq m \leq M_t} \left\{ \frac{\alpha\varepsilon}{2} \|d_t \Phi^m\|_{L_2}^2 + \frac{q_0 K_0}{2L} \|\nabla T^m\|_{L_2}^2 + \frac{q_1 D_0}{2M} \|\nabla \mu^m\|_{L_2}^2 \right\} \\
& + k \sum_{m=2}^{M_t} \left\{ \frac{\alpha\varepsilon k}{2} \|d_t^2 \Phi^m\|_{L_2}^2 + \varepsilon \|d_t \nabla \Phi^m\|_{L_2}^2 + \frac{q_0}{L} \|d_t T^m\|_{L_2}^2 + \frac{q_1}{M} \|d_t \mu^m\|_{L_2}^2 \right. \\
& \left. + \frac{q_0 K_0 k}{2L} \|d_t \nabla T^m\|_{L_2}^2 + \frac{q_1 D_0 k}{2M} \|d_t \nabla \mu^m\|_{L_2}^2 \right\} \leq C\varepsilon^{-2}. \tag{3.49}
\end{aligned}$$

Proof. From the definition of f we have

$$f(\Phi^m) = \frac{1}{2} (|\Phi^m|^2 - 1) (\Phi^m + \Phi^{m-1}) + k d_t \Phi^m.$$

Multiplying the above identity by $\frac{1}{\varepsilon} d_t \Phi^m$ and integrating it over Ω we obtain

$$\begin{aligned}
\frac{1}{\varepsilon} (f(\Phi^m), d_t \Phi^m) &= \frac{1}{2\varepsilon} \left(|\Phi^m|^2 - 1, (\Phi^m + \Phi^{m-1}) \frac{\Phi^m - \Phi^{m-1}}{k} \right) \\
&+ \frac{1}{2\varepsilon} (|\Phi^m|^2 - 1, k d_t \Phi^m d_t \Phi^m) \\
&= \frac{1}{2\varepsilon} (|\Phi^m|^2 - 1, d_t (|\Phi^m|^2 - 1)) + \frac{k}{2\varepsilon} (|\Phi^m|^2 - 1, |d_t \Phi^m|^2).
\end{aligned}$$

Using the identity

$$(d_t U^m, U^m) = \frac{1}{2} d_t \|U^m\|_{L_2}^2 + \frac{k}{2} \|d_t U^m\|_{L_2}^2 \tag{3.50}$$

in the first term on the right hand side, we obtain

$$\begin{aligned}
\frac{1}{\varepsilon}(f(\Phi^m), d_t\Phi^m) &= \frac{1}{2\varepsilon} \left(\frac{1}{2}d_t\|\Phi^m\|^2 - 1\|_{L_2}^2 + \frac{k}{2}\|d_t(|\Phi^m|^2 - 1)\|_{L_2}^2 \right) + \\
&\quad \frac{k}{2\varepsilon}(|\Phi^m|^2, |d_t\Phi^m|^2) - \frac{k}{2\varepsilon}\|d_t\Phi^m\|_{L_2}^2 \\
&\geq \frac{1}{4\varepsilon}d_t\|\Phi^m\|^2 - 1\|_{L_2}^2 + \\
&\quad \frac{k}{4\varepsilon}\|d_t|\Phi^m|^2\|_{L_2}^2 - \frac{k}{2\varepsilon}\|d_t\Phi^m\|_{L_2}^2. \tag{3.51}
\end{aligned}$$

In order to verify (a), we choose $u_h = d_t\Phi^m$ in (3.47a), $v_h = q_0L^{-1}T^m$ in (3.47b) and $w_h = q_1M^{-1}\mu^m$ in (3.47c) and add the resulting equations. This leads to

$$\begin{aligned}
&\alpha\varepsilon(d_t\Phi^m, d_t\Phi^m) + \varepsilon(\nabla\Phi^m, \nabla d_t\Phi^m) + \frac{1}{\varepsilon}(f(\Phi^m), d_t\Phi^m) + \frac{q_0}{L}(d_tT^m, T^m) \\
&+ \frac{q_0}{L}(K^m\nabla T^m, \nabla T^m) + \frac{q_1}{M}(d_t\mu^m, \mu^m) + \frac{q_1}{M}(D^m\nabla\mu^m, \nabla\mu^m) = 0.
\end{aligned}$$

Now using (3.50) and the estimate in (3.51) for $\frac{1}{\varepsilon}(f(\Phi^m), d_t\Phi^m)$ we obtain

$$\begin{aligned}
&\frac{\varepsilon}{2}d_t\|\nabla\Phi^m\|_{L_2}^2 + \frac{1}{4\varepsilon}d_t\|\Phi^m\|^2 - 1\|_{L_2}^2 + \frac{q_0}{2L}d_t\|T^m\|_{L_2}^2 + \frac{q_1}{2M}d_t\|\mu^m\|_{L_2}^2 \\
&+ \alpha\varepsilon\|d_t\Phi^m\|_{L_2}^2 + \frac{\varepsilon k}{2}\|d_t\nabla\Phi^m\|_{L_2}^2 + \frac{k}{4\varepsilon}\|d_t|\Phi^m|^2\|_{L_2}^2 + \frac{q_0k}{2L}\|d_tT^m\|_{L_2}^2 \\
&+ \frac{q_1k}{2M}\|d_t\mu^m\|_{L_2}^2 + \frac{q_0K_0}{L}\|\nabla T^m\|_{L_2}^2 + \frac{q_1D_0}{M}\|\nabla\mu^m\|_{L_2}^2 \leq \frac{k}{2\varepsilon}\|d_t\Phi^m\|_{L_2}^2 \tag{3.52}
\end{aligned}$$

Assume that k satisfies

$$\alpha\varepsilon - \frac{k}{2\varepsilon} \geq (1 - c_0)\alpha\varepsilon \tag{3.53}$$

for some $0 < c_0 < 1$, that is, $k \leq 2c_0\alpha\varepsilon^2$. This guarantees that all coefficients on the left hand side are positive. Now, after multiplying (3.52) by k , summing over m from 1 to M_ℓ and using (3.17b) we get the assertion (a).

We need an intermediate estimate before we prove assertion (b). By taking the test function d_tT^m for equation (3.47b) and using the identity

$$\begin{aligned}
(K^m\nabla T^m, d_t\nabla T^m) &= \frac{1}{2}d_t(K^m\nabla T^m, \nabla T^m) + \frac{k}{2}(K^m d_t\nabla T^m, d_t\nabla T^m) \\
&\quad - \frac{1}{2}(d_tK^m\nabla T^{m-1}, \nabla T^{m-1}) \tag{3.54}
\end{aligned}$$

we get

$$\begin{aligned} \|d_t T^m\|_{L_2}^2 + \frac{1}{2}d_t(K^m \nabla T^m, \nabla T^m) + \frac{k}{2}(K^m d_t \nabla T^m, d_t \nabla T^m) \\ \leq \frac{1}{2}\|d_t T^m\|_{L_2}^2 + \frac{L^2}{2}\|d_t \Phi^m\|_{L_2}^2 + C\|\nabla T^{m-1}\|_{L_2}^2 \end{aligned}$$

where we used $d_t K^m = (K^m - K^{m-1})/k = K_t(\xi^m, \cdot)$, the assumption on K and Young's inequality.

Summing up the previous inequality over m after multiplying by k we obtain

$$\begin{aligned} K_0 \max_{1 \leq m \leq M_t} \|\nabla T^m\|_{L_2}^2 + k \sum_{m=1}^{M_t} \{ \|d_t T^m\|_{L_2}^2 + K_0 k \|d_t \nabla T^m\|_{L_2}^2 \} \\ \leq kL^2 \sum_{m=1}^{M_t} \|d_t \Phi^m\|_{L_2}^2 + k \sum_{m=1}^{M_t} \|\nabla T^{m-1}\|_{L_2}^2 + (K^0 \nabla T^0, \nabla T^0) \leq C\varepsilon^{-1} \quad (3.55) \end{aligned}$$

where we used the assertion (a) and (3.17d) in the last step. By applying the same procedure for equation (3.47c) we obtain a similar estimate

$$D_0 \max_{1 \leq m \leq M_t} \|\nabla \mu^m\|_{L_2}^2 + k \sum_{m=1}^{M_t} \{ \|d_t \mu^m\|_{L_2}^2 + D_0 k \|d_t \nabla \mu^m\|_{L_2}^2 \} \leq C\varepsilon^{-1} \quad (3.56)$$

Equation (3.47a) for $m = 1$, $u_h = d_t \Phi^1$ gives us

$$\alpha\varepsilon(d_t \Phi^1, d_t \nabla \Phi^1) + \varepsilon(\nabla \Phi^1, d_t \Phi^1) + \frac{1}{\varepsilon}(f(\Phi^1), d_t \Phi^1) - q_0(T^1, d_t \Phi^1) - q_1(\mu^1, d_t \Phi^1) = 0.$$

According to (3.17c), we have

$$\varepsilon(\nabla \Phi^0, d_t \nabla \Phi^1) + \frac{1}{\varepsilon}(f(\Phi^0), d_t \Phi^1) - q_0(T^0, d_t \Phi^1) - q_1(\mu^0, d_t \Phi^1) \geq -C\varepsilon^{-\frac{1}{2}}\|d_t \Phi^1\|_{L_2}.$$

Hence, by subtracting this from the equation before we obtain

$$\begin{aligned} \alpha\varepsilon\|d_t \Phi^1\|_{L_2}^2 + \varepsilon k \|\nabla d_t \Phi^1\|_{L_2}^2 + \frac{k}{\varepsilon}(f'(\xi)d_t \Phi^1, d_t \Phi^1) \\ - q_0(T^1 - T^0, d_t \Phi^1) - q_1(\mu^1 - \mu^0, d_t \Phi^1) \leq C\varepsilon^{-\frac{1}{2}}\|d_t \Phi^1\|_{L_2}. \end{aligned}$$

With the inequalities

$$\begin{aligned} \frac{k}{\varepsilon}(f'(\xi)d_t \Phi^1, d_t \Phi^1) &\geq -\frac{k}{\varepsilon}\|d_t \Phi^1\|_{L_2}^2 \\ C\varepsilon^{-\frac{1}{2}}\|d_t \Phi^1\|_{L_2} &\leq \frac{\alpha\varepsilon}{6}\|d_t \Phi^1\|_{L_2}^2 + \tilde{C}\varepsilon^{-2} \\ q_0(T^1 - T^0, d_t \Phi^1) &\leq \frac{\alpha\varepsilon}{6}\|d_t \Phi^1\|_{L_2}^2 + C\varepsilon^{-1}(\|T^1\|_{L_2}^2 + \|T^0\|_{L_2}^2), \end{aligned}$$

(and a similar inequality for the remaining term involving μ) we get

$$\begin{aligned} \left(\frac{\alpha\varepsilon}{2} - \frac{k}{\varepsilon}\right) \|d_t\Phi^1\|_{L_2}^2 + \varepsilon k \|\nabla d_t\Phi^1\|_{L_2}^2 &\leq C\varepsilon^{-1}(\varepsilon^{-1} + \|T^1\|_{L_2}^2 + \\ &+ \|\mu^1\|_{L_2}^2 + \|T^0\|_{L_2}^2 + \|\mu^0\|_{L_2}^2). \end{aligned}$$

Using condition (3.53) (with $0 < c_0 < 1/4$), (3.17), we obtain

$$(1 - 4c_0)\frac{\alpha\varepsilon}{2} \|d_t\Phi^1\|_{L_2}^2 \leq C\varepsilon^{-2}. \quad (3.57)$$

Now we come to the assertion (b).

(b) Applying the difference operator d_t to (3.47a) and using the test function $d_t\Phi^m$ we get

$$\begin{aligned} \alpha\varepsilon(d_t^2\Phi^m, d_t\Phi^m) + \varepsilon(d_t\nabla\Phi^m, \nabla d_t\Phi^m) + \frac{1}{\varepsilon}(d_t f(\Phi^m), d_t\Phi^m) \\ - q_0(d_t T^m, d_t\Phi^m) - q_1(d_t\mu^m, d_t\Phi^m) = 0. \end{aligned}$$

We add equation (3.47b) with $v_h = q_0 L^{-1} d_t T^m$ and equation (3.47c) with $w_h = q_1 M^{-1} d_t \mu^m$ to the above equation. Then we use the identity (3.54) and the inequality

$$\begin{aligned} \frac{1}{\varepsilon}(d_t f(\Phi^m), d_t\Phi^m) &= \frac{1}{\varepsilon} \left(\frac{f(\Phi^m) - f(\Phi^{m-1})}{k}, d_t\Phi^m \right) \\ &= \frac{1}{\varepsilon} (f'(\xi) d_t\Phi^m, d_t\Phi^m) \\ &\geq -\frac{1}{\varepsilon} \|d_t\Phi^m\|_{L_2}^2 \end{aligned}$$

to get

$$\begin{aligned} \frac{\alpha\varepsilon}{2} d_t \|d_t\Phi^m\|_{L_2}^2 + \frac{\alpha\varepsilon k}{2} \|d_t^2\Phi^m\|_{L_2}^2 + \varepsilon \|d_t\nabla\Phi^m\|_{L_2}^2 + \frac{q_0}{L} \|d_t T^m\|_{L_2}^2 \\ + \frac{q_0}{2L} d_t (K^m \nabla T^m, \nabla T^m) + \frac{q_0 k}{2L} (K^m d_t \nabla T^m, d_t \nabla T^m) + \frac{q_1}{M} \|d_t \mu^m\|_{L_2}^2 \\ + \frac{q_1}{2M} d_t (D^m \nabla \mu^m, \nabla \mu^m) + \frac{q_1 k}{2M} (D^m d_t \nabla \mu^m, d_t \nabla \mu^m) \leq \frac{1}{\varepsilon} \|d_t\Phi^m\|_{L_2}^2 \\ + \frac{q_0}{2L} (d_t K^m \nabla T^{m-1}, \nabla T^{m-1}) + \frac{q_1}{2M} (d_t D^m \nabla \mu^{m-1}, \nabla \mu^{m-1}). \quad (3.58) \end{aligned}$$

Summation over m after multiplying by k and use of (a), (3.55), (3.56) and (3.57) gives the assertion (b).

3.4.2 Discrete spectrum estimates

To establish bounds for the global error, we also need a discrete version of the spectrum estimate of Theorem 3.6. Let

$$C_1 := \max_{|\xi| \leq 2C_0} |f''(\xi)|$$

and let C_2 be the smallest positive ε -independent constant such that

$$\begin{aligned} \operatorname{ess\,sup}_J \|\varphi - P_h \varphi\|_{L^\infty} &\leq C_2 h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \operatorname{ess\,sup}_J \|\varphi\|_{H^2} \\ &\leq C C_2 h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \varepsilon^{-\frac{3}{2}}, \end{aligned}$$

where C is a constant with $\|\varphi\|_{H^2} \leq C\varepsilon^{-\frac{3}{2}}$ (cf. Lemma 3.2).

Lemma 3.7 *Suppose (3.18), Lemma 3.2 and Theorem 3.6 are valid, and ε_0, C_0 are the constants there. Let $\varepsilon_1 := \min \left\{ \varepsilon_0, \sqrt{C_1/\alpha} \right\}$. Then for $\varepsilon \in (0, \varepsilon_1]$ the following estimate holds:*

$$\inf_{0 \neq \psi \in H^1} \frac{\varepsilon \|\nabla \psi\|_{L_2}^2 + \varepsilon^{-1} (f'(P_h \varphi) \psi, \psi)}{\alpha \varepsilon \|\psi\|_{L_2}^2} \geq -2C_0, \quad (3.59)$$

provided that h satisfies

$$h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \leq (C C_1 C_2)^{-1} C_0 \alpha \varepsilon^{\frac{7}{2}}.$$

Proof. We have

$$\begin{aligned} \operatorname{ess\,sup}_J \|P_h \varphi\|_{L^\infty} &\leq \operatorname{ess\,sup}_J \{ \|\varphi\|_{L^\infty} + \|\varphi - P_h \varphi\|_{L^\infty} \} \\ &\leq C_0 + C C_2 h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \varepsilon^{-\frac{3}{2}} \\ &\leq C_0 + C_1^{-1} C_0 \alpha \varepsilon^2 \leq 2C_0. \end{aligned} \quad (3.60)$$

Using the Mean Value Theorem and the definition of C_1 and C_2 and the assumption on h , we obtain

$$\begin{aligned} \operatorname{ess\,sup}_J \|f'(P_h \varphi) - f'(\varphi)\|_{L^\infty} &\leq \sup_{|\xi| \leq 2C_0} |f''(\xi)| \operatorname{ess\,sup}_J \|P_h \varphi - \varphi\|_{L^\infty} \\ &\leq C C_1 C_2 h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \varepsilon^{-\frac{3}{2}} \\ &\leq C_0 \alpha \varepsilon^2. \end{aligned}$$

We use the inequality $a \geq b - |a - b|$ to get

$$f'(P_h \varphi) \geq f'(\varphi) - |f'(P_h \varphi) - f'(\varphi)| \geq f'(\varphi) - C_0 \alpha \varepsilon^2. \quad (3.61)$$

The above inequality in view of (3.42) implies that

$$\begin{aligned} & \inf_{0 \neq \psi \in H^1} \frac{\varepsilon \|\nabla \psi\|_{L_2}^2 + \varepsilon^{-1} (f'(P_h \varphi) \psi, \psi)}{\alpha \varepsilon \|\psi\|_{L_2}^2} \\ & \geq \inf_{0 \neq \psi \in H^1} \frac{\varepsilon \|\nabla \psi\|_{L_2}^2 + \varepsilon^{-1} (f'(\varphi) \psi, \psi)}{\alpha \varepsilon \|\psi\|_{L_2}^2} - C_0 \geq -2C_0, \end{aligned}$$

and this completes the proof. \square

3.5 Error estimates

Now we are in a position to state the main result which contains error estimates for the discrete solutions. Before that, we need a weak formulation of the phase field system. Multiplying the equations (3.1) by test functions (u, v, w) , we get the following equations for the weak solution (φ, T, μ) :

$$\alpha \varepsilon (\varphi_t, u) + \varepsilon (\nabla \varphi, \nabla u) + \frac{1}{\varepsilon} (f(\varphi), u) = q_0(T, u) + q_1(\mu, u) \quad (3.62a)$$

$$(T_t, v) + (K \nabla T, \nabla v) + L(\varphi_t, v) = 0 \quad (3.62b)$$

$$(\mu_t, w) + (D \nabla \mu, \nabla w) + M(\varphi_t, w) = 0 \quad (3.62c)$$

for all $(u, v, w) \in [H^1(\Omega)]^3$. We formulate now the following theorem.

Theorem 3.7 *Assume that $\{(\Phi^m, T^m, \mu^m)\}_{m=0}^{M_t}$ is the solution of (3.47) for the time partition J_k and a mesh \mathcal{T}_h . Assume that (3.17) holds. Let the following mesh constraints*

$$(1) \quad k \leq \min\{2c_0 \alpha \varepsilon^2, C \varepsilon^{\frac{10+N}{4}}\} \quad \text{with } 0 < c_0 < 1/4$$

$$(2) \quad h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \leq (CC_1 C_2)^{-1} C_0 \alpha \varepsilon^{\frac{7}{2}}$$

$$(3) \quad k^2 \varepsilon^{-6} + h^4 A(\varepsilon) \leq C \varepsilon^{\frac{2(10+N)}{4-N}}$$

be valid with

$$A(\varepsilon) = h^{\frac{4-N}{2}} \varepsilon^{-\frac{11}{2}} + \varepsilon^{-\max\{6, 2\xi_1\}} \quad (3.63)$$

and for $N = 2, 3$. Then the solution of (3.47) satisfies the error estimates

$$(i) \quad \max_{0 \leq m \leq M_t} \|\varphi(t_m) - \Phi^m\|_{L_2} \leq C \left(k \varepsilon^{-\frac{7}{2}} + h^2 [A(\varepsilon)]^{\frac{1}{2}} \varepsilon^{-\frac{1}{2}} \right),$$

$$(ii) \quad \left(k \sum_{m=1}^{M_t} \|T(t_m) - T^m\|_{L_2}^2 \right)^{1/2} \leq C \left(k \varepsilon^{-3} + h^2 [A(\varepsilon)]^{\frac{1}{2}} \right)$$

$$(iii) \quad \left(k \sum_{m=1}^{M_t} \|\mu(t_m) - \mu^m\|_{L_2}^2 \right)^{1/2} \leq C \left(k \varepsilon^{-3} + h^2 [A(\varepsilon)]^{\frac{1}{2}} \right)$$

$$\begin{aligned}
\text{(iv)} \quad & \max_{0 \leq m \leq M_t} \left\| k \sum_{j=1}^m \nabla(T(t_j) - T^j) \right\|_{L_2} \leq C \left(k^{\frac{1}{2}} \varepsilon^{-3} + h^2 k^{-\frac{1}{2}} [A(\varepsilon)]^{\frac{1}{2}} + h \varepsilon^{-\frac{5}{2}} \right) \\
\text{(v)} \quad & \max_{0 \leq m \leq M_t} \left\| k \sum_{j=1}^m \nabla(\mu(t_j) - \mu^j) \right\|_{L_2} \leq C \left(k^{\frac{1}{2}} \varepsilon^{-3} + h^2 k^{-\frac{1}{2}} [A(\varepsilon)]^{\frac{1}{2}} + h \varepsilon^{-\frac{5}{2}} \right) \\
\text{(vi)} \quad & \left(k \sum_{m=1}^{M_t} \|\nabla(\varphi(t_m) - \Phi^m)\|_{L_2}^2 \right)^{1/2} \leq C \left(k \varepsilon^{-\frac{9}{2}} + h^2 [A(\varepsilon)]^{\frac{1}{2}} \varepsilon^{-\frac{3}{2}} + h \varepsilon^{-\frac{3}{2}} \right) \\
\text{(vii)} \quad & \left(k \sum_{m=1}^{M_t} \|\nabla(T(t_m) - T^m)\|_{L_2}^2 \right)^{1/2} \leq C \left(k \varepsilon^{-3} + h^2 [A(\varepsilon)]^{\frac{1}{2}} + h \varepsilon^{-\frac{5}{2}} \right) \\
\text{(viii)} \quad & \left(k \sum_{m=1}^{M_t} \|\nabla(\mu(t_m) - \mu^m)\|_{L_2}^2 \right)^{1/2} \leq C \left(k \varepsilon^{-3} + h^2 [A(\varepsilon)]^{\frac{1}{2}} + h \varepsilon^{-\frac{5}{2}} \right) \\
\text{(ix)} \quad & \max_{0 \leq m \leq M_t} \|\varphi(t_m) - \Phi^m\|_{L_\infty} \leq C \left(h^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \varepsilon^{-\frac{3}{2}} \right. \\
& \quad \left. + h^{-\frac{N}{2}} \left(k \varepsilon^{-\frac{7}{2}} + h^2 [A(\varepsilon)]^{\frac{1}{2}} \varepsilon^{-\frac{1}{2}} \right) \right).
\end{aligned}$$

Proof. We divide the proof of the theorem into three parts. In Part 1 we use the weak and discrete equations to derive a basic inequality making use of the definition of the elliptic projections and the energy estimates (in Lemma 3.2). Part 2 is devoted to an estimate of the terms arising from the nonlinearity. The stability estimates (in Lemma 3.6) and the discrete spectrum estimate (in Lemma 3.7) are used in this part. The final part includes induction steps which yield an important inequality. With the help of this inequality, the properties of the elliptic projections and the energy estimates we prove the assertions of the theorem.

Part 1. We begin by defining the global errors as follows:

$$E_\varphi^m := \varphi(t_m) - \Phi^m, \quad E_T^m := T(t_m) - T^m, \quad E_\mu^m := \mu(t_m) - \mu^m. \quad (3.64)$$

Denote

$$\begin{aligned}
\Theta_\varphi^m &:= \varphi(t_m) - P_h \varphi(t_m), & \Upsilon_\varphi^m &:= P_h \varphi(t_m) - \Phi^m, \\
\Theta_T^m &:= T(t_m) - P_h^{K(t_m)} T(t_m), & \Upsilon_T^m &:= P_h^{K(t_m)} T(t_m) - T^m, \\
\Theta_\mu^m &:= \mu(t_m) - P_h^{D(t_m)} \mu(t_m), & \Upsilon_\mu^m &:= P_h^{D(t_m)} \mu(t_m) - \mu^m
\end{aligned} \quad (3.65)$$

so that

$$E_\varphi^m = \Theta_\varphi^m + \Upsilon_\varphi^m, \quad E_T^m = \Theta_T^m + \Upsilon_T^m, \quad E_\mu^m = \Theta_\mu^m + \Upsilon_\mu^m.$$

We can estimate the part of the error with Θ_u^m for $u = \varphi, T, \mu$ by the properties of the elliptic projections and the energy estimates. To estimate the

remaining part with Υ_u^m we first derive some basic equations. Using the weak equations (3.62), the definition of the elliptic projections (3.43) at time t_m and the discrete equations (3.47), we obtain

$$\begin{aligned} \alpha\varepsilon(d_t\Upsilon_\varphi^m, u_h) + \varepsilon(\nabla\Upsilon_\varphi^m, \nabla u_h) + \frac{1}{\varepsilon}(f(P_h\varphi(t_m)) - f(\Phi^m), u_h) = \\ -\alpha\varepsilon(d_t\Theta_\varphi^m, u_h) + q_0(\Theta_T^m + \Upsilon_T^m, u_h) + q_1(\Theta_\mu^m + \Upsilon_\mu^m, u_h) \\ + \alpha\varepsilon(R_\varphi^m, u_h) - \frac{1}{\varepsilon}(f(\varphi(t_m)) - f(P_h\varphi(t_m)), u_h), \end{aligned} \quad (3.66)$$

$$\begin{aligned} (d_t\Upsilon_T^m, v_h) + (K(t_m)\nabla\Upsilon_T^m, \nabla v_h) = - (d_t\Theta_T^m, v_h) - L(d_t\Theta_\varphi^m + d_t\Upsilon_\varphi^m, v_h) \\ + ([K^m - K(t_m)]\nabla T(t_m), \nabla v_h) \\ + (R_T^m + LR_\varphi^m, v_h) \end{aligned} \quad (3.67)$$

and analogously

$$\begin{aligned} (d_t\Upsilon_\mu^m, w_h) + (D(t_m)\nabla\Upsilon_\mu^m, \nabla w_h) = - (d_t\Theta_\mu^m, w_h) - M(d_t\Theta_\varphi^m + d_t\Upsilon_\varphi^m, w_h) \\ + ([D^m - D(t_m)]\nabla\mu(t_m), \nabla w_h) \\ + (R_\mu^m + MR_\varphi^m, w_h) \end{aligned} \quad (3.68)$$

where R_u^m is defined by

$$R_u^m := d_t u(t_m) - u_t(t_m), \quad \text{for } u = \varphi, T, \mu.$$

In order to deal with the terms involving $d_t\Upsilon_\varphi^m$, we need a preparatory step for the equations (3.67) and (3.68). We do the following step for equation (3.67) since for (3.68) it is done analogously. First, replacing the super index in (3.67) by j and summing over j from 1 to m gives

$$\begin{aligned} \sum_{j=1}^m (d_t\Upsilon_T^j, v_h) + \sum_{j=1}^m (K(t_m)\nabla\Upsilon_T^j, \nabla v_h) = - \sum_{j=1}^m (d_t\Theta_T^j + L(d_t\Theta_\varphi^j + d_t\Upsilon_\varphi^j), v_h) \\ + \sum_{j=1}^m \{ ([K^j - K(t_j)]\nabla T(t_j), \nabla v_h) + ([K(t_m) - K(t_j)]\nabla\Upsilon_T^j, \nabla v_h) \} \\ + \sum_{j=1}^m (R_T^j + LR_\varphi^j, v_h). \end{aligned} \quad (3.69)$$

In the above, the term $\sum_{j=1}^m (K(t_m)\nabla\Upsilon_T^j, \nabla v_h)$ in the left was added in both sides of the equation which resulted from the summing step.

Define G_T^m by

$$G_T^m = k \sum_{j=1}^m \Upsilon_T^j, \quad G_T^0 = 0. \quad (3.70)$$

We have the identity

$$k \sum_{j=1}^m d_t U^j = U^m - U^0. \quad (3.71)$$

Now, multiplying the equation (3.69) by k , and using the above identity for $k \sum_{j=1}^m (d_t \Upsilon_T^j, v_h)$, we obtain the following equation:

$$\begin{aligned} (\Upsilon_T^m, v_h) + (K(t_m) \nabla G_T^m, \nabla v_h) &= -L(\Upsilon_\varphi^m, v_h) - (L\Theta_\varphi^m + \Theta_T^m, v_h) \\ &+ k \sum_{j=1}^m \{ ([K^j - K(t_j)] \nabla T(t_j), \nabla v_h) + ([K(t_m) - K(t_j)] \nabla \Upsilon_T^j, \nabla v_h) \} \\ &+ (k \sum_{j=1}^m [R_T^j + LR_\varphi^j], v_h) + (E_T^0 + LE_\varphi^0, v_h). \end{aligned} \quad (3.72)$$

For Υ_μ^m we have an analogous equation

$$\begin{aligned} (\Upsilon_\mu^m, w_h) + (D(t_m) \nabla G_\mu^m, \nabla w_h) &= -M(\Upsilon_\varphi^m, w_h) - (M\Theta_\varphi^m + \Theta_\mu^m, w_h) \\ &+ k \sum_{j=1}^m \{ ([D^j - D(t_j)] \nabla \mu(t_j), \nabla w_h) + ([D(t_m) - D(t_j)] \nabla \Upsilon_\mu^j, \nabla w_h) \} \\ &+ (k \sum_{j=1}^m [R_\mu^j + MR_\varphi^j], w_h) + (E_\mu^0 + ME_\varphi^0, w_h) \end{aligned} \quad (3.73)$$

where G_μ^m is defined in the same manner as in (3.70).

Now, we choose $u_h = \Upsilon_\varphi^m$ in (3.66), $v_h = q_0 L^{-1} \Upsilon_T^m$ in (3.72), and $w_h = q_1 M^{-1} \Upsilon_\mu^m$ in (3.73) and add the resulting equations. Then the mixed terms on the right hand side involving $(\Upsilon_\varphi^m, \Upsilon_T^m)$ and $(\Upsilon_\varphi^m, \Upsilon_\mu^m)$ cancel. This provides the possibility to obtain terms with the desired scaling (in terms of powers of ε) on the right hand side in the estimates to follow.

After multiplying the result of the adding by k , summing over m from 1 to ℓ ($\ell \leq M_\ell$) and using the formula (3.50) for $(d_t \Upsilon_\varphi^m, \Upsilon_\varphi^m)$ we obtain

$$\begin{aligned}
& k \sum_{m=1}^{\ell} \left\{ \frac{\alpha \varepsilon}{2} (d_t \|\Upsilon_\varphi^m\|_{L_2}^2 + k \|d_t \Upsilon_\varphi^m\|_{L_2}^2) + \frac{q_0}{L} \|\Upsilon_T^m\|_{L_2}^2 + \frac{q_1}{M} \|\Upsilon_\mu^m\|_{L_2}^2 + \varepsilon \|\nabla \Upsilon_\varphi^m\|_{L_2}^2 \right\} \\
& + k \sum_{m=1}^{\ell} \left\{ \frac{q_0}{L} (K(t_m) \nabla G_T^m, \nabla \Upsilon_T^m) + \frac{q_1}{M} (D(t_m) \nabla G_\mu^m, \nabla \Upsilon_\mu^m) \right\} + \\
& + \frac{k}{\varepsilon} \sum_{m=1}^{\ell} (f(P_h \varphi(t_m)) - f(\Phi^m), \Upsilon_\varphi^m) \\
& = k \sum_{m=1}^{\ell} \left\{ \frac{q_0}{L} (k \sum_{j=1}^m [R_T^j + LR_\varphi^j], \Upsilon_T^m) + \frac{q_1}{M} (k \sum_{j=1}^m [R_\mu^j + MR_\varphi^j], \Upsilon_\mu^m) \right\} + \\
& \frac{q_0 k}{L} \sum_{m=1}^{\ell} \left\{ (k \sum_{j=1}^m [K^j - K(t_j)] \nabla T(t_j), \nabla \Upsilon_T^m) + (k \sum_{j=1}^m [K(t_m) - K(t_j)] \nabla \Upsilon_T^j, \nabla \Upsilon_T^m) \right\} \\
& + \frac{q_1 k}{M} \sum_{m=1}^{\ell} \left\{ (k \sum_{j=1}^m [D^j - D(t_j)] \nabla \mu(t_j), \nabla \Upsilon_\mu^m) + (k \sum_{j=1}^m [D(t_m) - D(t_j)] \nabla \Upsilon_\mu^j, \nabla \Upsilon_\mu^m) \right\} \\
& + k \sum_{m=1}^{\ell} \alpha \varepsilon (R_\varphi^m, \Upsilon_\varphi^m) + s_1 - \frac{k}{\varepsilon} \sum_{m=1}^{\ell} (f(\varphi(t_m)) - f(P_h \varphi(t_m)), \Upsilon_\varphi^m) \quad (3.74)
\end{aligned}$$

where s_1 is defined by

$$\begin{aligned}
s_1 = k \sum_{m=1}^{\ell} \{ & q_0 (\Theta_T^m, \Upsilon_\varphi^m) + q_1 (\Theta_\mu^m, \Upsilon_\varphi^m) - q_0 (\Theta_\varphi^m, \Upsilon_T^m) - \alpha \varepsilon (d_t \Theta_\varphi^m, \Upsilon_\varphi^m) \\
& - q_0 L^{-1} (\Theta_T^m, \Upsilon_T^m) - q_1 (\Theta_\varphi^m, \Upsilon_\mu^m) - q_1 M^{-1} (\Theta_\mu^m, \Upsilon_\mu^m) \\
& + q_0 L^{-1} (E_T^0 + LE_\varphi^0, \Upsilon_T^m) + q_1 M^{-1} (E_\mu^0 + ME_\varphi^0, \Upsilon_\mu^m) \}.
\end{aligned}$$

In the following we estimate some terms in the left hand side of (3.74) from below and the terms on the right hand side from above in a suitable manner that is required for later steps. We start with the following term on the left, leaving out the constant factor $q_0 L^{-1}$:

$$k \sum_{m=1}^{\ell} (K(t_m) \nabla G_T^m, \nabla \Upsilon_T^m).$$

Using $d_t G_T^m = \Upsilon_T^m$ (see (3.70) for the definition of G_T^m) and a similar identity as (3.54), the above term equals to

$$\begin{aligned} k \sum_{m=1}^{\ell} (K(t_m) \nabla G_T^m, \nabla d_t G_T^m) &= \frac{k}{2} \sum_{m=1}^{\ell} d_t (K(t_m) \nabla G_T^m, \nabla G_T^m) + \\ &+ \frac{k^2}{2} \sum_{m=1}^{\ell} (K(t_m) d_t \nabla G_T^m, d_t \nabla G_T^m) \\ &- \frac{k}{2} \sum_{m=1}^{\ell} (d_t K(t_m) \nabla G_T^{m-1}, \nabla G_T^{m-1}). \end{aligned}$$

and the right hand side can be written as

$$\begin{aligned} &\frac{1}{2} (K(t_m) \nabla G_T^\ell, \nabla G_T^\ell) + \frac{k^2}{2} \sum_{m=1}^{\ell} (K(t_m) \nabla \Upsilon_T^m, \nabla \Upsilon_T^m) \\ &- \frac{k}{2} \sum_{m=1}^{\ell} (d_t K(t_m) \nabla G_T^{m-1}, \nabla G_T^{m-1}). \end{aligned}$$

By estimating the first two terms of it from below, we finally obtain

$$\begin{aligned} k \sum_{m=1}^{\ell} (K(t_m) \nabla G_T^m, \nabla \Upsilon_T^m) &\geq \frac{K_0}{2} \|\nabla G_T^\ell\|_{L_2}^2 + \frac{K_0 k^2}{2} \sum_{m=1}^{\ell} \|\nabla \Upsilon_T^m\|_{L_2}^2 \\ &- \frac{k}{2} \sum_{m=1}^{\ell} (d_t K(t_m) \nabla G_T^{m-1}, \nabla G_T^{m-1}). \end{aligned} \quad (3.75)$$

Analogously, we get the estimate

$$\begin{aligned} k \sum_{m=1}^{\ell} (D(t_m) \nabla G_\mu^m, \nabla \Upsilon_\mu^m) &\geq \frac{D_0}{2} \|\nabla G_\mu^\ell\|_{L_2}^2 + \frac{D_0 k^2}{2} \sum_{m=1}^{\ell} \|\nabla \Upsilon_\mu^m\|_{L_2}^2 \\ &- \frac{k}{2} \sum_{m=1}^{\ell} (d_t D(t_m) \nabla G_\mu^{m-1}, \nabla G_\mu^{m-1}). \end{aligned} \quad (3.76)$$

The last terms on the above two inequalities move to the right hand side and we estimate them from above by

$$Ck \sum_{m=1}^{\ell-1} \{ \|\nabla G_T^m\|_{L_2}^2 + \|\nabla G_\mu^m\|_{L_2}^2 \} \quad (3.77)$$

where the constant C depends on the $\|\partial_t K_{ij}\|_{L_\infty(J \times \Omega)}$ and $\|\partial_t D_{ij}\|_{L_\infty(J \times \Omega)}$.

We now move to the right hand side of equation (3.74). Using the definition of G_T^m we get

$$s_2 := k \sum_{m=1}^{\ell} \left(k \sum_{j=1}^m [R_T^j + LR_\varphi^j], \Upsilon_T^m \right) = k \sum_{m=1}^{\ell} \left(k \sum_{j=1}^m [R_T^j + LR_\varphi^j], d_t G_T^m \right).$$

With the following discrete summation by parts formula

$$\sum_{m=1}^{\ell} (d_t f^m, g^m) = \frac{1}{k} [(f^\ell, g^\ell) - (f^0, g^0)] - \sum_{m=1}^{\ell} (f^{m-1}, d_t g^m) \quad (3.78)$$

in the above we obtain

$$\begin{aligned} s_2 &= \left(k \sum_{j=1}^{\ell} [R_T^j + LR_\varphi^j], G_T^\ell \right) - k^2 \sum_{m=1}^{\ell} \left(d_t \sum_{j=1}^m [R_T^j + LR_\varphi^j], G_T^{m-1} \right) \\ &= \left(k \sum_{m=1}^{\ell} [R_T^m + LR_\varphi^m], G_T^\ell \right) - k \sum_{m=1}^{\ell} (R_T^m + LR_\varphi^m, G_T^{m-1}). \end{aligned}$$

The term is estimated by using elementary inequalities as

$$\begin{aligned} s_2 &\leq \frac{K_0}{12} \|\nabla G_T^\ell\|_{L_2}^2 + \frac{k}{4} \sum_{m=1}^{\ell} \|\Upsilon_T^m\|_{L_2}^2 + Ck \sum_{m=1}^{\ell-1} \|\nabla G_T^m\|_{L_2}^2 \\ &\quad + Ck \sum_{m=1}^{\ell} (\|R_\varphi^m\|_{H^{-1}}^2 + \|R_T^m\|_{H^{-1}}^2). \end{aligned} \quad (3.79)$$

Analogously, we have an estimate

$$\begin{aligned} k \sum_{m=1}^{\ell} \left(k \sum_{j=1}^m [R_\mu^j + MR_\varphi^j], \Upsilon_\mu^m \right) &\leq \frac{D_0}{12} \|\nabla G_\mu^\ell\|_{L_2}^2 + \frac{k}{4} \sum_{m=1}^{\ell} \|\Upsilon_\mu^m\|_{L_2}^2 \\ &\quad + Ck \sum_{m=1}^{\ell-1} \|\nabla G_\mu^m\|_{L_2}^2 + Ck \sum_{m=1}^{\ell} (\|R_\varphi^m\|_{H^{-1}}^2 + \|R_\mu^m\|_{H^{-1}}^2). \end{aligned} \quad (3.80)$$

Let us consider now the next term of (3.74)

$$\begin{aligned} s_3 &:= \frac{q_0 k}{L} \sum_{m=1}^{\ell} \left(k \sum_{j=1}^m [K^j - K(t_j)] \nabla T(t_j), d_t \nabla G_T^m \right) \\ &\quad + \frac{q_1 k}{M} \sum_{m=1}^{\ell} \left(k \sum_{j=1}^m [D^j - D(t_j)] \nabla \mu(t_j), d_t \nabla G_\mu^m \right). \end{aligned}$$

We proceed as for the term s_2 , i.e. use (3.78) and obtain

$$s_3 \leq \frac{q_0 K_0}{12L} \|\nabla G_T^\ell\|_{L_2}^2 + \frac{q_1 D_0}{12M} \|\nabla G_\mu^\ell\|_{L_2}^2 + Ck \sum_{m=1}^{\ell-1} \{ \|\nabla G_T^m\|_{L_2}^2 + \|\nabla G_\mu^m\|_{L_2}^2 \} + \\ Ck \sum_{m=1}^{\ell} \{ \|[K^m - K(t_m)]\nabla T(t_m)\|_{L_2}^2 + \|[D^m - D(t_m)]\nabla \mu(t_m)\|_{L_2}^2 \}. \quad (3.81)$$

For the term

$$s_4 := k \sum_{m=1}^{\ell} \left(k \sum_{j=1}^m [K(t_m) - K(t_j)] \nabla \Upsilon_T^j, d_t \nabla G_T^m \right),$$

we apply the summation by parts formula (3.78) and use $d_t G_T^m = \Upsilon_T^m$ and $G_T^m = 0$ to get

$$s_4 = (\nabla G_T^\ell, k \sum_{j=1}^{\ell} [K(t_\ell) - K(t_j)] d_t \nabla G_T^j) \\ - k \sum_{m=1}^{\ell} (\nabla G_T^{m-1}, k d_t \sum_{j=1}^m [K(t_m) - K(t_j)] d_t \nabla G_T^j) \\ = (\nabla G_T^\ell, k \sum_{j=1}^{\ell} [K(t_\ell) - K(t_j)] d_t \nabla G_T^j).$$

Applying the summation by parts once more for

$$k \sum_{m=1}^{\ell} ([K(t_\ell) - K(t_m)] \nabla G_T^\ell, d_t \nabla G_T^m)$$

we obtain

$$s_4 = k \sum_{m=1}^{\ell} (\nabla G_T^{m-1}, d_t K^m \nabla G_T^\ell).$$

This term and an analogous term in (3.74) (with D, μ) are together estimated by

$$\frac{q_0 K_0}{12L} \|\nabla G_T^\ell\|_{L_2}^2 + \frac{q_1 D_0}{12M} \|\nabla G_\mu^\ell\|_{L_2}^2 + Ck \sum_{m=1}^{\ell-1} \{ \|\nabla G_T^m\|_{L_2}^2 + \|\nabla G_\mu^m\|_{L_2}^2 \}. \quad (3.82)$$

We now turn our attention to the remaining terms on the right hand side of (3.74). For the terms in the last line we have the estimates

$$\begin{aligned} k \sum_{m=1}^{\ell} \alpha \varepsilon (R_{\varphi}^m, \Upsilon_{\varphi}^m) &\leq k \sum_{m=1}^{\ell} \left\{ \frac{\alpha \varepsilon^3}{2} \|\nabla \Upsilon_{\varphi}^m\|_{L_2}^2 + \frac{\alpha \varepsilon}{6} \|\Upsilon_{\varphi}^m\|_{L_2}^2 \right\} \\ &+ Ck \sum_{m=1}^{\ell} (\varepsilon + \varepsilon^{-1}) \|R_{\varphi}^m\|_{H^{-1}}^2, \end{aligned} \quad (3.83)$$

and

$$\begin{aligned} &\frac{k}{\varepsilon} \sum_{m=1}^{\ell} |(f(\varphi(t_m)) - f(P_h \varphi(t_m)), \Upsilon_{\varphi}^m)| \\ &\leq k \sum_{m=1}^{\ell} \frac{1}{\varepsilon} |(f'(\xi) \Theta_{\varphi}^m, \Upsilon_{\varphi}^m)| \leq k \sum_{m=1}^{\ell} \left\{ \frac{\alpha \varepsilon}{6} \|\Upsilon_{\varphi}^m\|_{L_2}^2 + \frac{C}{\varepsilon^3} \|\Theta_{\varphi}^m\|_{L_2}^2 \right\}. \end{aligned} \quad (3.84)$$

What remains in the last line is the term which we denoted by s_1 . Elementary inequalities result in

$$\begin{aligned} |s_1| &\leq k \sum_{m=1}^{\ell} \left\{ \frac{\alpha \varepsilon}{6} \|\Upsilon_{\varphi}^m\|_{L_2}^2 + \frac{q_0}{4L} \|\Upsilon_T^m\|_{L_2}^2 + \frac{q_1}{4M} \|\Upsilon_{\mu}^m\|_{L_2}^2 \right\} \\ &+ Ck \sum_{m=1}^{\ell} \left\{ \varepsilon \|d_t \Theta_{\varphi}^m\|_{L_2}^2 + \|\Theta_{\varphi}^m\|_{L_2}^2 + (1 + \varepsilon^{-1}) (\|\Theta_T^m\|_{L_2}^2 + \|\Theta_{\mu}^m\|_{L_2}^2) \right\} \\ &+ C \left\{ \|E_{\varphi}^0\|_{L_2}^2 + \|E_T^0\|_{L_2}^2 + \|E_{\mu}^0\|_{L_2}^2 \right\} \end{aligned} \quad (3.85)$$

where we have taken care of the required scalings for terms $\|\Upsilon_u^m\|_{L_2}^2$ for $u = \varphi, T, \mu$. Employing the estimates (3.75)–(3.77) and (3.79)–(3.85) in (3.74), we obtain

$$\begin{aligned} &\frac{\alpha \varepsilon}{2} \|\Upsilon_{\varphi}^{\ell}\|_{L_2}^2 + \frac{q_0 K_0}{4L} \|\nabla G_T^{\ell}\|_{L_2}^2 + \frac{q_1 D_0}{4M} \|\nabla G_{\mu}^{\ell}\|_{L_2}^2 + k \sum_{m=1}^{\ell} \left\{ \frac{\alpha \varepsilon k}{2} \|d_t \Upsilon_{\varphi}^m\|_{L_2}^2 \right. \\ &+ \frac{q_0}{2L} \|\Upsilon_T^m\|_{L_2}^2 + \frac{q_1}{2M} \|\Upsilon_{\mu}^m\|_{L_2}^2 + \frac{q_0 K_0 k}{2L} \|\nabla \Upsilon_T^m\|_{L_2}^2 + \frac{q_1 D_0 k}{2M} \|\nabla \Upsilon_{\mu}^m\|_{L_2}^2 \\ &\left. + \left(\varepsilon - \frac{\alpha \varepsilon^3}{2} \right) \|\nabla \Upsilon_{\varphi}^m\|_{L_2}^2 \right\} + \frac{k}{\varepsilon} \sum_{m=1}^{\ell} (f(P_h \varphi(t_m)) - f(\Phi^m), \Upsilon_{\varphi}^m) \\ &\leq S + k \sum_{m=1}^{\ell} \left\{ \frac{\alpha \varepsilon}{2} \|\Upsilon_{\varphi}^m\|_{L_2}^2 + C (\|\nabla G_T^m\|_{L_2}^2 + \|\nabla G_{\mu}^m\|_{L_2}^2) \right\} \end{aligned} \quad (3.86)$$

where

$$\begin{aligned}
S := & Ck \sum_{m=1}^{\ell} \left\{ (1 + \varepsilon + \varepsilon^{-1}) \|R_{\varphi}^m\|_{H^{-1}}^2 + \|R_T^m\|_{H^{-1}}^2 + \|R_{\mu}^m\|_{H^{-1}}^2 + \varepsilon \|d_t \Theta_{\varphi}^m\|_{L_2}^2 \right. \\
& + (1 + \varepsilon^{-3}) \|\Theta_{\varphi}^m\|_{L_2}^2 + (1 + \varepsilon^{-1}) \|\Theta_T^m\|_{L_2}^2 + (1 + \varepsilon^{-1}) \|\Theta_{\mu}^m\|_{L_2}^2 \\
& + \|[K^m - K(t_m)] \nabla T(t_m)\|_{L_2}^2 + \|[D^m - D(t_m)] \nabla \mu(t_m)\|_{L_2}^2 \left. \right\} \\
& + \frac{\alpha \varepsilon}{2} \|\Upsilon_{\varphi}^0\|_{L_2}^2 + C \left\{ \|E_{\varphi}^0\|_{L_2}^2 + \|E_T^0\|_{L_2}^2 + \|E_{\mu}^0\|_{L_2}^2 \right\}. \tag{3.87}
\end{aligned}$$

We bound now S with the help of the energy estimates of Lemma 3.2 and the stability estimates of Lemma 3.6. The properties of the elliptic projections (3.44)–(3.46) are also employed. We start with the term involving

$$R_{\varphi}^m = d_t \varphi(t_m) - \varphi_t(t_m) = -\frac{1}{k} \int_{t_{m-1}}^{t_m} (s - t_{m-1}) \varphi_{tt}(s) ds$$

and use (vii) of Lemma 3.2 to get

$$\begin{aligned}
k \sum_{m=1}^{\ell} \|R_{\varphi}^m\|_{H^{-1}}^2 &= \frac{1}{k} \sum_{m=1}^{\ell} \left\| \int_{t_{m-1}}^{t_m} (s - t_{m-1}) \varphi_{tt}(s) ds \right\|_{H^{-1}}^2 \\
&\leq \frac{1}{k} \sum_{m=1}^{\ell} \left[\int_{t_{m-1}}^{t_m} (s - t_{m-1})^2 ds \right] \left[\int_{t_{m-1}}^{t_m} \|\varphi_{tt}(s)\|_{H^{-1}}^2 ds \right] \\
&\leq k^2 \int_0^{t_{\ell}} \|\varphi_{tt}(s)\|_{H^{-1}}^2 ds \leq Ck^2 \varepsilon^{-5},
\end{aligned}$$

and similarly from (xii) and (xiii) of the same lemma we deduce that

$$\begin{aligned}
k \sum_{m=1}^{\ell} \|R_T^m\|_{H^{-1}}^2 &\leq k^2 \int_0^{t_{\ell}} \|T_{tt}(s)\|_{H^{-1}}^2 ds \leq Ck^2 \varepsilon^{-5}, \\
k \sum_{m=1}^{\ell} \|R_{\mu}^m\|_{H^{-1}}^2 &\leq k^2 \int_0^{t_{\ell}} \|\mu_{tt}(s)\|_{H^{-1}}^2 ds \leq Ck^2 \varepsilon^{-5}.
\end{aligned}$$

With (vi) of Lemma 3.2, we obtain

$$k \sum_{m=1}^{\ell} \|\Theta_{\varphi}^m\|_{L_2}^2 = k \sum_{m=1}^{\ell} \|(\varphi - P_h \varphi)(t_m)\|_{L_2}^2 \leq Ch^4 \text{ess sup}_{[0, t_{\ell}]} \|\varphi\|_{H^2}^2 \leq Ch^4 \varepsilon^{-3},$$

and (x) and (xi) results in the analogous estimates

$$\begin{aligned} k \sum_{m=1}^{\ell} \|\Theta_T^m\|_{L_2}^2 &\leq Ch^4 \operatorname{ess\,sup}_{[0,t_\ell]} \|T\|_{H^2}^2 \leq Ch^4 \varepsilon^{-5}, \\ k \sum_{m=1}^{\ell} \|\Theta_\mu^m\|_{L_2}^2 &\leq Ch^4 \operatorname{ess\,sup}_{[0,t_\ell]} \|\mu\|_{H^2}^2 \leq Ch^4 \varepsilon^{-5}. \end{aligned}$$

For the next terms, we assume that the approximation K^m of the heat conductivity $K(t_m)$ satisfies

$$\|K^m - K(t_m)\|_{L_2(\Omega, \mathbb{R}^{N \times N})}^2 \leq Ch^4 \|K(t_m)\|_{H^2(\Omega, \mathbb{R}^{N \times N})}^2 \leq Ch^4 \quad (3.88)$$

with constant C for all $t_m \in J_k$. Then, with (a) of Lemma 3.3 we obtain

$$k \sum_{m=1}^{\ell} \|[K^m - K(t_m)] \nabla T(t_m)\|_{L_2}^2 \leq Ch^4 \varepsilon^{-\max\{5, 2\xi_1\}} \quad (3.89)$$

The same condition as (3.88) is assumed for the diffusion coefficient D and the analogous term (with μ, D instead of T, K) in S is also estimated by $Ch^4 \varepsilon^{-\max\{5, 2\xi_1\}}$.

To estimate the remaining terms of S , we assume that the initial value approximations (φ^0, T^0, μ^0) satisfy

$$\|u_0 - u(0)\|_{L_2}^2 \leq Ch^4 \|u_0\|_{H^2}^2, \quad \text{for } u = \varphi, T, \mu.$$

Elliptic projections of initial functions satisfy for example, the above requirement. Using (3.17), we obtain then

$$\begin{aligned} \|E_\varphi^0\|_{L_2}^2 &\leq Ch^4 \|\varphi_0\|_{H^2}^2 \leq Ch^4 \varepsilon^{-3}, \\ \|E_T^0\|_{L_2}^2 &\leq Ch^4 \|T_0\|_{H^2}^2 \leq Ch^4 \varepsilon^{-1}, \\ \|E_\mu^0\|_{L_2}^2 &\leq Ch^4 \|\mu_0\|_{H^2}^2 \leq Ch^4 \varepsilon^{-1} \end{aligned}$$

and

$$\varepsilon \|\Upsilon_\varphi^0\|_{L_2}^2 \leq \varepsilon (\|E_\varphi^0\|_{L_2}^2 + \|\Theta_\varphi^0\|_{L_2}^2) \leq C\varepsilon h^4 \|\varphi_0\|_{H^2}^2 \leq Ch^4 \varepsilon^{-2}.$$

Finally, using the energy estimates we obtain for the remaining term of S

$$\begin{aligned} \varepsilon k \sum_{m=1}^{\ell} \|d_t \Theta_\varphi^m\|_{L_2}^2 &= \varepsilon k \sum_{m=1}^{\ell} \left\| \frac{1}{k} \int_{t_{m-1}}^{t_m} (\varphi - P_h \varphi)_t(s) ds \right\|_{L_2}^2 \\ &\leq \varepsilon \sum_{m=1}^{\ell} \int_{t_{m-1}}^{t_m} \|(\varphi - P_h \varphi)_t(s)\|_{L_2}^2 ds \\ &= \varepsilon \int_0^{t_\ell} \|(\varphi - P_h \varphi)_t(s)\|_{L_2}^2 ds \\ &\leq C\varepsilon h^4 \int_0^{t_\ell} \|\varphi_t(s)\|_{H^2}^2 ds \leq Ch^4 \varepsilon^{-\max\{4, 2\xi_1 - 1\}}. \end{aligned}$$

Collecting all the above estimates we obtain

$$S \leq C (k^2 \varepsilon^{-6} + h^4 \varepsilon^{-\max\{6, 2\xi_1\}}). \quad (3.90)$$

By the above we conclude the Part 1 of the proof. What we have achieved so far is the inequality (3.86) with S estimated by (3.90).

Part 2. In this part we deal with the nonlinear term on the left hand side of equation (3.86). For this we shall use the discrete spectrum estimate of Lemma 3.7.

Using the following identity for $f(\varphi) = \varphi^3 - \varphi$,

$$f(a) - f(b) = (a - b)[f'(a) + (a - b)^2 - 3(a - b)a], \quad \forall a, b \in \mathbb{R}$$

with $a - b = P_h \varphi(t_m) - \Phi^m = \Upsilon_\varphi^m$ we get

$$\begin{aligned} (f(P_h \varphi(t_m)) - f(\Phi^m), \Upsilon_\varphi^m) &= (f'(P_h \varphi(t_m)) \Upsilon_\varphi^m, \Upsilon_\varphi^m) + ((\Upsilon_\varphi^m)^3, \Upsilon_\varphi^m) \\ &\quad - 3((\Upsilon_\varphi^m)^2 P_h \varphi(t_m), \Upsilon_\varphi^m) \\ &\geq (f'(P_h \varphi(t_m)) \Upsilon_\varphi^m, \Upsilon_\varphi^m) + \|\Upsilon_\varphi^m\|_{L_4}^4 - C \|\Upsilon_\varphi^m\|_{L_3}^3 \end{aligned}$$

where the boundedness of $P_h \varphi$ in the L_∞ norm (cf. (3.60)) has been taken into account.

Considering this estimate and (3.90) in (3.86) we obtain

$$\begin{aligned} &\frac{\alpha \varepsilon}{2} \|\Upsilon_\varphi^\ell\|_{L_2}^2 + \frac{q_0 K_0}{4L} \|\nabla G_T^\ell\|_{L_2}^2 + \frac{q_1 D_0}{4M} \|\nabla G_\mu^\ell\|_{L_2}^2 + \\ &k \sum_{m=1}^{\ell} \left\{ \frac{\alpha \varepsilon k}{2} \|d_t \Upsilon_\varphi^m\|_{L_2}^2 + \frac{q_0}{2L} \|\Upsilon_T^m\|_{L_2}^2 + \frac{q_1}{2M} \|\Upsilon_\mu^m\|_{L_2}^2 + \frac{\alpha \varepsilon^3}{2} \|\nabla \Upsilon_\varphi^m\|_{L_2}^2 \right. \\ &\quad \left. + \frac{q_0 K_0 k}{2L} \|\nabla \Upsilon_T^m\|_{L_2}^2 + \frac{q_1 D_0 k}{2M} \|\nabla \Upsilon_\mu^m\|_{L_2}^2 + \frac{1}{\varepsilon} \|\Upsilon_\varphi^m\|_{L_4}^4 \right\} + \\ &k \sum_{m=1}^{\ell} (1 - \alpha \varepsilon^2) \left[\varepsilon \|\nabla \Upsilon_\varphi^m\|_{L_2}^2 + \frac{1}{\varepsilon} (f'(P_h \varphi(t_m)) \Upsilon_\varphi^m, \Upsilon_\varphi^m) \right] \\ &\leq k \sum_{m=1}^{\ell} \left\{ \frac{\alpha \varepsilon}{2} \|\Upsilon_\varphi^m\|_{L_2}^2 + C (\|\nabla G_T^m\|_{L_2}^2 + \|\nabla G_\mu^m\|_{L_2}^2) \right\} + \frac{Ck}{\varepsilon} \sum_{m=1}^{\ell} \|\Upsilon_\varphi^m\|_{L_3}^3 + \\ &k \sum_{m=1}^{\ell} \alpha \varepsilon |(f'(P_h \varphi(t_m)) \Upsilon_\varphi^m, \Upsilon_\varphi^m)| + C (k^2 \varepsilon^{-6} + h^4 \varepsilon^{-\max\{6, 2\xi_1\}}). \quad (3.91) \end{aligned}$$

Now comes an important step in the estimation. We bound the last term of the left hand side by the discrete spectrum estimate (cf. Lemma 3.7), that

is,

$$\begin{aligned} (1 - \alpha\varepsilon^2) & \left[\varepsilon \|\nabla \Upsilon_\varphi^m\|_{L_2}^2 + \frac{1}{\varepsilon} (f'(P_h\varphi(t_m)) \Upsilon_\varphi^m, \Upsilon_\varphi^m) \right] \\ & \geq (1 - \alpha\varepsilon^2) (-2C_0\alpha\varepsilon \|\Upsilon_\varphi^m\|_{L_2}^2) \geq -2C_0\alpha\varepsilon \|\Upsilon_\varphi^m\|_{L_2}^2 \end{aligned} \quad (3.92)$$

The above term having the required suitable factor is combined with the first term in the sum on the right hand side of inequality (3.91). Moreover, using the uniform boundedness of $f'(P_h\varphi(t_m))$ in ε we obtain

$$k \sum_{m=1}^{\ell} \alpha\varepsilon |(f'(P_h\varphi(t_m)) \Upsilon_\varphi^m, \Upsilon_\varphi^m)| \leq k \sum_{m=1}^{\ell} C\alpha\varepsilon \|\Upsilon_\varphi^m\|_{L_2}^2.$$

Considering the above in (3.91) results in

$$\begin{aligned} & \frac{\alpha\varepsilon}{2} \|\Upsilon_\varphi^\ell\|_{L_2}^2 + \frac{q_0 K_0}{4L} \|\nabla G_T^\ell\|_{L_2}^2 + \frac{q_1 D_0}{4M} \|\nabla G_\mu^\ell\|_{L_2}^2 + \\ & k \sum_{m=1}^{\ell} \left\{ \frac{\alpha\varepsilon k}{2} \|d_t \Upsilon_\varphi^m\|_{L_2}^2 + \frac{q_0}{2L} \|\Upsilon_T^m\|_{L_2}^2 + \frac{q_1}{2M} \|\Upsilon_\mu^m\|_{L_2}^2 + \frac{\alpha\varepsilon^3}{2} \|\nabla \Upsilon_\varphi^m\|_{L_2}^2 \right. \\ & \quad \left. + \frac{q_0 K_0 k}{2L} \|\nabla \Upsilon_T^m\|_{L_2}^2 + \frac{q_1 D_0 k}{2M} \|\nabla \Upsilon_\mu^m\|_{L_2}^2 + \frac{1}{\varepsilon} \|\Upsilon_\varphi^m\|_{L_4}^4 \right\} \\ & \leq \tilde{C} k \sum_{m=1}^{\ell} \left\{ \frac{\alpha\varepsilon}{2} \|\Upsilon_\varphi^m\|_{L_2}^2 + \frac{q_0 K_0}{4L} \|\nabla G_T^m\|_{L_2}^2 + \frac{q_1 D_0}{4M} \|\nabla G_\mu^m\|_{L_2}^2 \right\} \\ & \quad + \frac{Ck}{\varepsilon} \sum_{m=1}^{\ell} \|\Upsilon_\varphi^m\|_{L_3}^3 + C (k^2 \varepsilon^{-6} + h^4 \varepsilon^{-\max\{6, 2\xi_1\}}). \end{aligned} \quad (3.93)$$

We are now almost ready for obtaining a final useful inequality. For that, it remains to estimate the first term in the last line of (3.93). Summing $E_\varphi^m = kd_t E_\varphi^m + E_\varphi^{m-1}$ over all the elements of the triangulation \mathcal{T}_h , we get

$$\|E_\varphi^m\|_{L_3}^3 \leq C \sum_{\mathcal{K} \in \mathcal{T}_h} (k^3 \|d_t E_\varphi^m\|_{L_3(\mathcal{K})}^3 + \|E_\varphi^{m-1}\|_{L_3(\mathcal{K})}^3).$$

At first, using an interpolation of L_3 between L_2 and H^2 , we obtain

$$\begin{aligned} \|E_\varphi^{m-1}\|_{L_3(\mathcal{K})}^3 & \leq C \|E_\varphi^{m-1}\|_{L_2(\mathcal{K})}^{\frac{12-N}{4}} \|E_\varphi^{m-1}\|_{H^2(\mathcal{K})}^{\frac{N}{4}} \\ & \leq C \|E_\varphi^{m-1}\|_{L_2(\mathcal{K})}^{\frac{12-N}{4}} (\|\Delta E_\varphi^{m-1}\|_{L_2(\mathcal{K})}^{\frac{N}{4}} + \|E_\varphi^{m-1}\|_{L_2(\mathcal{K})}^{\frac{N}{4}}) \\ & \leq C \|E_\varphi^{m-1}\|_{L_2(\mathcal{K})}^{\frac{12-N}{4}} \varepsilon^{-\frac{3N}{8}} \end{aligned}$$

where the last step results from Lemmas 3.2 (energy estimates, (vi)) and 3.6 (the stability estimates, (a)).

Similarly, we also have

$$\begin{aligned} k^3 \|d_t E_\varphi^m\|_{L_3(\mathcal{K})}^3 &\leq Ck^3 \|d_t E_\varphi^m\|_{L_2(\mathcal{K})}^{\frac{12-N}{4}} (\|d_t \Delta E_\varphi^m\|_{L_2(\mathcal{K})}^{\frac{N}{4}} + \|d_t E_\varphi^m\|_{L_2(\mathcal{K})}^{\frac{N}{4}}) \\ &\leq Ck^{\frac{12-N}{4}} \|d_t E_\varphi^m\|_{L_2(\mathcal{K})}^{\frac{12-N}{4}} \varepsilon^{-\frac{3N}{8}} \end{aligned}$$

Summing the above two inequalities over all $\mathcal{K} \in \mathcal{T}_h$ we obtain

$$\|E_\varphi^m\|_{L_3}^3 \leq C\varepsilon^{-\frac{3N}{8}} \left\{ \|E_\varphi^{m-1}\|_{L_2}^{\frac{12-N}{4}} + k^{\frac{12-N}{4}} \|d_t E_\varphi^m\|_{L_2}^{\frac{12-N}{4}} \right\}. \quad (3.94)$$

In view of the definition of the error E_φ^m , we have

$$\begin{aligned} \|\Upsilon_\varphi^m\|_{L_3}^3 &\leq C \left\{ \|\Theta_\varphi^m\|_{L_3}^3 + \varepsilon^{-\frac{3N}{8}} \left(\|\Theta_\varphi^{m-1}\|_{L_2}^{\frac{12-N}{4}} + k^{\frac{12-N}{4}} \|d_t \Theta_\varphi^m\|_{L_2}^{\frac{12-N}{4}} \right. \right. \\ &\quad \left. \left. + \|\Upsilon_\varphi^{m-1}\|_{L_2}^{\frac{12-N}{4}} + k^{\frac{12-N}{4}} \|d_t \Upsilon_\varphi^m\|_{L_2}^{\frac{12-N}{4}} \right) \right\}. \end{aligned}$$

Summing over m from 1 to ℓ results in the term to be estimated:

$$\begin{aligned} \frac{Ck}{\varepsilon} \sum_{m=1}^{\ell} \|\Upsilon_\varphi^m\|_{L_3}^3 &\leq C\varepsilon^{-\frac{8+3N}{8}} k \sum_{m=1}^{\ell} \left\{ \|\Theta_\varphi^m\|_{L_3}^3 \varepsilon^{\frac{3N}{8}} + \|\Theta_\varphi^{m-1}\|_{L_2}^{\frac{12-N}{4}} \right. \\ &\quad \left. + (\|\Theta_\varphi^m\|_{L_2} + \|\Theta_\varphi^{m-1}\|_{L_2})^{\frac{12-N}{4}} + \|\Upsilon_\varphi^{m-1}\|_{L_2}^{\frac{12-N}{4}} \right. \\ &\quad \left. + k^2 \|d_t \Upsilon_\varphi^m\|_{L_2}^2 (\|\Upsilon_\varphi^m\|_{L_2} + \|\Upsilon_\varphi^{m-1}\|_{L_2})^{\frac{4-N}{4}} \right\}. \quad (3.95) \end{aligned}$$

We start with the terms involving the Θ_φ^i . Using (3.44) and Lemma 3.2, we get

$$\begin{aligned} k \sum_{m=1}^{\ell} \|\Theta_\varphi^m\|_{L_2}^{\frac{12-N}{4}} &= k \sum_{m=1}^{\ell} \|\varphi(t_m) - P_h \varphi(t_m)\|_{L_2}^{\frac{12-N}{4}} \\ &\leq C(h^2 \|\varphi\|_{L_\infty(J; H^2)})^{\frac{12-N}{4}} \leq Ch^{\frac{12-N}{2}} \varepsilon^{-\frac{3(12-N)}{8}} \end{aligned}$$

and the same estimate holds with m inside the sum replaced by $m-1$. With the interpolation we also obtain

$$\begin{aligned} k \sum_{m=1}^{\ell} \|\Theta_\varphi^m\|_{L_3}^3 &\leq Ck \sum_{m=1}^{\ell} \|\varphi(t_m) - P_h \varphi(t_m)\|_{H^{\frac{N}{6}}}^3 \\ &\leq Ck \sum_{m=1}^{\ell} \|\varphi(t_m) - P_h \varphi(t_m)\|_{L_2}^{\frac{6-N}{2}} \|\varphi(t_m) - P_h \varphi(t_m)\|_{H^1}^{\frac{N}{2}} \\ &\leq Ch^{\frac{12-N}{2}} \varepsilon^{-\frac{9}{2}} \end{aligned}$$

where again Lemma 3.2 and approximation properties of the elliptic projections were used.

Therefore, we reach to the fact that all the Θ related terms on the right hand side of (3.95) are bounded by

$$Ch^{\frac{12-N}{2}}\varepsilon^{-\frac{11}{2}}. \quad (3.96)$$

For the very last term of (3.95), we use $\|\Phi^m\|_{L_4} \leq C\varepsilon$ which follows from the stability estimates (Lemma 3.6) and (3.18) to obtain

$$\begin{aligned} & C\varepsilon^{-\frac{8+3N}{8}}k^2 \sum_{m=1}^{\ell} k \|d_t \Upsilon_{\varphi}^m\|_{L_2}^2 (\|\Upsilon_{\varphi}^m\|_{L_2} + \|\Upsilon_{\varphi}^{m-1}\|_{L_2})^{\frac{4-N}{4}} \\ & \leq C\varepsilon^{-\frac{6+N}{4}}k^2 \sum_{m=1}^{\ell} k \|d_t \Upsilon_{\varphi}^m\|_{L_2}^2. \end{aligned}$$

However, notice that this term can be absorbed to the first term in the sum on the left hand side of (3.93), if k satisfies

$$C\varepsilon^{-\frac{6+N}{4}}k \leq \frac{\alpha\varepsilon}{4},$$

that is,

$$k \leq C\varepsilon^{\frac{10+N}{4}}. \quad (3.97)$$

Recall that this requirement was one of the assumptions of the theorem. Therefore with (3.95)–(3.97), we obtain

$$\begin{aligned} & \frac{\alpha\varepsilon}{2} \|\Upsilon_{\varphi}^{\ell}\|_{L_2}^2 + \frac{q_0 K_0}{4L} \|\nabla G_T^{\ell}\|_{L_2}^2 + \frac{q_1 D_0}{4M} \|\nabla G_{\mu}^{\ell}\|_{L_2}^2 + \\ & k \sum_{m=1}^{\ell} \left\{ \frac{\alpha\varepsilon k}{4} \|d_t \Upsilon_{\varphi}^m\|_{L_2}^2 + \frac{q_0}{2L} \|\Upsilon_T^m\|_{L_2}^2 + \frac{q_1}{2M} \|\Upsilon_{\mu}^m\|_{L_2}^2 + \frac{\alpha\varepsilon^3}{2} \|\nabla \Upsilon_{\varphi}^m\|_{L_2}^2 \right. \\ & \quad \left. + \frac{q_0 K_0 k}{2L} \|\nabla \Upsilon_T^m\|_{L_2}^2 + \frac{q_1 D_0 k}{2M} \|\nabla \Upsilon_{\mu}^m\|_{L_2}^2 + \frac{1}{\varepsilon} \|\Upsilon_{\varphi}^m\|_{L_4}^4 \right\} \quad (3.98) \\ & \leq \tilde{C}k \sum_{m=1}^{\ell} \left\{ \frac{\alpha\varepsilon}{2} \|\Upsilon_{\varphi}^m\|_{L_2}^2 + \frac{q_0 K_0}{4L} \|\nabla G_T^m\|_{L_2}^2 + \frac{q_1 D_0}{4M} \|\nabla G_{\mu}^m\|_{L_2}^2 \right\} \\ & \quad + C \left[k^2 \varepsilon^{-6} + h^4 A(\varepsilon) \right] + C\varepsilon^{-\frac{8+3N}{8}}k \sum_{m=1}^{\ell} \|\Upsilon_{\varphi}^{m-1}\|_{L_2}^{\frac{12-N}{4}} \end{aligned}$$

where

$$A(\varepsilon) = h^{\frac{4-N}{2}}\varepsilon^{-\frac{11}{2}} + \varepsilon^{-\max\{6, 2\xi_1\}}. \quad (3.99)$$

We conclude by the above Part 2 and move to the final part of the proof.

Part 3. We employ an induction argument in this part. Suppose there exists two positive constants $c_1(\mathcal{T}, \Omega)$ and $c_2(\mathcal{T}, \Omega)$ independent of ε , k and h such that

$$\begin{aligned} & \max_{0 \leq m \leq \ell} \left\{ \frac{\alpha\varepsilon}{4} \|\Upsilon_\varphi^m\|_{L_2}^2 + \frac{q_0 K_0}{4L} \|\nabla G_T^m\|_{L_2}^2 + \frac{q_1 D_0}{4M} \|\nabla G_\mu^m\|_{L_2}^2 \right\} + \\ & k \sum_{m=1}^{\ell} \left\{ \frac{\alpha\varepsilon k}{4} \|d_t \Upsilon_\varphi^m\|_{L_2}^2 + \frac{q_0}{2L} \|\Upsilon_T^m\|_{L_2}^2 + \frac{q_1}{2M} \|\Upsilon_\mu^m\|_{L_2}^2 + \frac{\alpha\varepsilon^3}{2} \|\nabla \Upsilon_\varphi^m\|_{L_2}^2 \right. \\ & \quad \left. + \frac{q_0 K_0 k}{2L} \|\nabla \Upsilon_T^m\|_{L_2}^2 + \frac{q_1 D_0 k}{2M} \|\nabla \Upsilon_\mu^m\|_{L_2}^2 + \frac{1}{\varepsilon} \|\Upsilon_\varphi^m\|_{L_4}^4 \right\} \\ & \leq c_1 [k^2 \varepsilon^{-6} + h^4 A(\varepsilon)] \exp(c_2 t_\ell) \end{aligned} \quad (3.100)$$

holds for sufficiently small h and k satisfying the mesh conditions in the theorem. For the start of the induction ($\ell = 0$) the inequality (3.100) holds trivially, since

$$\frac{\alpha\varepsilon}{4} \|\Upsilon_\varphi^0\|_{L_2}^2 \leq C\varepsilon \|\varphi_0\|_{L_2}^2 \leq Ch^4 \varepsilon^{-2}. \quad (3.101)$$

We recover the $(\ell + 1)$ -th step of the induction from the above assumption. The exponent in the last term of (3.98) which is greater than 2 enables us to recover (3.100) at $\ell + 1$ -th step by applying the discrete Gronwall inequality (see Lemma 3.1). In the following we explain this using some simple notations. Suppose for $a_m, b_m \geq 0$, we have $\varepsilon^\beta k a_0^{1+\gamma} \leq B(\varepsilon, k, h)$, and for all $0 < \ell \leq M_\ell$:

$$a_\ell + k \sum_{m=1}^{\ell} b_m \leq B(\varepsilon, k, h) + c_2 k \sum_{m=1}^{\ell} a_m + c_3 \varepsilon^\beta k \sum_{m=1}^{\ell} a_{m-1}^{1+\gamma} \quad (3.102)$$

holds with $\gamma > 0$ and constants c_2, c_3 independent of k, h, ε . We want to have the following inequality for all $0 < \ell \leq M_\ell$ under certain conditions on $B(k, h, \varepsilon)$:

$$\frac{1}{2} \max_{0 \leq m \leq \ell} \{a_m\} + k \sum_{m=1}^{\ell} b_m \leq c_1 B(\varepsilon, k, h) \exp(c_2 t_\ell) \quad (3.103)$$

where $c_1 = c_1(\mathcal{T})$ depends only on c_2, c_3 . The constant $c_1(\mathcal{T})$ is finite for $\mathcal{T} < \infty$. Assume now the inequality (3.103) holds for ℓ . Then from (3.102) with $\ell + 1$, for $k \leq 1/(2c_2)$ we get

$$\frac{a_{\ell+1}}{2} + k \sum_{m=1}^{\ell+1} b_m \leq B(\varepsilon, k, h) + c_2 k \sum_{m=1}^{\ell} a_m + c_3 \varepsilon^\beta k \sum_{m=1}^{\ell} a_m^{1+\gamma}.$$

Using (3.103) for the last two terms on the right hand side we obtain

$$\begin{aligned} \frac{a_{\ell+1}}{2} + k \sum_{m=1}^{\ell+1} b_m &\leq B(\varepsilon, k, h) + 2c_2 t_\ell c_1 B(\varepsilon, k, h) \exp(c_2 t_\ell) \\ &\quad + c_3 t_\ell \varepsilon^\beta [2c_1 B(\varepsilon, k, h) \exp(c_2 t_\ell)]^{1+\gamma}. \end{aligned}$$

We can bound the right hand side from above by $c_1 B(\varepsilon, k, h) \exp(c_2 t_{\ell+1})$ if

$$\varepsilon^\beta [B(\varepsilon, k, h)]^{1+\gamma} \leq c_4 B(\varepsilon, k, h), \quad (3.104)$$

i.e.

$$B(\varepsilon, k, h) \leq C \varepsilon^{-\beta/\gamma}, \quad (3.105)$$

and this completes the induction. In the above $C = (c_4)^{1/\gamma}$ depends on \mathcal{T} , but doesn't depend on k, h and ε .

In our situation we have $a_m = \frac{\alpha\varepsilon}{2} \|\Upsilon_\varphi^m\|_{L_2}^2$ and

$$\beta = -\frac{10+N}{4}, \quad \gamma = \frac{4-N}{8}.$$

Moreover, $B(k, h, \varepsilon) = C[k^2\varepsilon^{-6} + h^4 A(\varepsilon)]$ and using (3.101) the condition for a_0 is also fulfilled, i.e.

$$\varepsilon^\beta k \left[\frac{\alpha\varepsilon}{4} \|\Upsilon_\varphi^0\|_{L_2}^2 \right]^{1+\gamma} \leq C k h^{\frac{12-N}{2}} \varepsilon^{-\frac{11}{2}} \leq B(\varepsilon, k, h).$$

The mesh requirement (3.105) can be written as

$$k^2 \varepsilon^{-6} + h^4 A(\varepsilon) \leq C \varepsilon^{\frac{2(10+N)}{4-N}} \quad (3.106)$$

which is condition (3) in the formulation of the theorem. We have then (3.100) for all $\ell \leq M_\ell$, provided that k and h satisfies (3.106).

Finally, the estimates of the theorem can be derived using (3.100), (3.44)–(3.46), Lemma 3.2 and the definition of the error E_u^m for $u = \varphi, T, \mu$.

(i) We have

$$\begin{aligned} \max_{0 \leq m \leq M_\ell} \|\varphi(t_m) - \Phi^m\|_{L_2}^2 &\leq C \max_{0 \leq m \leq M_\ell} \|\varphi(t_m) - P_h \varphi(t_m)\|_{L_2}^2 + C \max_{0 \leq m \leq M_\ell} \|\Upsilon_\varphi^m\|_{L_2}^m \\ &\leq C h^4 \operatorname{ess\,sup}_J \|\varphi\|_{H^2}^2 + C \varepsilon^{-1} (k^2 \varepsilon^{-6} + h^4 A(\varepsilon)) \\ &\leq C [h^4 \varepsilon^{-3} + k^2 \varepsilon^{-7} + h^4 A(\varepsilon) \varepsilon^{-1}] \end{aligned}$$

and the assertion follows.

(ii) For the assertion, use (3.100) and Lemma 3.2 to obtain

$$\begin{aligned} k \sum_{m=1}^{M_t} \|T(t_m) - T^m\|_{L_2}^2 &\leq Ck \sum_{m=1}^{M_t} \|T(t_m) - P_h T(t_m)\|_{L_2}^2 + Ck \sum_{m=1}^{M_t} \|\Upsilon_T^m\|_{L_2}^2 \\ &\leq Ch^4 \operatorname{ess\,sup}_J \|T\|_{H^2}^2 + C [k^2 \varepsilon^{-6} + h^4 A(\varepsilon)] \\ &\leq C [h^4 \varepsilon^{-5} + k^2 \varepsilon^{-6} + h^4 A(\varepsilon)] \end{aligned}$$

which yields the assertion.

Analogously, we obtain

$$k \sum_{m=1}^{M_t} \|\mu(t_m) - \mu^m\|_{L_2}^2 \leq C [h^4 \varepsilon^{-5} + k^2 \varepsilon^{-6} + h^4 A(\varepsilon)]$$

which gives the assertion (iii).

(iv) The definition of G_T^m and the estimate

$$\begin{aligned} \max_{0 \leq m \leq M_t} \left\| k \sum_{j=1}^m \nabla(T(t_j) - T^j) \right\|_{L_2}^2 &\leq C \max_{0 \leq m \leq M_t} \left\{ \left\| k \sum_{j=1}^m \nabla \Theta_T^j \right\|_{L_2}^2 + \|\nabla G_T^m\|_{L_2}^2 \right\} \\ &\leq Ch^2 \operatorname{ess\,sup}_J \|T\|_{H^2}^2 + C [k^2 \varepsilon^{-6} + h^4 A(\varepsilon)] \end{aligned}$$

together with Lemma 3.2 yields (iv).

(v) Again, we have

$$\max_{0 \leq m \leq M_t} \left\| k \sum_{j=1}^m \nabla(\mu(t_j) - \mu^j) \right\|_{L_2}^2 \leq C \max_{0 \leq m \leq M_t} \left\{ \left\| k \sum_{j=1}^m \nabla \Theta_\mu^j \right\|_{L_2}^2 + \|\nabla G_\mu^m\|_{L_2}^2 \right\}$$

which immediately implies (v) in view of (3.100).

Furthermore, we also obtain

$$\begin{aligned} \varepsilon^3 k \sum_{m=1}^{M_t} \|\nabla(\varphi(t_m) - \Phi^m)\|_{L_2}^2 &\leq C\varepsilon^3 k \sum_{m=1}^{M_t} \|\nabla \Theta_\varphi^m\|_{L_2}^2 + C\varepsilon^3 k \sum_{m=1}^{M_t} \|\nabla \Upsilon_\varphi^m\|_{L_2}^2 \\ &\leq C\varepsilon^3 h^2 \operatorname{ess\,sup}_J \|\varphi\|_{H^2}^2 + C [k^2 \varepsilon^{-6} + h^4 A(\varepsilon)] \\ &\leq C [h^2 + k^2 \varepsilon^{-6} + h^4 A(\varepsilon)] \end{aligned}$$

which finishes the proof of (vi) of the theorem.

Moreover,

$$\begin{aligned} k \sum_{m=1}^{M_t} \|\nabla(T(t_m) - T^m)\|_{L_2}^2 &\leq Ck \sum_{m=1}^{M_t} \|\nabla \Theta_T^m\|_{L_2}^2 + Ck \sum_{m=1}^{M_t} \|\nabla \Upsilon_T^m\|_{L_2}^2 \\ &\leq C (h^2 \varepsilon^{-5} + k^{-1} [k^2 \varepsilon^{-6} + h^4 A(\varepsilon)]) \end{aligned}$$

which gives the assertion (vii). The assertion (viii) is proved analogously as (vii).

The last assertion (ix) of the theorem follows from (3.45) and the inverse inequality

$$\|v_h\|_{L_\infty} \leq Ch^{-\frac{N}{2}} \|v_h\|_{L_2}, \quad (3.107)$$

which holds for all $v_h \in V_h$. That is,

$$\begin{aligned} \max_{0 \leq m \leq M_t} \|\varphi(t_m) - \Phi^m\|_{L_\infty}^2 &\leq C \max_{0 \leq m \leq M_t} \|\varphi(t_m) - P_h \varphi(t_m)\|_{L_\infty}^2 + C \max_{0 \leq m \leq M_t} \|\Upsilon_\varphi^m\|_{L_\infty}^2 \\ &\leq Ch^{4-N} |\ln h|^{3-N} \operatorname{ess\,sup}_J \|\varphi\|_{H^2}^2 \\ &\quad + Ch^{-N} \max_{0 \leq m \leq M_t} \|\Upsilon_\varphi^m\|_{L_2}^2 \\ &\leq Ch^{4-N} |\ln h|^{3-N} \varepsilon^{-3} + Ch^{-N} [k^2 \varepsilon^{-7} + h^4 A(\varepsilon) \varepsilon^{-1}]. \end{aligned}$$

This completes the proof of Theorem 3.7. \square

Remark 3.1 *Assumption (1) of the theorem is necessary for the stability estimates (Lemma 3.6) and the estimation of a term which arises from the nonlinearity of the function $f(\varphi)$ (see (3.95) and (3.97)). The next assumption (2) was a condition for the discrete spectrum estimates of Lemma 3.7 which we used in the proof (see (3.92)). The final assumption was required for the estimation of a term which also comes from the nonlinearity (see (3.95) and (3.106)).*

We can also prove the following theorem.

Theorem 3.8 *Under the assumptions and mesh conditions of Theorem 3.7 the following error estimates hold:*

- (i) $\max_{0 \leq m \leq M_t} \|\Phi^m\|_{L_\infty} \leq C$
- (ii) $\max_{0 \leq m \leq M_t} \|T(t_m) - T^m\|_{L_2} \leq C \left(k\varepsilon^{-\frac{17}{4}} + h^2 [A(\varepsilon)]^{\frac{1}{2}} [\varepsilon^{-\frac{5}{4}} + k^{-\frac{1}{2}}] \right)$
- (iii) $\max_{0 \leq m \leq M_t} \|\mu(t_m) - \mu^m\|_{L_2} \leq C \left(k\varepsilon^{-\frac{17}{4}} + h^2 [A(\varepsilon)]^{\frac{1}{2}} [\varepsilon^{-\frac{5}{4}} + k^{-\frac{1}{2}}] \right)$
- (iv) $\max_{0 \leq m \leq M_t} \|T(t_m) - T^m\|_{L_\infty} \leq Ch^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \varepsilon^{-\frac{5}{2}} +$
 $Ch^{-\frac{N}{2}} (k\varepsilon^{-3} + h^2 [A(\varepsilon)]^{\frac{1}{2}}) [\varepsilon^{-\frac{5}{4}} + k^{-\frac{1}{2}}]$
- (v) $\max_{0 \leq m \leq M_t} \|\mu(t_m) - \mu^m\|_{L_\infty}^2 \leq Ch^{\frac{4-N}{2}} |\ln h|^{\frac{3-N}{2}} \varepsilon^{-\frac{5}{2}} +$
 $Ch^{-\frac{N}{2}} (k\varepsilon^{-3} + h^2 [A(\varepsilon)]^{\frac{1}{2}}) [\varepsilon^{-\frac{5}{4}} + k^{-\frac{1}{2}}]$

where $A(\varepsilon)$ is defined as in (3.63) and C is independent of ε .

Proof. (i) Estimate (ix) of Theorem 3.7 implies that there exist $h_0 > 0$ and $k_0 > 0$ such that

$$\max_{0 \leq m \leq M_t} \|\varphi(t_m) - \Phi^m\|_{L_\infty} \leq C$$

holds for $h < h_0, k < k_0$. Then the inequality

$$\|\Phi^m\|_{L_\infty} \leq \|\varphi(t_m)\|_{L_\infty} + \|\varphi(t_m) - \Phi^m\|_{L_\infty}$$

and the boundedness of φ in the L_∞ norm confirms the claim.

For the next assertions of the theorem, we need some preparatory steps. By choosing $u_h = -L\Upsilon_T^m - M\Upsilon_\mu^m$ in (3.66), $v_h = \alpha\varepsilon\Upsilon_T^m$ in (3.67) and $w_h = \alpha\varepsilon\Upsilon_\mu^m$ in (3.68) and summing up the resulting equations we obtain

$$\begin{aligned} & \alpha\varepsilon[(d_t\Upsilon_T^m, \Upsilon_T^m) + (d_t\Upsilon_\mu^m, \Upsilon_\mu^m) + (K(t_m)\nabla\Upsilon_T^m, \nabla\Upsilon_T^m) + (D(t_m)\nabla\Upsilon_\mu^m, \Upsilon_\mu^m)] \\ &= L\varepsilon(\nabla\Upsilon_\varphi^m, \nabla\Upsilon_T^m) + M\varepsilon(\nabla\Upsilon_\varphi^m, \nabla\Upsilon_\mu^m) + \alpha\varepsilon(R_T^m, \Upsilon_T^m) + \alpha\varepsilon(R_\mu^m, \Upsilon_\mu^m) \\ & \quad - q_0(\Theta_T^m + \Upsilon_T^m, L\Upsilon_T^m + M\Upsilon_\mu^m) - q_1(\Theta_\mu^m + \Upsilon_\mu^m, L\Upsilon_T^m + M\Upsilon_\mu^m) \\ & \quad + \frac{L}{\varepsilon}(f(\varphi(t_m)) - f(\Phi^m), \Upsilon_T^m) + \frac{M}{\varepsilon}(f(\varphi(t_m)) - f(\Phi^m), \Upsilon_\mu^m) \\ & \quad + \alpha\varepsilon([K^m - K(t_m)]\nabla T^m, \nabla\Upsilon_T^m) + \alpha\varepsilon([D^m - D(t_m)]\nabla\mu^m, \nabla\Upsilon_\mu^m) \\ & \quad - \alpha\varepsilon(d_t\Theta_T^m, \Upsilon_T^m) - \alpha\varepsilon(d_t\Theta_\mu^m, \Upsilon_\mu^m). \end{aligned}$$

Using (3.50) in the above equation we get

$$\begin{aligned} & \alpha\varepsilon\left(\frac{1}{2}d_t\|\Upsilon_T^m\|_{L_2}^2 + \frac{k}{2}\|d_t\Upsilon_T^m\|_{L_2}^2 + \frac{1}{2}d_t\|\Upsilon_\mu^m\|_{L_2}^2 + \frac{k}{2}\|d_t\Upsilon_\mu^m\|_{L_2}^2\right) + \\ & \alpha\varepsilon(K_0\|\nabla\Upsilon_T^m\|_{L_2}^2 + D_0\|\nabla\Upsilon_\mu^m\|_{L_2}^2) \\ & \leq \alpha\varepsilon[(R_\mu^m, \Upsilon_\mu^m) + (R_T^m, \Upsilon_T^m) - (d_t\Theta_T^m, \Upsilon_T^m) - (d_t\Theta_\mu^m, \Upsilon_\mu^m)] + L\varepsilon(\nabla\Upsilon_\varphi^m, \nabla\Upsilon_T^m) \\ & \quad + M\varepsilon(\nabla\Upsilon_\varphi^m, \nabla\Upsilon_\mu^m) - Lq_0(\Theta_T^m, \Upsilon_T^m) - Lq_1(\Theta_\mu^m, \Upsilon_T^m) - Mq_0(\Theta_T^m, \Upsilon_\mu^m) \\ & \quad - Mq_1(\Theta_\mu^m, \Upsilon_\mu^m) - (Lq_1 + Mq_0)(\Upsilon_T^m, \Upsilon_\mu^m) - Lq_0(\Upsilon_T^m, \Upsilon_T^m) - Mq_1(\Upsilon_\mu^m, \Upsilon_\mu^m) \\ & \quad + \alpha\varepsilon([K^m - K(t_m)]\nabla T^m, \nabla\Upsilon_T^m) + \alpha\varepsilon([D^m - D(t_m)]\nabla\mu^m, \nabla\Upsilon_\mu^m) \\ & \quad + \frac{L}{\varepsilon}(f(\varphi(t_m)) - f(\Phi^m), \Upsilon_T^m) + \frac{M}{\varepsilon}(f(\varphi(t_m)) - f(\Phi^m), \Upsilon_\mu^m). \end{aligned}$$

The Mean Value Theorem applied to the last two terms and some easy manipulations on other terms of the right hand side gives

$$\begin{aligned} & \frac{\alpha\varepsilon}{2}(d_t\|\Upsilon_T^m\|_{L_2}^2 + d_t\|\Upsilon_\mu^m\|_{L_2}^2) + \frac{\alpha\varepsilon k}{2}(\|d_t\Upsilon_T^m\|_{L_2}^2 + \|d_t\Upsilon_\mu^m\|_{L_2}^2) \\ & + \alpha\varepsilon(K_0\|\nabla\Upsilon_T^m\|_{L_2}^2 + D_0\|\nabla\Upsilon_\mu^m\|_{L_2}^2) \leq C\{\varepsilon^{-\frac{1}{2}}\|E_\varphi^m\|_{L_2}^2 \\ & + \varepsilon^{-\frac{3}{2}}(\|\Upsilon_T^m\|_{L_2}^2 + \|\Upsilon_\mu^m\|_{L_2}^2) + \varepsilon^2\|\nabla\Upsilon_\varphi^m\|_{L_2}^2 + \|\nabla\Upsilon_T^m\|_{L_2}^2 + \|\nabla\Upsilon_\mu^m\|_{L_2}^2 \\ & + \varepsilon\|[K^m - K(t_m)]\nabla T^m\|_{L_2}^2 + \varepsilon\|[D^m - D(t_m)]\nabla\mu^m\|_{L_2}^2 \\ & + \|\Theta_T^m\|_{L_2}^2 + \|\Theta_\mu^m\|_{L_2}^2 + \varepsilon\|d_t\Theta_T^m\|_{L_2}^2 + \varepsilon\|d_t\Theta_\mu^m\|_{L_2}^2 + \varepsilon\|R_T^m\|_{H^{-1}}^2 + \varepsilon\|R_\mu^m\|_{H^{-1}}^2\}. \end{aligned}$$

Summing over m from 1 to ℓ after multiplying by k gives us

$$\begin{aligned}
& \|\Upsilon_T^\ell\|_{L_2}^2 + \|\Upsilon_\mu^\ell\|_{L_2}^2 + k \sum_{m=1}^{\ell} (k \|d_t \Upsilon_T^m\|_{L_2}^2 + k \|d_t \Upsilon_\mu^m\|_{L_2}^2) \\
& \leq \|\Upsilon_T^0\|_{L_2}^2 + \|\Upsilon_\mu^0\|_{L_2}^2 + Ck \sum_{m=1}^{\ell} \{ \varepsilon^{-\frac{3}{2}} \|E_\varphi^m\|_{L_2}^2 + \varepsilon^{-\frac{5}{2}} (\|\Upsilon_T^m\|_{L_2}^2 + \|\Upsilon_\mu^m\|_{L_2}^2) \\
& \quad + \varepsilon \|\nabla \Upsilon_\varphi^m\|_{L_2}^2 + \varepsilon^{-1} (\|\nabla \Upsilon_T^m\|_{L_2}^2 + \|\nabla \Upsilon_\mu^m\|_{L_2}^2) + \varepsilon^{-1} (\|\Theta_T^m\|_{L_2}^2 + \|\Theta_\mu^m\|_{L_2}^2) \\
& \quad + \varepsilon \|[K^m - K(t_m)]\nabla T^m\|_{L_2}^2 + \varepsilon \|[D^m - D(t_m)]\nabla \mu^m\|_{L_2}^2 \\
& \quad + \|d_t \Theta_T^m\|_{L_2}^2 + \|d_t \Theta_\mu^m\|_{L_2}^2 + \|R_T^m\|_{H^{-1}}^2 + \|R_\mu^m\|_{H^{-1}}^2 \}.
\end{aligned}$$

Now using inequality (3.100), (i) of the Theorem 3.7, (3.89) and similar estimates we used in the proof of Theorem 3.7 on the right hand side (see (3.87)), we get the following:

$$\begin{aligned}
\|\Upsilon_T^\ell\|_{L_2}^2 + \|\Upsilon_\mu^\ell\|_{L_2}^2 + k \sum_{m=1}^{\ell} (k \|d_t \Upsilon_T^m\|_{L_2}^2 + k \|d_t \Upsilon_\mu^m\|_{L_2}^2) \\
\leq C(\varepsilon^{-\frac{5}{2}} + k^{-1})[k^2 \varepsilon^{-6} + h^4 A(\varepsilon)] \quad (3.108)
\end{aligned}$$

where A is defined by (3.63).

Now with the help of (3.108) we can derive the estimates of the theorem. Assertion (ii) follows from

$$\begin{aligned}
\max_{0 \leq m \leq M_t} \|T(t_m) - T^m\|_{L_2}^2 & \leq C \max_{0 \leq m \leq M_t} \|\Theta_T^m\|_{L_2}^2 + C \max_{0 \leq m \leq M_t} \|\Upsilon_T^m\|_{L_2}^2 \\
& \leq C(h^4 \varepsilon^{-5} + (\varepsilon^{-\frac{5}{2}} + k^{-1})[k^2 \varepsilon^{-6} + h^4 A(\varepsilon)]),
\end{aligned}$$

and (3.45). Assertion (iii) is proved analogously.

The estimate (iv) follows from (3.108) and (3.107), that is,

$$\begin{aligned}
\max_{0 \leq m \leq M_t} \|T(t_m) - T^m\|_{L_\infty}^2 & \leq \max_{0 \leq m \leq M_t} \|\Theta_T^m\|_{L_\infty}^2 + \max_{0 \leq m \leq M_t} \|\Upsilon_T^m\|_{L_\infty}^2 \\
& \leq Ch^{4-N} |\ln h|^{3-N} \text{ess sup}_J \|T\|_{H^2} \\
& \quad + Ch^{-N} \max_{0 \leq m \leq M_t} \|\Upsilon_T^m\|_{L_2}^2 \\
& \leq Ch^{4-N} |\ln h|^{3-N} \varepsilon^{-5} \\
& \quad + Ch^{-N} (\varepsilon^{-\frac{5}{2}} + k^{-1})[k^2 \varepsilon^{-6} + h^4 A(\varepsilon)].
\end{aligned}$$

The last estimate (v) for μ can be derived analogously as (iv) and this concludes the proof of Theorem 3.8. \square

Chapter 4

Numerical experiments for the discretization error

In this chapter we present and analyze an experimental technique to determine the dependence of the error on the interface thickness ε . We will assume a certain form of the error function and determine the parameters of the function by performing some numerical experiments. The parameters of the error function are identified by the least squares method. For the nonlinear least square problem arising from the estimation of the parameters of the error function, we employ a Newton method with line search. The observed power of ε^{-1} is relatively small and justify the theoretical prediction that the dependence of the error on ε^{-1} is of low polynomial order.

4.1 Approximate error and experiments

We reserve the notation $E(h)$ to represent the error between the finite element solution U_h computed on a grid with a mesh size h and the exact solution U in a certain norm $\|\cdot\|$. Notice that if the numerical method is of p -th order, then we have for small h

$$E(h) \approx Ch^p,$$

with a constant C independent of h .

In case of the exact solution being unknown one can approximate it by a reference solution \bar{U} which is computed on a sufficiently fine grid. The error on the h -grid can be approximated by $U_h - \bar{U}$. Let $\bar{E}(h)$ be the approximate error on the grid with mesh size h ,

$$\bar{E}(h) = \|U_h - \bar{U}\|.$$

In order to study the dependence of the error constants on ε , we shall consider the error of a finite element solution in the L_2 -norm at a fixed time

$\bar{t} \in [0, \mathcal{T}]$. We assume that the approximate error for the phase field variable φ has the following form:

$$\bar{E}_\varphi(h, \varepsilon) := \|\Phi^\varepsilon(\cdot, \bar{t}) - \Phi_h^\varepsilon(\cdot, \bar{t})\|_{L_2(\Omega)} = Ch^p \varepsilon^{-q} \quad (4.1)$$

with constants C, p and q independent of h and ε . For an ε , the reference solution is denoted by Φ^ε and the solution on a grid with mesh size h by Φ_h^ε . Error functions \bar{E}_T and \bar{E}_c which correspond to the variables T and c are defined analogously.

Our primary goal is to determine the parameters C, p and q of the error functions by some numerical experiments. For this purpose, we solve the phase field problem for different values of the pair (ε, h) and compute the approximate errors. The time steps in the tests are chosen by the relation $k = Ch^2$ with C being a fixed constant. In the next section we formulate the task of the parameter determination as a least squares problem.

4.2 Nonlinear least squares problem

We solve the phase field problem for values of the pair (h_i, ε_j) for $i = 1, \dots, m_2, j = 1, \dots, m_1$ and then compute the approximate errors

$$\bar{E}_{ij} = \bar{E}(h_i, \varepsilon_j) = \|\Phi^{\varepsilon_j}(\cdot, \bar{t}) - \Phi_{h_i}^{\varepsilon_j}(\cdot, \bar{t})\|_{L_2(\Omega)}.$$

Our aim is to find C, p and q such that $\bar{E}(h_i, \varepsilon_j)$ is as close as possible to $Ch_i^p \varepsilon_j^{-q}$ in a sense that the sum of squares of differences for all i, j is minimal. For simplicity of the presentation, we denote $m = m_1 m_2$ and use the following notations:

$$x = (x_1, x_2, x_3)^\top = (\ln C, p, q)^\top$$

We also use index $\ell = (i - 1)m_1 + j$ which goes from 1 to m .

Being equipped with the above terminology we consider the following least square problem:

$$\min_{x \in \mathbb{R}^3} F(x) = \min_{x \in \mathbb{R}^3} \frac{1}{2} \|\mathbf{g}(x) - \mathbf{b}\|^2 \quad (4.2)$$

where

$$\begin{aligned} \mathbf{b} &= (b_1, \dots, b_m)^\top \quad \text{with } b_\ell = b_{(i-1)m_1+j} = \bar{E}_{ij}, \\ \mathbf{g}(x) &= (g_1(x), \dots, g_m(x))^\top \quad \text{with } g_\ell(x) = e^{x_1} h_i^{x_2} \varepsilon_j^{-x_3} \end{aligned}$$

for $\ell = 1, \dots, m$ (or equivalently $i = 1, \dots, m_2, j = 1, \dots, m_1$) and $\|\cdot\|$ is the Euclidean norm.

Define the components of the residual vector

$$\mathbf{r}(x) = (r_1(x), \dots, r_m(x))^\top$$

by

$$r_\ell(x) = g_\ell(x) - b_\ell$$

for $\ell = 1, \dots, m$.

We can write the objective function $F(x)$ in (4.2) also in the following form:

$$F(x) = \frac{1}{2} \mathbf{r}(x)^\top \mathbf{r}(x) = \frac{1}{2} \sum_{\ell=1}^m r_\ell(x)^2 = \frac{1}{2} \sum_{i=1}^{m_2} \sum_{j=1}^{m_1} r_{(i-1)m_1+j}^2(x).$$

Notice that the functions $g_\ell(x)$ are continuously differentiable and the elements of the Jacobian matrix $\mathbf{J}(x) \in \mathbb{R}^{m \times 3}$ are given by

$$J_{\ell s}(x) = \frac{\partial r_\ell(x)}{\partial x_s}$$

for $\ell = 1, \dots, m$ and $s = 1, 2, 3$.

The first derivative of $F(x)$, $\nabla F(x) \in \mathbb{R}^3$ is computed by

$$\nabla F(x) = \sum_{\ell=1}^m r_\ell(x) \nabla r_\ell(x) = \mathbf{J}(x)^\top \mathbf{r}(x)$$

and the second derivative $\nabla^2 F(x) \in \mathbb{R}^{3 \times 3}$ is given by

$$\begin{aligned} \nabla^2 F(x) &= \sum_{\ell=1}^m (\nabla r_\ell(x) \cdot \nabla r_\ell(x)^\top + r_\ell(x) \nabla^2 r_\ell(x)) \\ &= \mathbf{J}(x)^\top \mathbf{J}(x) + \mathbf{S}(x), \end{aligned}$$

with

$$\mathbf{S}(x) := \sum_{\ell=1}^m r_\ell(x) \nabla^2 r_\ell(x) \quad \text{and} \quad \nabla^2 r_\ell(x) = \left(\frac{\partial^2 r_\ell}{\partial x_p \partial x_q} \right)_{p,q=1}^3.$$

We approximate F by a quadratic function, i.e. assume the following representation is valid:

$$\begin{aligned} F(x) &\approx F(\bar{x}) + \nabla F(\bar{x})^\top (x - \bar{x}) + \frac{1}{2} (x - \bar{x})^\top \nabla^2 F(\bar{x}) (x - \bar{x}) \\ &= \frac{1}{2} \mathbf{r}(\bar{x})^\top \mathbf{r}(\bar{x}) + \mathbf{r}(\bar{x})^\top \mathbf{J}(\bar{x}) (x - \bar{x}) + \\ &\quad \frac{1}{2} (x - \bar{x})^\top (\mathbf{J}(\bar{x})^\top \mathbf{J}(\bar{x}) + \mathbf{S}(\bar{x})) (x - \bar{x}) \end{aligned}$$

around \bar{x} . Then the $i + 1$ -th step of the Newton method combined with the line search is as follows:

- Compute the descent direction $d^{(i)}$ from

$$(\mathbf{J}(x^{(i)})^\top \mathbf{J}(x^{(i)}) + \mathbf{S}(x^{(i)})) d^{(i)} = -\mathbf{J}(x^{(i)})^\top \mathbf{r}(x^{(i)})$$

- Set

$$x^{(i+1)} = x^{(i)} + \lambda^{(i)} d^{(i)}$$

for some $\lambda^{(i)}$ which makes $x^{(i+1)}$ an acceptable next iterate.

If the Hessian matrix

$$\mathbf{H}(x^{(i)}) = \mathbf{J}(x^{(i)})^\top \mathbf{J}(x^{(i)}) + \mathbf{S}(x^{(i)})$$

in the first step of the algorithms is not positive definite, we modify it by $\mathbf{H}(x^{(i)}) + \nu \mathbf{I}$ with a sufficiently large positive ν and solve

$$(\mathbf{H}(x^{(i)}) + \nu \mathbf{I}) d^{(i)} = -\mathbf{J}(x^{(i)})^\top \mathbf{r}(x^{(i)})$$

to get a descent direction $d^{(i)}$.

The line search in the last step starts with $\lambda^{(i)} = 1$ and checks the condition

$$F(x^{(i)} + \lambda^{(i)} d^{(i)}) \leq F(x^{(i)}) + \alpha \lambda^{(i)} \nabla F(x^{(i)})^\top d^{(i)}$$

for some $\alpha \in (0, 1)$. If the condition is not satisfied then we halve $\lambda^{(i)}$ and repeat the procedure till we find a suitable step length.

For our problem (4.2), we have

$$\mathbf{J}(x) = \begin{pmatrix} J_{11} & J_{12} & J_{13} \\ J_{21} & J_{22} & J_{23} \\ \vdots & \vdots & \vdots \\ J_{m1} & J_{m2} & J_{m3} \end{pmatrix}$$

with

$$\begin{aligned} J_{\ell,1} &= e^{x_1} h_i^{x_2} \varepsilon_j^{-x_3} \\ J_{\ell,2} &= e^{x_1} h_i^{x_2} \varepsilon_j^{-x_3} \ln h_i \\ J_{\ell,3} &= -e^{x_1} h_i^{x_2} \varepsilon_j^{-x_3} \ln \varepsilon_j \end{aligned}$$

and

$$\nabla^2 r_\ell(x) = e^{x_1} h_i^{x_2} \varepsilon_j^{-x_3} \begin{pmatrix} 1 & \ln h_i & -\ln \varepsilon_j \\ \ln h_i & (\ln h_i)^2 & -\ln h_i \ln \varepsilon_j \\ -\ln \varepsilon_j & -\ln h_i \ln \varepsilon_j & (\ln \varepsilon_j)^2 \end{pmatrix}$$

for $\ell = 1, \dots, m$.

If $x^* = (x_1^*, x_2^*, x_3^*)^\top$ is a solution of problem (4.2) then we have

$$(C, p, q) = (e^{x_1^*}, x_2^*, x_3^*).$$

4.3 Linear least squares problem

We consider the following least squares problem

$$\min_{x \in \mathbb{R}^3} \|\mathbf{g}(x) - \mathbf{b}\|^2 \quad (4.3)$$

with $g_\ell(x) = \ln(e^{x_1} h_i^{x_2} \varepsilon_j^{-x_3})$ and $b_\ell = \ln \bar{E}_{ij}$ for $\ell = 1, \dots, m$, where we again used the notation $x = (x_1, x_2, x_3) = (\ln C, p, q)$. The residuals $r_\ell(x) = b_\ell - g_\ell(x)$ are defined by

$$\begin{aligned} r_{(i-1)m_1+j}(\mathbf{x}) &= \ln \bar{E}_{ij} - \ln(e^{x_1} h_i^{x_2} \varepsilon_j^{-x_3}) \\ &= \ln \bar{E}_{ij} - (x_1 + x_2 \ln h_i - x_3 \ln \varepsilon_j), \end{aligned} \quad (4.4)$$

$i = 1, \dots, m_1$ and $j = 1, \dots, m_2$. We observe that the residuals are now linear functions of x_1, x_2 and x_3 . By taking logarithms of the error function and the data we obtained a linear least squares problem which is simple to solve. Problem (4.3) can be written as

$$\min_{x \in \mathbb{R}^3} \|\mathbf{A}x - \mathbf{b}\|^2$$

with a matrix $\mathbf{A} \in \mathbb{R}^{m \times 3}$ and a vector $\mathbf{b} \in \mathbb{R}^m$. The ℓ -th row of the matrix \mathbf{A} is given by

$$A_\ell = (1 \quad \ln h_i \quad -\ln \varepsilon_j)$$

and $b_\ell = \ln \bar{E}_{ij}$. This problem is equivalent to the finding of the solution of the linear system $\mathbf{A}x = \mathbf{b}$. The matrix \mathbf{A} has full rank, thus the solution $x^* = (x_1^*, x_2^*, x_3^*)$ of the normal equations

$$\mathbf{A}^T \mathbf{A}x = \mathbf{A}^T \mathbf{b} \quad (4.5)$$

is unique. If x^* is the solution of (4.5), it solves (4.3) as well and we get the desired parameters by $(C, p, q) = (e^{x_1^*}, x_2^*, x_3^*)$. The linear least squares problem doesn't necessarily have the same solution as the nonlinear least squares problem of Section 4.2. We will compare both results.

4.4 Data and numerical scheme

In this section we shall briefly discuss the data used for the experiments. We consider the phase field system (2.7) from Section 2.3 on square domains in \mathbb{R}^2 . In the computations, we used slightly modified functions

$$f(\varphi) = \frac{1}{2}(\varphi^3 - \varphi), \quad (4.6)$$

$$q = q(T, c, \varphi) = -\frac{16[s]_E}{15\sigma}(T - T_A c - T_B(1 - c))(\varphi^2 - 1)^2. \quad (4.7)$$

The above dependence on φ of the function q keeps the values of the phase field φ in the range $[-1, 1]$. For pure solid or pure liquid the function vanishes. The function $D = D(\varphi)$ is defined by (2.6) with $d_S = 0.8$ and $d_L = 1$. The constant M in the function $M(c) = Mc(1 - c)$ is chosen as

$$M = \frac{1}{2} \ln \frac{m_L}{m_S},$$

where m_S, m_L are the slopes of the solidus and liquidus lines in a phase diagram. We use $m_S = 2m_L$. The heat conductivity K is chosen as constant 1 in both phases. The initial data are

$$\varphi_0(x) = \tanh\left(\frac{\|\mathbf{x}\| - r_0}{2\varepsilon}\right), \quad T_0(x) = (T_A - T_B)c_L + T_B - T_U \quad (4.8)$$

with T_U being the undercooling temperature. For the concentration, we have either

$$c_0(x) = \begin{cases} c_S, & \|\mathbf{x}\| \leq r_0 \\ c_L, & \text{else} \end{cases} \quad \text{or} \quad c_0(x) = \frac{c_L - c_S}{2} \tanh\left(\frac{\|\mathbf{x}\| - r_0}{2\varepsilon}\right) + \frac{c_L + c_S}{2} \quad (4.9)$$

as initial function. We selected $T_A = 0, T_B = 0.5, c_S = 0.2$ and $c_L = 0.4$. The undercooling T_U varies between 0.22 and 0.3. The selection of initial functions corresponds to the situation that a solid seed of radius r_0 is placed in the liquid. Since the liquid surrounding the seed is undercooled below the equilibrium temperature, the solid seed grows as the time advances.

In the following, we make a short description of the numerical scheme used for the solution of the phase field system. The finite element space of continuous piecewise linear functions associated with a triangulation of Ω is denoted as usual by V_h . The scheme we used for the solution is as follows:

Find $(\Phi^m, T^m, C^m) \in [V_h]^3$, $m = 1, 2, \dots, n$ such that for every $(u_h, v_h, w_h) \in [V_h]^3$, we have

$$\begin{aligned} \alpha\varepsilon(d_t\Phi^m, u_h) + \varepsilon(\nabla\Phi^m, \nabla u_h) + \frac{1}{\varepsilon}(f(\Phi^{m-1}), u_h) \\ + (q(T^{m-1}, C^{m-1}, \Phi^{m-1}), u_h) = 0 \\ (d_tT^m, v_h) + (K\nabla T^m, \nabla v_h) + L(d_t\Phi^m, v_h) = 0 \quad (4.10) \\ (d_tC^m, w_h) + (D(\Phi^m)\nabla C^m, \nabla w_h) + (D(\Phi^m)M(C^{m-1})\nabla\Phi^m, w_h) = 0. \end{aligned}$$

Here $(\Phi^0, T^0, C^0) \in [V_h]^3$ is the starting value, $d_tU^m = \frac{U^m - U^{m-1}}{k}$ and k is the time step. The scheme allows us to solve the system sequentially, the part of the system corresponding to the phase field equation is solved first.

4.4.1 Results in two dimensions

In this section, we present some numerical results. We make tests using several values of the parameter ε and h and compute the approximate errors for all possible pairs of values. Then we solve the least squares problem described in Sections 4.2 and 4.3 and determine the parameters of the error functions \bar{E}_ψ , $\psi = \varphi, T, c$. The computations for the first test are done on uniform grids with mesh size

$$h_i = \frac{1}{N_i} \quad \text{for } N_i = 2^{8+i}, \quad i = 0, 1, 2 \quad (4.11)$$

and

$$\varepsilon_j = 0.01 + 0.005j, \quad \text{for } j = 0, 1, \dots, 6. \quad (4.12)$$

The values of the parameters h and ε are chosen in such a way that the grid is capable to capture the thin interface of length $O(\varepsilon)$ between solid and liquid. The solution for mesh size $h = 2^{-11}$ was used as reference solution for each value of ε . We choose $T_U = 0.22$ for the first test. The errors for phase field, temperature and concentration variables are considered independently. The results from test (T1) is summarized in Table 4.1 (linear least squares) and Table 4.2 (nonlinear least squares). They demonstrate that the dependence of the error constants on ε^{-1} is of low polynomial order. We conclude from the results that in computations for small values of ε it is possible to use reasonable time step and mesh sizes such that the amount of work required remains affordable. This can be done without much loss on the quality of the numerical solution. In the next test (T2) we have chosen a higher initial

	C	p	q		C	p	q
\bar{E}_φ	1.7081	1.5251	0.5468	\bar{E}_φ	2.1593	1.5133	0.4719
\bar{E}_T	0.9090	1.9446	0.7531	\bar{E}_T	1.4361	1.7728	0.4190
\bar{E}_c	0.0886	1.4071	0.5017	\bar{E}_c	0.0926	1.4101	0.4940
	C	p	q		C	p	q
\bar{E}_φ	2.1687	1.4933	0.4391	\bar{E}_φ	2.0164	1.4756	0.4291
\bar{E}_T	1.3063	1.6627	0.2830	\bar{E}_T	1.0375	1.5878	0.2269
\bar{E}_c	0.0960	1.4111	0.4852	\bar{E}_c	0.0984	1.4112	0.4778

Table 4.1: (T1): Linear least squares method. Parameters of the error functions at $t_1 = 6.4\text{E}-05$ (top left), $t_2 = 0.000128$ (top right), $t_3 = 0.000192$ (bottom left) and $t_4 = 0.000256$.

	C	p	q		C	p	q
\bar{E}_φ	1.1346	1.4572	0.5616	\bar{E}_φ	1.4809	1.4185	0.4424
\bar{E}_T	1.5486	1.9494	0.6235	\bar{E}_T	2.1539	1.7212	0.2445
\bar{E}_c	0.0499	1.3037	0.5108	\bar{E}_c	0.0528	1.3067	0.5002
	C	p	q		C	p	q
\bar{E}_φ	1.4516	1.3893	0.4034	\bar{E}_φ	1.3031	1.3678	0.3972
\bar{E}_T	1.7097	1.5973	0.1241	\bar{E}_T	1.1417	1.5112	0.0978
\bar{E}_c	0.0551	1.3067	0.4882	\bar{E}_c	0.0568	1.3060	0.4785

Table 4.2: (T1): Nonlinear least squares method. Parameters of the error functions at $t_1 = 6.4\text{E}-05$ (top left), $t_2 = 0.000128$ (top right), $t_3 = 0.000192$ (bottom left) and $t_4 = 0.000256$.

undercooling $T_U = 0.25$. The results are summarized in Tables 4.3 and 4.4. We can observe here an increase of the negative powers of ε in the error function E_T . This can be explained by the initial constant T_0 . Because of this the error E_T at small t is relatively large compared to the errors at later times.

	C	p	q		C	p	q
\bar{E}_φ	0.8516	1.4014	0.5066	\bar{E}_φ	0.8520	1.4025	0.5090
\bar{E}_T	0.0008	1.4047	1.3696	\bar{E}_T	0.0011	1.4049	1.3329
\bar{E}_c	0.0859	1.3977	0.4948	\bar{E}_c	0.0861	1.3977	0.4942

Table 4.3: (T2): $T_U = 0.25$ and linear least squares. Parameters of the error functions at $t_1 = 9.6\text{E}-06$ (left), $t_2 = 1.28\text{E}-05$.

	C	p	q		C	p	q
\bar{E}_φ	0.4820	1.2933	0.5084	\bar{E}_φ	0.4818	1.2948	0.5116
\bar{E}_T	0.0005	1.2933	1.3246	\bar{E}_T	0.0008	1.2941	1.2819
\bar{E}_c	0.0489	1.2878	0.4926	\bar{E}_c	0.0491	1.2879	0.4920

Table 4.4: (T2): $T_U = 0.25$ and nonlinear least squares. Parameters of the error functions at $t_1 = 9.6\text{E}-06$ (left), $t_2 = 1.28\text{E}-05$.

4.5 Tests for an anisotropic model

One of the interesting applications of phase field models is the simulation of dendritic growth. Therefore, it is interesting to see the dependence of the error on ε for anisotropic phase field models. We can apply the presented techniques for the determination of the parameters of the error function in this case as well.

In the tests we use the anisotropic phase field system introduced in Section 2.3, i.e. the model equations are (2.12), (2.7b) and (2.7c) with data (4.8) and (4.9). The part of the scheme which is different from the isotropic case (4.10) is

$$\begin{aligned} \alpha\varepsilon(d_t\Phi^m, u_h) + \varepsilon(\eta^2(\nabla\Phi^{m-1})\nabla\Phi^m, \nabla u_h) + (\mathbf{s}(\nabla\Phi^{m-1}), \nabla u_h) \\ + \frac{1}{\varepsilon}(f(\Phi^{m-1}), u_h) + (q(T^{m-1}, C^{m-1}, \Phi^{m-1}), u_h) = 0 \end{aligned}$$

where the components of $\mathbf{s} = (s_1, s_2)^\top$ is defined analogously to (2.14) in two dimensions. Through the numerical experiments we intend to see the dependence of the error on the parameter ε for the anisotropic case. The parameters as well as initial functions are the same as for the isotropic case. The small solid seed placed in the liquid grows with time and dendrite arms build along the coordinate axes due to the introduced four fold anisotropy.

4.5.1 Results for the anisotropic model

In the tests, the strength of anisotropy is chosen as $\delta_4 = 0.05$. This value is relatively big and leads to a fast growth of dendrite arms along the coordinate axes. The computations for the first two tests are done on uniform grids with mesh size

$$h_i = \frac{1}{N_i} \quad \text{for } N_i = 2^{7+i}, \quad i = 0, 1, 2$$

and $\varepsilon_j = 0.01 + 0.005j$, for $j = 0, 1, \dots, 8$. From the test results we can conclude that the introduction of anisotropy into the model doesn't imply a considerable change of the dependence of the error on ε . The results remain similar to the case without anisotropy. The results for test (T3) for the anisotropic model are summarized in Table 4.5 and Table 4.6. In (T3), the value $T_U = 0.3$ is used. The errors at time $t_1 = 3.2\text{E}-05$ are displayed in Figure 4.1. In Figure 4.2 we have compared the results of the linear and nonlinear least squares methods. The comparison is made for the error function for the phase field at time t_1 . For the convenience of the comparison, we displayed the functions for fixed values of h . Each row corresponds to a certain value of fixed h . The plots in the left column shows the quality of the data fitting. The curves with the legend "measured" correspond to

	C	p	q		C	p	q
\bar{E}_φ	2.2016	1.3880	0.3976	\bar{E}_φ	2.6539	1.3957	0.3550
\bar{E}_T	0.0094	1.2963	0.9164	\bar{E}_T	0.0334	1.3382	0.7415
\bar{E}_c	1.0332	1.4211	0.1017	\bar{E}_c	0.7850	1.4139	0.1282

Table 4.5: (T3): Linear least squares. Parameters of the error functions for the anisotropic model, $T_U = 0.3$, $t_1 = 3.2\text{E}-05$ (left) and $t_2 = 6.4\text{E}-05$.

	C	p	q		C	p	q
\bar{E}_φ	1.3351	1.2786	0.3791	\bar{E}_φ	1.6365	1.2897	0.3368
\bar{E}_T	0.0061	1.1494	0.8298	\bar{E}_T	0.0227	1.2232	0.6859
\bar{E}_c	1.0248	1.4059	0.0822	\bar{E}_c	0.7695	1.3965	0.1090

Table 4.6: (T3): Nonlinear least squares. Parameters of the error functions for the anisotropic model, $T_U = 0.3$, $t_1 = 3.2\text{E}-05$ (left) and $t_2 = 6.4\text{E}-05$.

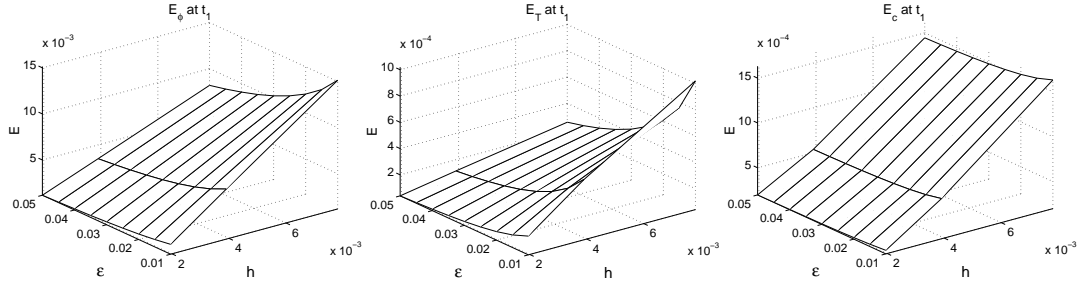


Figure 4.1: (T3): Error behaviours at t_1

$(\varepsilon, \bar{E}(h_i, \varepsilon))$ for $h_1 = 1/128$, $h_2 = 1/256$, $h_3 = 1/512$. The curves with “fitted (linear)” correspond to $(\varepsilon, Ch_i^p \varepsilon^{-q})$ where $(C, p, q) = (2.2016, 1.3880, 0.3976)$ (cf. Table 4.5) is determined by the linear least squares method. For the “fitted (nonlinear)” the values $(C, p, q) = (1.3351, 1.2786, 0.3791)$ are from Table 4.6. The second column shows the deviations of two fitted data from the “measured” data. For the next test (T4) we have chosen a lower undercooling temperature $T_U = 0.25$ than the one used for the test (T3). We also have here different final times for the measurement of the errors. The results of this test are shown in Table 4.7 and Table 4.8 for linear and nonlinear least squares methods.

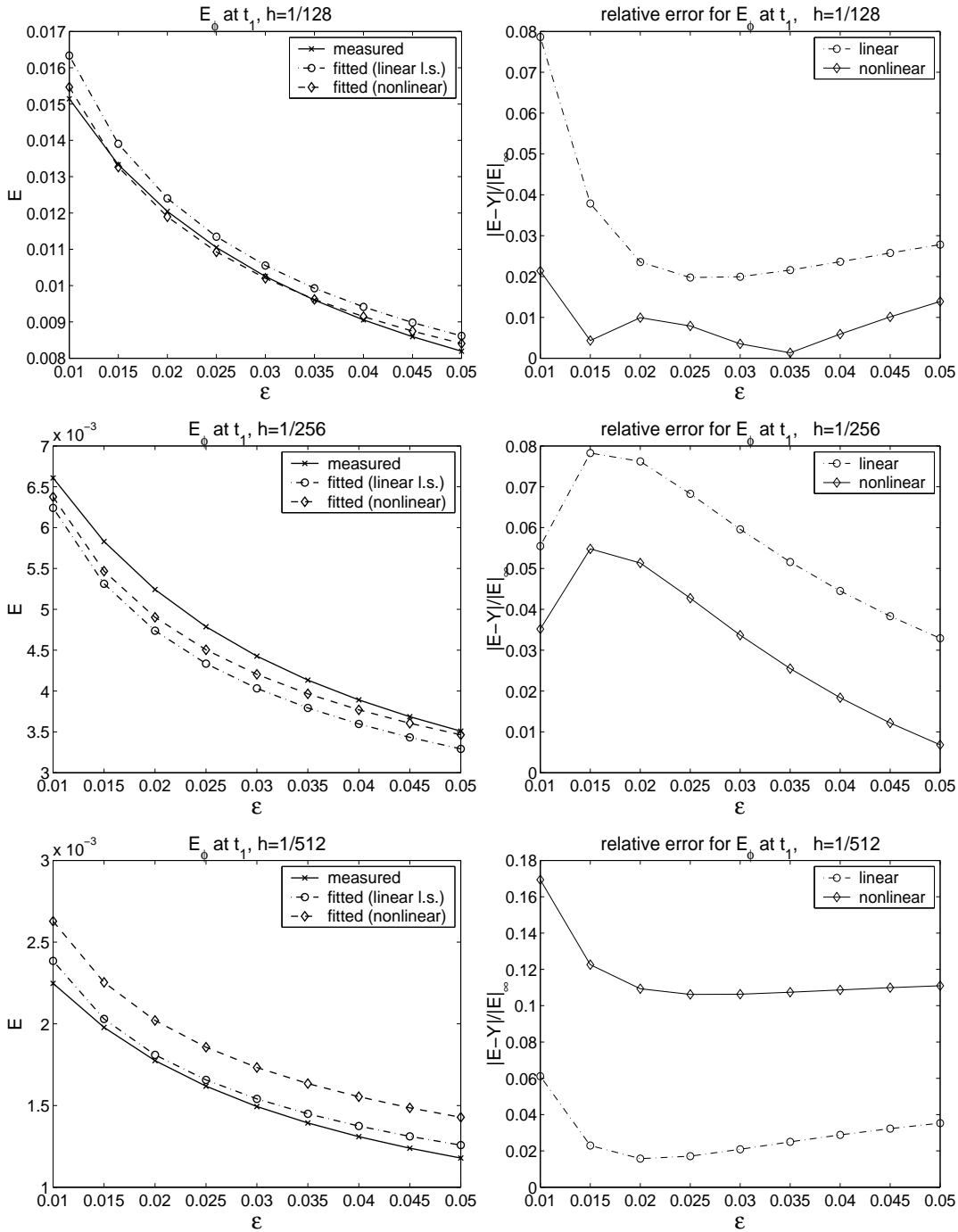


Figure 4.2: (T3): Comparison of the two methods for \bar{E}_φ at t_1 .

4.5.2 Some tests in three dimensions

In this section we make some experiments for the anisotropic problem in three dimensions. The computations are done on uniform grids with mesh

	C	p	q		C	p	q
\bar{E}_φ	7.2978	1.4087	0.3099	\bar{E}_φ	8.6454	1.4155	0.2621
\bar{E}_T	0.1904	1.3619	0.5548	\bar{E}_T	0.5112	1.3847	0.3583
\bar{E}_c	1.3981	1.4013	0.1386	\bar{E}_c	1.2908	1.4105	0.1437

Table 4.7: (T4): Linear least squares. Parameters of the error functions for the anisotropic model, $t_1 = 1.28\text{E}-04$ (left) and $t_2 = 2.56\text{E}-04$.

	C	p	q		C	p	q
\bar{E}_φ	4.3121	1.2999	0.2991	\bar{E}_φ	5.0503	1.3073	0.2554
\bar{E}_T	0.1209	1.2487	0.5189	\bar{E}_T	0.3108	1.2763	0.3406
\bar{E}_c	0.7500	1.2773	0.1325	\bar{E}_c	0.6966	1.2902	0.1411

Table 4.8: (T4): Nonlinear least squares. Parameters of the error functions for the anisotropic model, $t_1 = 1.28\text{E}-04$ (left) and $t_2 = 2.56\text{E}-04$.

size $h_i = \frac{1}{N_i}$ for $N_1 = 96, N_2 = 192$, and $\varepsilon_j = 0.015 + 0.0025j$ for $j = 0, 1, \dots, 4$. The reference solution is computed on the grid with $h = 1/384$. The results of test (T5) are presented in Table 4.9 and 4.10. We have chosen $\delta_4 = 0.05$ and $T_U = 0.25$ in the computations. The results in three dimensions also demonstrate the low polynomial dependence of the error on ε^{-1} . The result obtained by nonlinear and linear least squares methods does not differ significantly in the tests for both two and three dimensions.

	C	p	q		C	p	q
\bar{E}_φ	0.2533	1.6854	0.4688	\bar{E}_φ	0.2535	1.6874	0.4747
\bar{E}_T	0.0002	1.6438	1.2281	\bar{E}_T	0.0007	1.6528	1.0900
\bar{E}_c	0.2533	1.6854	0.4688	\bar{E}_c	0.0264	1.6838	0.4500

Table 4.9: (T5): Three dimensions and linear least squares. Parameters of the error functions, $t_1 = 3.2\text{E}-05$ (left) and $t_2 = 6.4\text{E}-05$.

	C	p	q		C	p	q
\bar{E}_φ	0.2564	1.6849	0.4654	\bar{E}_φ	0.2561	1.6870	0.4718
\bar{E}_T	0.0002	1.6373	1.1971	\bar{E}_T	0.0007	1.6485	1.0626
\bar{E}_c	0.0263	1.6818	0.4504	\bar{E}_c	0.0267	1.6821	0.4461

Table 4.10: (T5): Three dimensions and nonlinear least squares. Parameters of the error functions, $t_1 = 6.4\text{E}-05$ (left) and $t_2 = 1.28\text{E}-04$.

Chapter 5

Adaptive simulation of dendritic crystals

In this chapter we consider numerical simulations of dendritic structures by the phase field model introduced in Chapter 2. In Section 2.3 we discussed models for the growth of dendritic structures. Here, we address some modeling and implementation aspects, the data and the numerical scheme. We compare numerical results of simulations for different strengths of the anisotropy and different undercooling temperatures.

5.1 The problem

Consider the anisotropic system for binary alloys consisting of equations (2.12), (2.7b) and (2.7c). At the beginning of the simulation, we have a small solid seed placed in an undercooled melt. This situation can be reflected by an initial phase field function chosen as in (4.8). The choice of the tanh function is justified since the function is the principal term in the asymptotic expansions near the interface (cf. Appendix A.1). Far from the interface the values are near to ± 1 and we have a smooth transition from -1 to $+1$ over the interface region. The initial solid seed has radius r_0 . In Figure 5.1 a simplified (c, T) phase diagram with linear solidus and liquidus lines in the neighborhood of $(0, T_B)$ is shown. The diagram corresponds to the situation that the solute is rejected into the liquid as the solid seed grows. The liquid has a higher solute concentration than the solid. The liquid should be undercooled to facilitate the growth. Therefore, the temperature at the beginning can be set to a value which lies below the equilibrium melting temperature which corresponds to the initial composition of the alloy as in (4.8). If the initial undercooling T_U is big, then the solidification at the beginning is rapid. As the liquid heats up due to the release of latent heat

at the interface the growth of the crystal slows down. The concentration at time $t = 0$ is chosen as constant c_L in liquid and c_S in solid phases as in (4.9). The relations between the parameters can be established from the phase diagram chosen. We choose homogeneous Neumann boundary conditions for

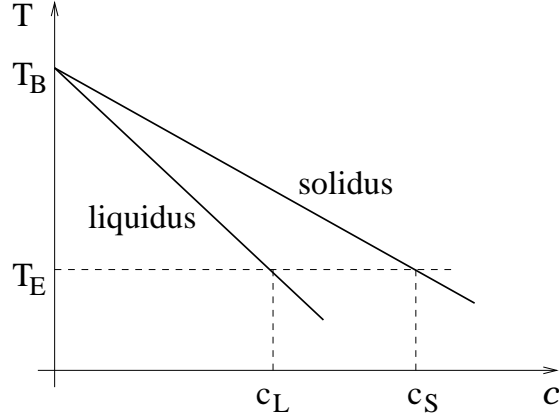


Figure 5.1: A simplified phase diagram

the equations. We specify now the data functions. The functions $f(\varphi)$ and $q(T, c, \varphi)$ are chosen as in (4.6) and (4.7). The heat conductivity K takes the same constant value in both phases, and the solute diffusivity $D(\varphi)$ is defined with solute diffusivities d_L, d_S in liquid and solid, respectively. The diffusivity in the solid is less than that in the liquid ($d_S < d_L$). Finally, in the function $M(c) = \frac{1}{2} \ln \frac{m_L}{m_S} c(1-c)$ the slopes m_S, m_L of the solidus and liquidus lines are taken from the simplified phase diagram.

5.1.1 Discretization

In the following, we introduce the numerical scheme. Introduce a partition $\{t_m\}_{m=0}^\ell$ of the time interval $(0, \mathcal{T}]$ by $t_m - t_{m-1} = k$ for $m = 1, \dots, \ell$.

Let $u^m = u(t_m, \cdot)$ for $u = \varphi, T, c$. We use the following semi-implicit time discrete problem:

Find $(\varphi^m, T^m, c^m) \in [H^1(\Omega)]^3$ such that

$$\begin{aligned} \alpha \varepsilon (d_t \varphi^m, u) + \varepsilon (\eta^2 (\nabla \varphi^{m-1}) \nabla \varphi^m, \nabla u) + \varepsilon (\mathbf{s}(\nabla \varphi^{m-1}), \nabla u) \\ + \frac{1}{\varepsilon} (f(\varphi^{m-1}), u) + (q(T^{m-1}, c^{m-1}, \varphi^{m-1}), u) = 0 \end{aligned} \quad (5.1a)$$

$$(d_t T^m, v) + (K \nabla T^m, \nabla v) + L (d_t \varphi^m, \nabla v) = 0 \quad (5.1b)$$

$$(d_t c^m, w) + (D(\varphi^m) \nabla c^m, \nabla w) + (D(\varphi^m) M(c^{m-1}) \nabla \varphi^m, \nabla w) = 0 \quad (5.1c)$$

for all $(u, v, w) \in [H^1(\Omega)]^3$ and $m = 1, \dots, \ell$. The function \mathbf{s} is defined as in (2.13).

To obtain a fully discrete system, we introduce a space discretization with a finite dimensional space of $H^1(\Omega)$. Let \mathcal{T}_h be a quasi-uniform triangulation of the domain Ω and V_h the corresponding finite element space. Moreover, let $\{\psi_j(x)\}_{j=1}^n$ be a set of basis functions of V_h .

We consider the discrete space $\{t_m\}_{m=1}^\ell \times V_h$ and denote by $\Phi_h^m(x)$, $T_h^m(x)$ and $C_h^m(x)$ the approximations of the solutions in this space. The representations of the discrete solution by basis functions of V_h are

$$\Phi_h^m(x) = \sum_{j=1}^n \Phi_j^m \psi_j(x), \quad T_h^m(x) = \sum_{j=1}^n T_j^m \psi_j(x), \quad C_h^m(x) = \sum_{j=1}^n C_j^m \psi_j(x) \quad (5.2)$$

where T_j^m , c_j^m , ϕ_j^m are constants. Introducing (5.2) to the time discrete system (i.e. the system (5.1) with φ^m , T^m , c^m replaced by Φ_h^m , T_h^m , C_h^m) and choosing basis functions ψ_i , $i = 1, \dots, n$ as test functions u, v, w , we obtain linear systems of equations for $\{\Phi_j^m\}_{j=1}^n$, $\{T_j^m\}_{j=1}^n$ and $\{C_j^m\}_{j=1}^n$.

5.1.2 Implementation and adaptive grid

In this section we address some aspects of the implementation. In the numerical simulations we use the C++ finite element library `deal.II` [20]. We make computations with bilinear elements using adaptive grids. As we will see from the numerical results it is sufficient to have a grid which is locally fine in the interface region and coarse away from the interface. Employing adaptive grids greatly reduces the computational work. In the following we make a brief description of the grid adapting procedure.

Denote the grid at time t_m by G^m and the solution on the grid by (Φ^m, T^m, C^m) . Suppose that we have local error indicators $\eta_{\Phi, K'}$, $\eta_{T, K'}$, $\eta_{C, K'}$ for each cell $K' \in G^m$. We omitted the superscript for the solution for simplicity of the notation. Define the total cell error $\eta_{K'}$ by

$$\eta_{K'} = \sqrt{\eta_{\Phi, K'}^2 + \eta_{T, K'}^2 + \eta_{C, K'}^2}$$

for each cell $K' \in G^m$, and the total error η_{total} by

$$\eta_{\text{total}}^2 := \sum_{K' \in G^m} \eta_{K'}^2. \quad (5.3)$$

The tolerance for the total error tol^{m+1} at time t_{m+1} can be computed from the energy norms of the solution (Φ^m, T^m, C^m) . Naturally, we set the tolerances for the cell errors by $\text{tol}_{\text{cell}}^{m+1} = \text{tol}^{m+1} / \sqrt{\mathcal{N}}$ where \mathcal{N} is the number of cells in G^m .

We use the following strategy for the grid adaption. Suppose that we have a grid, the solution on the grid and an error tolerance. At time t_{m+1} we compute the solutions $(\Phi^{m+1}, T^{m+1}, C^{m+1})$ on G^m and determine the cell error $(\eta_{K'})$ and total error (η_{total}) corresponding to this solution. If η_{total} is below a given tolerance tol^{m+1} we move to the next time step, otherwise we perform refinement and coarsening on G^m . We take a loop over all cells of G^m and mark the cells with $\eta_{K'} > \beta_1 \text{tol}_{\text{cell}}^{m+1}$ for refinement and the cells with $\eta_{K'} < \beta_2 \text{tol}_{\text{cell}}^{m+1}$ for coarsening. The parameters are for the purpose of controlling the number of cells to be refined or coarsened and satisfy $\beta_2 < 1 < \beta_1$. After the refinement and coarsening we repeat the procedure till we obtain an admissible grid. One could as well work with varying tolerances in each refinement and coarsening step. We summarize the above in the following algorithm:

Given: A grid G^m , solution (Φ^m, T^m, C^m) and tolerance tol^{m+1} .

1. Compute $(\Phi^{m+1}, T^{m+1}, C^{m+1})$ on G^m .
2. Estimate cell errors $\eta_{U,K'}$ for each $K' \in G^m$ and $U = \Phi^{m+1}, T^{m+1}, C^{m+1}$. Compute η_{total} by (5.3).
3. If $\eta_{\text{total}} > \text{tol}^{m+1}$ refine and coarsen G^m and go to 2. else set $m := m + 1$ and go to 1.

We use a gradient recovery error estimator by Kelly et al. [1] in the computations. It is defined as

$$\eta_{K'}^2 = \frac{h}{24} \int_{\partial K'} \left[\frac{\partial u_X}{\partial n} \right]^2 ds$$

where u_X is a finite element approximation of u and K' is a cell of the triangulation and

$$\left[\frac{\partial u_X}{\partial n} \right] = \left[\frac{\partial u_X}{\partial n_{K'}} \right] \Big|_{K'} + \left[\frac{\partial u_X}{\partial n_J} \right] \Big|_J$$

is the discontinuity in the finite element approximation to the gradient across the edge between neighbouring cells K' and J . Here, $[\cdot]$ denotes the jump of the argument over a face.

For the linear systems we use the Conjugate Gradient (CG) method with the preconditioning by Symmetric Successive Overrelaxation (SSOR). The relaxation parameter is chosen as $w = 1.2$ and the residual tolerance for the CG-iteration is set to $1\text{E}-12$. For the computations with $\varepsilon = 0.01$ we used the time step $k = 0.0001$. For the other values of ε ($0.005 - 0.02$) similar results are obtained. A typical parameter and data set in two dimensions is shown in Table 5.1.

α	3.0	r_0	0.1	ε	0.01
T_U	0.3	K	1	d_L	1.0
T_A	0.0	c_S	0.2	d_S	0.8
T_B	0.5	c_L	0.4	σ	0.00032

Table 5.1: Material and computational parameters

5.2 Numerical results

In this section we present computations of the dendritic crystals in two and three space dimensions. Results of the simulations using different strengths of anisotropy and undercooling temperatures are discussed.

5.2.1 Results in two dimensions

In Figure 5.2 we displayed the evolution of the interface for dendritic structures with four principal directions of the growth. For big (initial) undercooling temperatures, we have a steeper temperature gradient ahead of the interface. Therefore the latent heat which is released at the interface during the solidification is transported away easily, this causes fast growth in the chosen directions. By comparing the sizes of a solidified area at a fixed time we can observe this behaviour. The next set of pictures (Figure 5.3) shows

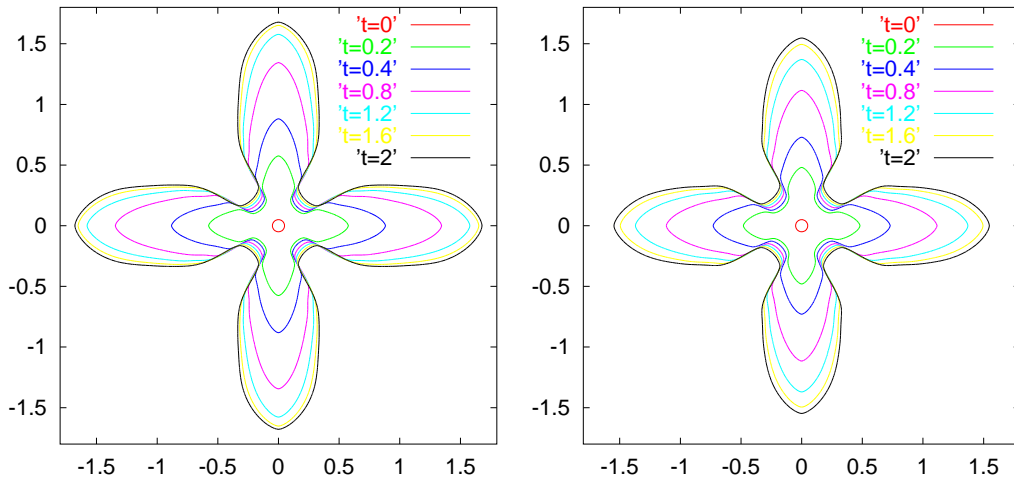


Figure 5.2: Positions of the interface for $\varepsilon = 0.01$, $\delta_4 = 0.05$ and different initial undercooling temperatures. Left: $T_U = 0.3$, right: $T_U = 0.28$

typical phase field, temperature and concentration profiles for a simulation. The solid is the hottest part of the system. We can also observe the higher

concentration at the interface in the figure corresponding to the solute pile-up. Due to the symmetry of the four fold anisotropy the computations are done in one quarter of the domain. The grid (a quarter of it) at the time $t = 1.5$ has 25377 degrees of freedom. The error indicator we use produces reasonable grids for our problem. We would have needed 262144 degrees of freedom, if we were to use a uniform grid which is as fine as the interface region of the adapted grid. The degrees of freedom and the number of nodes are not the same in the grid since we have hanging nodes in the grid. The values of the solution at hanging nodes are determined by the interpolations and they are eliminated from the linear system we solve at each time step.

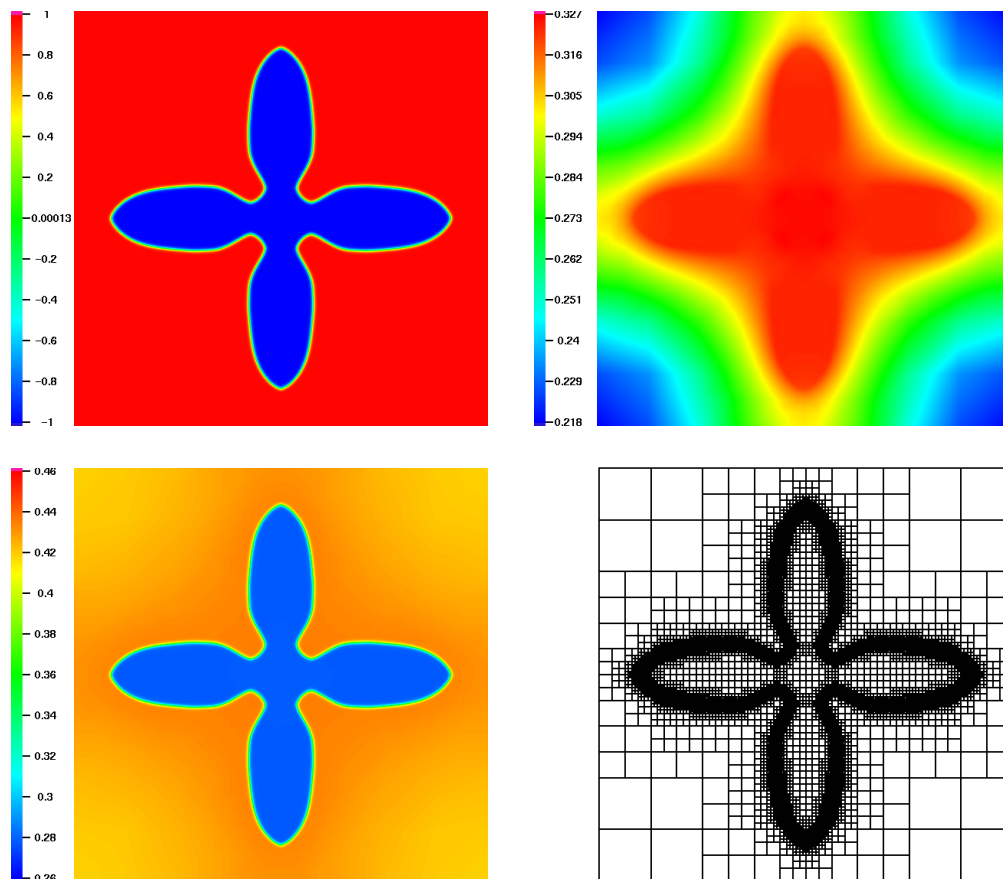


Figure 5.3: Phase field (top left), temperature (top right), concentration (bottom left) and grids at $t = 1.5$ for simulations using $\varepsilon = 0.01$, $\delta_4 = 0.05$ and $T_U = 0.3$

In Figure 5.5 we present the evolution of the interface for dendritic structures with six arms. We used the strength of the anisotropy $\delta_6 = 0.01$, the inter-

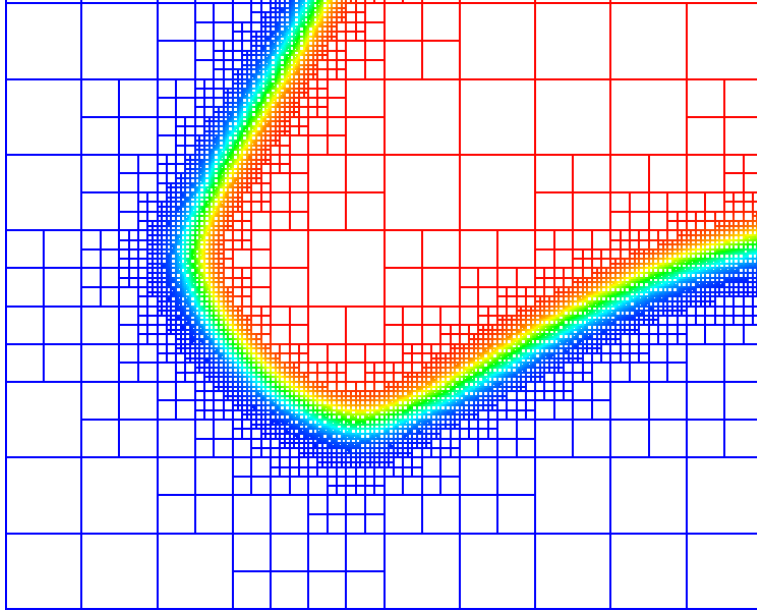


Figure 5.4: Interfacial region zoomed.

face thickness parameter $\varepsilon = 0.01$ and compared the results for two different initial undercooling temperatures.

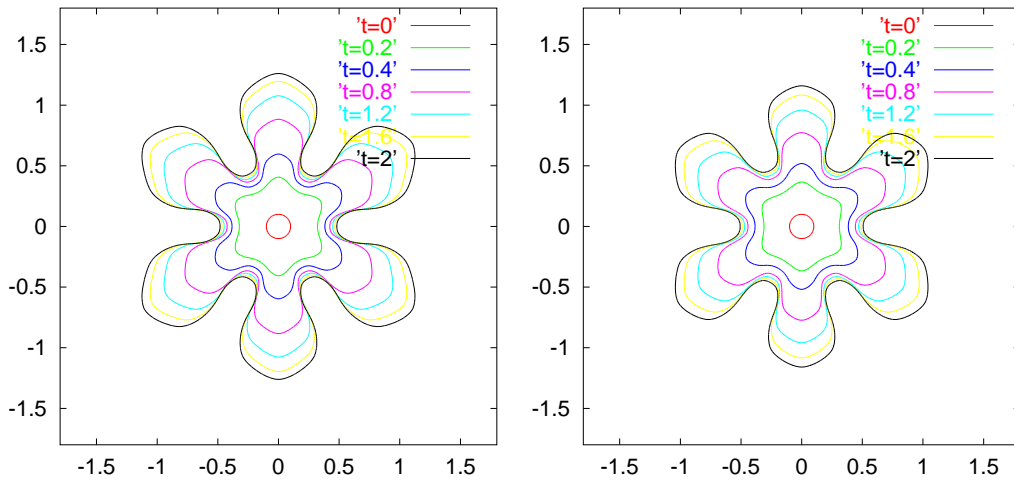


Figure 5.5: Six fold anisotropy: Positions of the interface for a simulation with $\varepsilon = 0.01$, $\delta_6 = 0.01$ and different initial undercooling temperatures. Left: $T_U = 0.3$, right: $T_U = 0.28$

Figure 5.6 shows the cross sections of the phase field and temperature at

several times. In Figure 5.7 we compare the concentrations along one arm of the (four fold) crystals for simulations with two different initial undercoolings. The cutting plane for figures 5.6 and 5.7 is $y = 0$ on the (x, y, u) (for $u = \varphi, T, c$) surface. Naturally, the growth is faster for a big initial undercooling. Then the resulting fast growth permits the tip to reject more heat into the liquid and hence warming the surrounding liquid. Once the liquid temperature exceeds the equilibrium melting temperature (no undercooling) then the growth stops. This is the case as the interface approaches the boundary of the computational domain. As the interface advances the solute is rejected from the solid and excess solute is transported away from the interface through diffusion. As amount of the rejected solute increase, a solute pile up builds ahead of the interface and the concentration gradient becomes steeper there. This is seen in Figure 5.7. The concentration takes nearly constant values in each phases and has a jump over the interface when the interface approaches the boundary of the computational domain. The growth in this case is very slow or no growth since no undercooling is present.

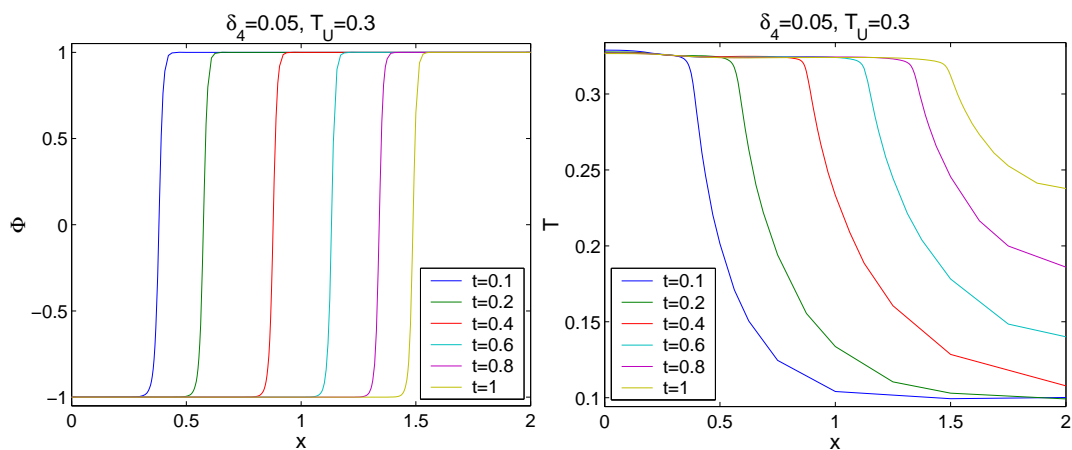


Figure 5.6: Cross sections of the phase field and the temperature by the plane $y = 0$

5.2.2 Results in three dimensions

The parameters for the simulations in three dimensions are basically the same as for the two dimensional case. In Figure 5.8 a level surface of the phase field for four fold anisotropy $\delta_4 = 0.05$ and $\varepsilon = 0.01$ is shown. The surface tension is chosen as $\sigma = 1.28\text{E}-03$ in this simulation. The computations are done in one octant of the domain due to the symmetry. The contours of the temperature field and the grid with edges coloured by the concentration

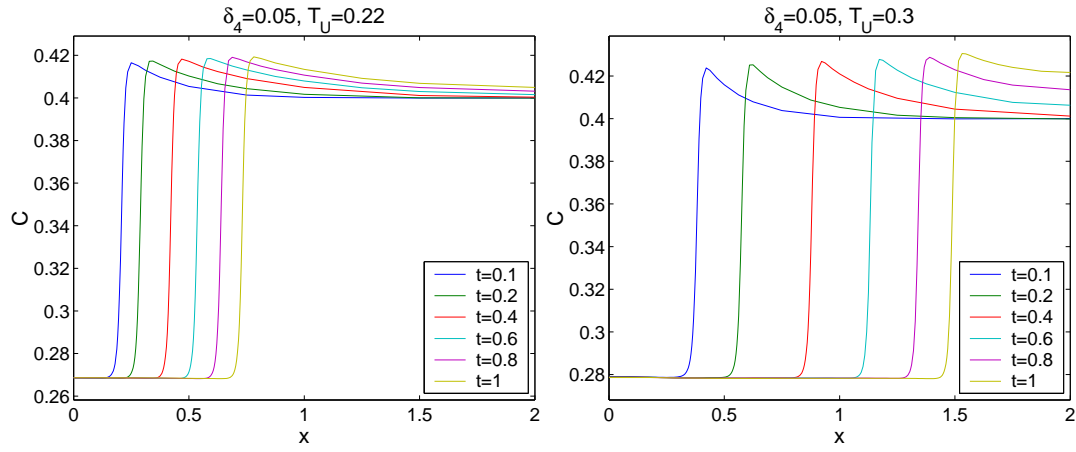


Figure 5.7: Cross sections of c by the plane $y = 0$

values are shown in Figure 5.9. The grid there has 547582 degrees of freedom.

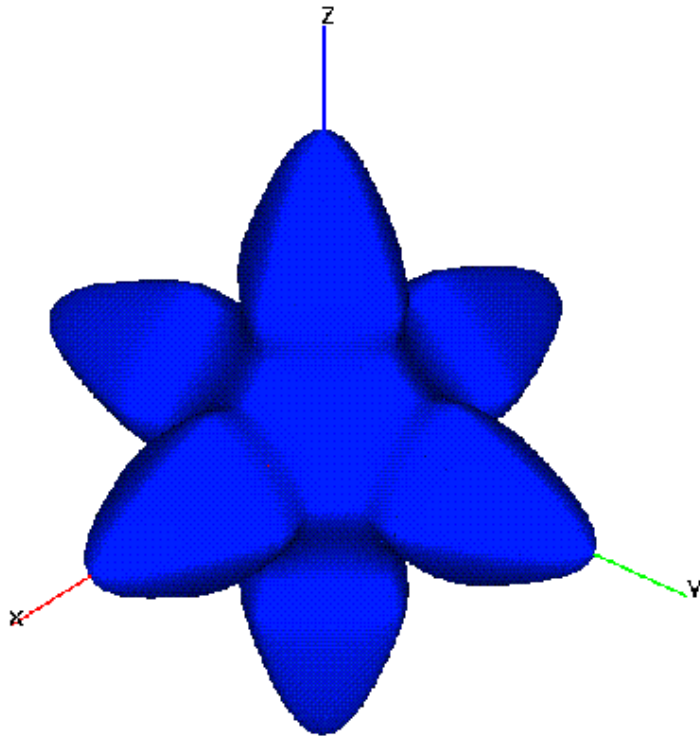


Figure 5.8: Level surface of the phase field $\{x : \varphi(t, x) = 0\}$ ($\delta_4 = 0.05, \varepsilon = 0.01$) at $t = 0.55$

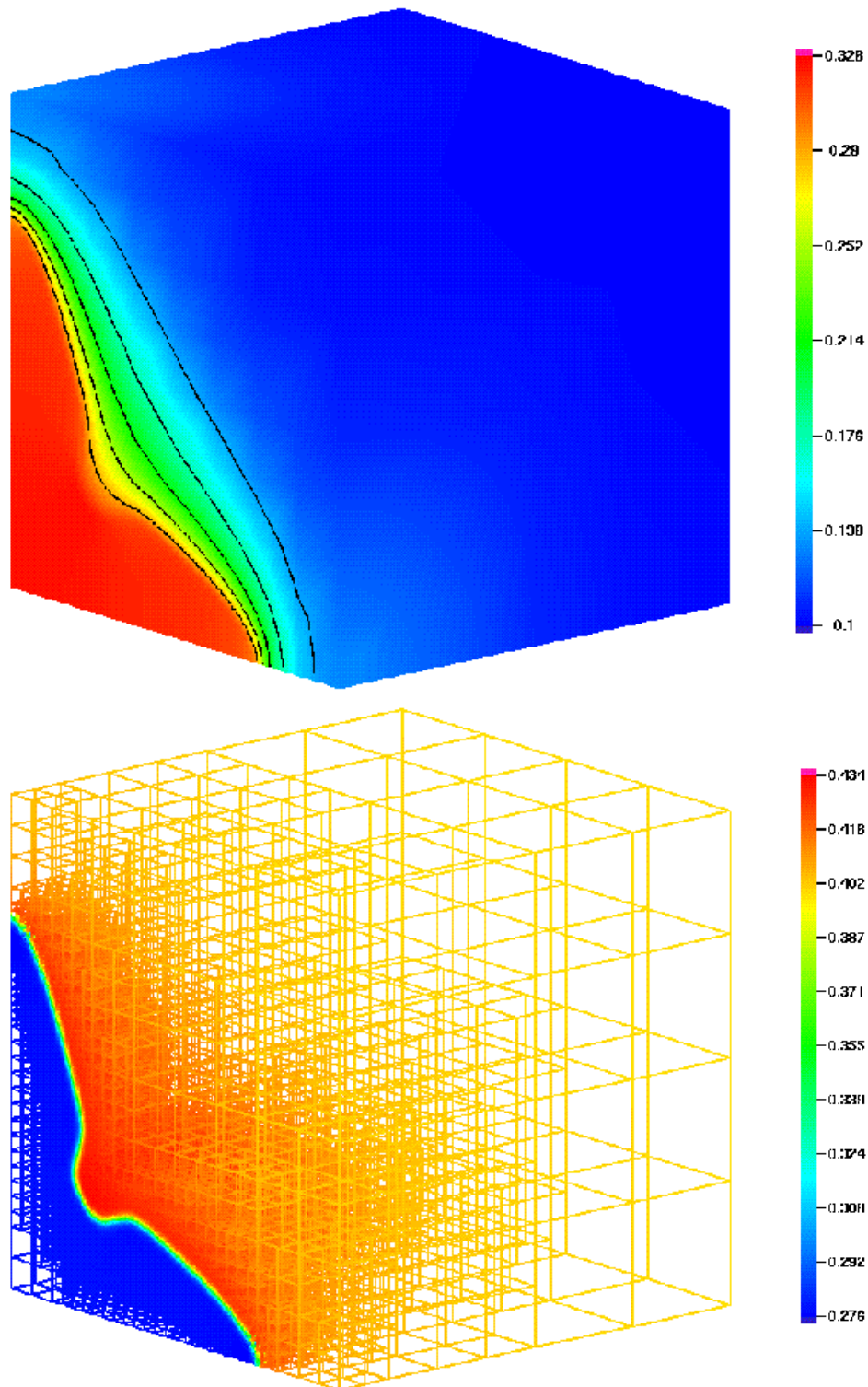


Figure 5.9: Contours of temperature T (top) and grid at $t = 0.55$ with edges coloured by the values of c (bottom)

A

Appendix

A.1 Formal asymptotic expansions

In this section we consider asymptotic expansions of the solution of a phase field system in the neighbourhood of the solid-liquid interface. The phase field system

$$\alpha\varepsilon\partial_t\varphi - \varepsilon\Delta\varphi + \frac{1}{\varepsilon}f(\varphi) + \frac{\delta}{\sigma}q(T, \mu) = 0 \quad (\text{A1.1})$$

$$\partial_t T - \nabla \cdot (K\nabla T) + L\partial_t\varphi = 0 \quad (\text{A1.2})$$

$$\partial_t\mu - \nabla \cdot (D\nabla\mu) + M\partial_t\varphi = 0 \quad (\text{A1.3})$$

is considered in $\Omega \in \mathbb{R}^N$ with $f(\varphi) = \varphi^3 - \varphi$ and scalar K, D . Let $(\varphi_\varepsilon, T_\varepsilon, \mu_\varepsilon)$ be the solution of the system with appropriate boundary conditions for parameter ε . We consider first the inner expansions (close to the interface) as we are interested in the behaviour of the solution in the interfacial region. For this purpose, we define local coordinates chosen in the neighbourhood of the solid liquid interface. Denote by $r_\varepsilon(t, x)$ the signed distance of x to the level set $\Gamma_\varepsilon(t) = \{x \in \mathbb{R}^N : \varphi_\varepsilon(t, x) = 0\}$ at time t . It is positive in the liquid, negative in the solid domain. Let $s_\varepsilon(t, x)$ be the projection of x on $\Gamma_\varepsilon(t)$ along the normal of $\Gamma_\varepsilon(t)$. The subscript ε in the local coordinates $(r_\varepsilon, s_\varepsilon)$ is omitted for simplicity. The coordinates satisfy

$$\begin{aligned} |\nabla r|^2 &= 1, \quad \nabla r \cdot \nabla s_i = 0 \quad \text{for } i = 1, \dots, N-1 \\ \partial_t r &= -v \end{aligned}$$

with v denoting the velocity of the interface. At the interface we have $\Delta r = \kappa$ with κ being the curvature of the interface.

In the neighbourhood of $\Gamma_\varepsilon(t)$, the solution of the phase field system is represented in new variables

$$\psi_\varepsilon(t, r, s) = \psi_0(t, r, s) + \varepsilon\psi_1(t, r, s) + \varepsilon^2\psi_2(t, r, s) + \dots, \quad (\text{A1.4})$$

for $\psi = \varphi, T, \mu$. We also define a scaling of r by $\rho = r/\varepsilon$. The definition of r implies that

$$\varphi_\varepsilon(t, 0, s) = 0. \quad (\text{A1.5})$$

We consider now outer expansions (away from the interface). The outer expansions are done in cartesian coordinates as

$$\Psi_\varepsilon(t, x) = \Psi_0(t, x) + \varepsilon\Psi_1(t, x) + \varepsilon^2\Psi_2(t, x) + \dots, \quad (\text{A1.6})$$

for $\Psi = \Phi, U, V$ with Φ, U and V corresponding to the variables φ, T and μ , respectively. The coefficient functions in the expansion are supposed to be bounded. The functions can be discontinuous at the interface. Plugging (A1.6) in (A1.1)–(A1.3) and equating the coefficients of powers of ε we get the outer problems of different orders. Expansions of K and D are included in what follows. We have

$$\begin{aligned} & \alpha\varepsilon(\partial_t\Phi_0 + \varepsilon\partial_t\Phi_1 + \dots) - \varepsilon(\Delta\Phi_0 + \varepsilon\Delta\Phi_1 + \dots) \\ & + \frac{1}{\varepsilon}f(\Phi_0 + \varepsilon\Phi_1 + \varepsilon^2\Phi_2 + \dots) \\ & + \frac{\delta}{\sigma}q(U_0 + \varepsilon U_1 + \varepsilon^2 U_2 + \dots, V_0 + \varepsilon V_1 + \varepsilon^2 V_2 + \dots) = 0, \end{aligned} \quad (\text{A1.7})$$

$$\begin{aligned} & \partial_t(U_0 + \varepsilon U_1 + \varepsilon^2 U_2 + \dots) \\ & - \nabla \cdot ((K_0 + \varepsilon K_1 + \varepsilon^2 K_2 + \dots)\nabla(U_0 + \varepsilon U_1 + \varepsilon^2 U_2 + \dots)) \\ & = -L(\partial_t\Phi_0 + \varepsilon\partial_t\Phi_1 + \varepsilon^2\partial_t\Phi_2 + \dots), \end{aligned} \quad (\text{A1.8})$$

$$\begin{aligned} & \partial_t(V_0 + \varepsilon V_1 + \varepsilon^2 V_2 + \dots) \\ & - \nabla \cdot ((D_0 + \varepsilon D_1 + \varepsilon^2 D_2 + \dots)\nabla(V_0 + \varepsilon V_1 + \varepsilon^2 V_2 + \dots)) \\ & = -M(\partial_t\Phi_0 + \varepsilon\partial_t\Phi_1 + \varepsilon^2\partial_t\Phi_2 + \dots). \end{aligned} \quad (\text{A1.9})$$

The *zero-th order outer problem* is set by collecting the coefficients of ε^{-1} in (A1.7), the coefficients of ε^0 in equations (A1.8) and (A1.9), i.e.

$$f(\Phi_0) = 0 \quad (\text{A1.10})$$

$$\partial_t U_0 - \nabla \cdot (K_0 \nabla U_0) + L \partial_t \Phi_0 = 0 \quad (\text{A1.11})$$

$$\partial_t V_0 - \nabla \cdot (D_0 \nabla V_0) + M \partial_t \Phi_0 = 0. \quad (\text{A1.12})$$

Similarly, we obtain the *first order outer problem*

$$f'(\Phi_0)\Phi_1 = -\frac{\delta}{\sigma}q(U_0, V_0) \quad (\text{A1.13})$$

$$\partial_t U_1 - \nabla \cdot (K_0 \nabla U_1) + L \partial_t \Phi_1 = \nabla \cdot (K_1 \nabla U_0) \quad (\text{A1.14})$$

$$\partial_t V_1 - \nabla \cdot (D_0 \nabla V_1) + M \partial_t \Phi_1 = \nabla \cdot (D_1 \nabla V_0). \quad (\text{A1.15})$$

Equation (A1.10) has solutions $\Phi_0 = \pm 1$ and $\Phi_0 = 0$. Then, for $r \neq 0$ (in solid or liquid domain) we have simple heat and diffusion equations for U_0 and V_0 in the zero-th order problem which can be solved with appropriate initial and boundary conditions. Similarly, higher order equations reduce to equations for Ψ_k only.

Matching conditions arise from the fact that inner and outer expansions describe the same function in an intermediate region with distance of order $\sqrt{\varepsilon}$ from the interface. For the matching conditions, cartesian coordinates in the function representing the outer expansions are expressed by the local coordinates $(\rho, s) = (r/\varepsilon, s)$.

In the region where the inner and outer expansions represent the same functions we equate the representations (A1.4) and (A1.6). We combine the expansion of $s \in \Gamma(t)$,

$$s(t) = s_0(t) + \varepsilon s_1(t) + \varepsilon^2 s_2(t) + \dots$$

with the outer expansions (A1.6) and expand the terms of the outer expansion in the Taylor series. Then we pass to the limits $\rho \rightarrow \pm\infty$ with ρ related to ε in suitable manner. By equating the coefficients of ε^0 and ε^1 in the resulting equation we obtain the following conditions:

$$\psi_0(t, \pm\infty, s) = \Psi_0(t, s_0(t)_\pm) \quad (\text{A1.16})$$

$$\psi_1(t, \rho, s) \sim \Psi_1(t, s_0(t)_\pm) + \rho \partial_r \Psi_0(t, s_0(t)_\pm) + y_1(t) \partial_r \Psi_0(t, s_0(t)_\pm) \quad (\text{A1.17})$$

(for large ρ) where $s_0(t)_\pm$ denote the limits of $s_0(t)$ from the liquid (+) side (for $\rho > 0$) or solid (-) side (for $\rho < 0$).

We turn now to the inner expansions applied to the phase field system (A1.1)–(A1.3). For the representation of the solutions in the (r, s) coordinates

$$u(t, x) \rightarrow \tilde{u}(t, r(x, t), s(x, t))$$

we need transformations of the differential operators present in the system.

$$\begin{aligned}
\partial_t u &= \partial_t \tilde{u} + \partial_r \tilde{u} \partial_t r + \sum_{i=1}^{N-1} \partial_{s_i} \tilde{u} \partial_t s_i \\
&= (\partial_t - v \partial_r + \partial_t s \cdot \nabla_s) \tilde{u} \\
\Delta u &= \nabla \cdot \left(\partial_r \tilde{u} \nabla r + \sum_{i=1}^{N-1} \partial_{s_i} \tilde{u} \nabla s_i \right) \\
&= \partial_r^2 \tilde{u} |\nabla r|^2 + \partial_r \tilde{u} \Delta r + \sum_{i=1}^{N-1} (\partial_{s_i}^2 \tilde{u} |\nabla s_i|^2 + \partial_{s_i} \tilde{u} \Delta s_i + \partial_{s_i}^2 \tilde{u} \nabla r \cdot \nabla s_i) \\
&= \left(\partial_r^2 + \Delta r \partial_r + \Delta s \cdot \nabla_s + \sum_{i=1}^{N-1} |\nabla s_i|^2 \partial_{s_i}^2 \right) \tilde{u} \\
\nabla \cdot (K \nabla u) &= \left(\partial_r (K \partial_r) + K \Delta r \partial_r + K \Delta s \cdot \nabla_s + \sum_{i=1}^{N-1} |\nabla s_i|^2 \partial_{s_i} (K \partial_{s_i}) \right) \tilde{u}.
\end{aligned}$$

For $\nabla \cdot (D \nabla)$ we have the same transformation formula as the last one with K replaced by D .

With the variable ρ , the differential operators transform according to

$$\begin{aligned}
\partial_t &\sim \partial_t - \varepsilon^{-1} v \partial_\rho + \partial_t s \cdot \nabla_s \\
\Delta &\sim \varepsilon^{-2} \partial_\rho^2 + \varepsilon^{-1} \Delta r \partial_\rho + \Delta s \cdot \nabla_s + \sum_{i=1}^{N-1} |\nabla s_i|^2 \partial_{s_i}^2 \\
\nabla \cdot (K \nabla) &\sim \varepsilon^{-2} \partial_\rho (K \partial_\rho) + \varepsilon^{-1} K \Delta r \partial_\rho + K \Delta s \cdot \nabla_s + \sum_{i=1}^{N-1} |\nabla s_i|^2 \partial_{s_i} (K \partial_{s_i}).
\end{aligned}$$

Transformation of variables in the phase field system results in

$$\begin{aligned}
&\alpha \varepsilon \partial_t \varphi_\varepsilon - \alpha v \partial_\rho \varphi_\varepsilon + \alpha \varepsilon \partial_t s \cdot \nabla_s \varphi_\varepsilon - \varepsilon^{-1} \partial_\rho^2 \varphi_\varepsilon - \Delta r \partial_\rho \varphi_\varepsilon \\
&\quad - \varepsilon \Delta s \cdot \nabla_s \varphi_\varepsilon - \varepsilon \sum_{i=1}^{N-1} |\nabla s_i|^2 \partial_{s_i}^2 \varphi_\varepsilon + \varepsilon^{-1} f(\varphi_\varepsilon) + \frac{\delta}{\sigma} q(T_\varepsilon, \mu_\varepsilon) = 0, \\
&\partial_t T_\varepsilon - \varepsilon^{-1} v \partial_\rho T_\varepsilon + \partial_t s \cdot \nabla_s T_\varepsilon - \varepsilon^{-2} \partial_\rho (K \partial_\rho T_\varepsilon) - \varepsilon^{-1} K \Delta r \partial_\rho T_\varepsilon - K \Delta s \cdot \nabla_s T_\varepsilon \\
&\quad - \sum_{i=1}^{N-1} |\nabla s_i|^2 \partial_{s_i} (K \partial_{s_i} T_\varepsilon) + L \partial_t \varphi_\varepsilon - L \varepsilon^{-1} v \partial_\rho \varphi_\varepsilon + L \partial_t s \cdot \nabla_s \varphi_\varepsilon = 0
\end{aligned}$$

where we omitted the tilde for simplicity of the notation. The equation for μ_ε has the same form as the equation for T_ε . Now, we apply the inner expansions

(A1.4) to the system and taken into account the expansions

$$\Delta r = \kappa_0 + \varepsilon \kappa_1 + \dots, \quad v = v_0 + \varepsilon v_1 + \dots$$

By equating the terms of same powers of ε in each side of the equations, we get sequences of problems for (φ_i, T_i, μ_i) .

The *zero-th order inner problem* is set by collecting the coefficients of ε^{-1} in the phase field equation, and the coefficients of ε^{-2} in the equations for T_ε and μ_ε :

$$-\partial_\rho^2 \varphi_0 + f(\varphi_0) = 0 \quad (\text{A1.18})$$

$$-\partial_\rho(K_0 \partial_\rho T_0) = 0 \quad (\text{A1.19})$$

$$-\partial_\rho(D_0 \partial_\rho \mu_0) = 0. \quad (\text{A1.20})$$

Equation (A1.18) is supplemented by the condition $\varphi_0(t, 0, s) = 0$ which results from (A1.5), and matching conditions of zero-th order (A1.16)

$$\varphi_0(t, \pm\infty, s) = \Phi_0|_{\Gamma_\pm} = \pm 1$$

with $\Phi_0|_{\Gamma_\pm}$ being the limit of Φ_0 from the liquid and solid sides. Equation (A1.18) with the given conditions determines φ_0 uniquely. Since we have $f(\varphi) = \varphi^3 - \varphi$,

$$\varphi_0(\rho) = \tanh\left(\frac{\rho}{\sqrt{2}}\right). \quad (\text{A1.21})$$

In a similar manner, the equations (A1.19) and (A1.20) are considered with the matching conditions (A1.16)

$$T_0(t, \pm\infty, s) = U_0|_{\Gamma_\pm} \quad (\text{A1.22})$$

and

$$\mu_0(t, \pm\infty, s) = V_0|_{\Gamma_\pm}. \quad (\text{A1.23})$$

Since the limit functions are bounded, after integrating the equations (A1.19), (A1.20), we find that T_0, μ_0 are independent of ρ , i.e.

$$T_0 = T_0(t, s), \quad \mu_0 = \mu_0(t, s). \quad (\text{A1.24})$$

The *first order inner problem* is set by collecting the coefficients of ε^0 in the phase field equation and the coefficients of ε^{-1} in the other two equations of the system:

$$-\partial_\rho^2 \varphi_1 + f'(\varphi_0) \varphi_1 = (\alpha v_0 + \kappa_0) \partial_\rho \varphi_0 - \frac{\delta}{\sigma} q(T_0, \mu_0) \quad (\text{A1.25})$$

$$-\partial_\rho(K_0 \partial_\rho T_1) = L v_0 \partial_\rho \varphi_0 \quad (\text{A1.26})$$

$$-\partial_\rho(D_0 \partial_\rho \mu_1) = M v_0 \partial_\rho \varphi_0 \quad (\text{A1.27})$$

where the independence of T_0, μ_0 on ρ has been taken into account.

The equation for φ_1 is linear and its right hand side depends on the solution of the problem of zero-th order. The differential operator $-\partial_\rho^2 + f'(\varphi_0)I$ has a nontrivial kernel which contains $\partial_\rho\varphi_0$. This implies that, for solvability, $\partial_\rho\varphi_0$ should be orthogonal to the right hand side, i.e.

$$\int_{\mathbb{R}} \left[(\alpha v_0 + \kappa_0) |\partial_\rho\varphi_0|^2 - \frac{\delta}{\sigma} q(T_0, \mu_0) \partial_\rho\varphi_0 \right] d\rho = 0.$$

Since T_0, μ_0 are ρ -independent, we get

$$(\alpha v_0 + \kappa_0) \int_{\mathbb{R}} |\partial_\rho\varphi_0|^2 d\rho = \frac{2\delta}{\sigma} q(T_0, \mu_0)$$

which corresponds to the Gibbs-Thomson condition with kinetic undercooling

$$\sigma(\alpha v_0 + \kappa_0) = q(T_0, \mu_0) \tag{A1.28}$$

provided that

$$\delta = \frac{1}{2} \int_{-\infty}^{+\infty} |\partial_\rho\varphi_0|^2 d\rho \tag{A1.29}$$

holds. For $\varphi_0 = \tanh \frac{\rho}{\sqrt{2}}$ we have $\delta = \frac{\sqrt{2}}{3}$.

Considering (A1.28), the equation (A1.25) turns into

$$-\partial_\rho^2\varphi_1 + f'(\varphi_0)\varphi_1 = (\alpha v_0 + \kappa_0) [\partial_\rho\varphi_0 - \delta].$$

It follows that $\varphi_1 = p(t, s)\theta_1(\rho)$, where $p(t, s) = \alpha v_0 + \kappa_0$ and $\theta_1(\rho)$ satisfies

$$-\theta_1'' + f'(\varphi_0)\theta_1 = \varphi_0' - \delta \tag{A1.30}$$

and

$$\theta_1(0) = 0, \quad \theta_1 \in L_\infty(\mathbb{R}) \tag{A1.31}$$

where the conditions arise from $\varphi_1(t, 0, s) = 0$ and the matching condition (A1.17) (the boundedness of Ψ_1).

Moreover, by (A1.29) we have

$$\int_{\mathbb{R}} (\delta - \varphi_0') \varphi_0' d\rho = 0,$$

so that the function θ_1 exists and is unique. Multiplying both sides of equation (A1.30) by φ_0'' and integrating over \mathbb{R} , we obtain

$$\begin{aligned}
0 &= \int_{\mathbb{R}} \varphi_0'' (\delta - \varphi_0') d\rho = \int_{\mathbb{R}} \varphi_0'' (\theta_1'' - f'(\varphi_0)\theta_1) d\rho \\
&= \int_{\mathbb{R}} (-\theta_1' \varphi_0''' - f'(\varphi_0)\theta_1 \varphi_0'') d\rho \\
&= \int_{\mathbb{R}} \theta_1' [-\varphi_0'' + f(\varphi_0)]' d\rho - \int_{\mathbb{R}} [f'(\varphi_0)\varphi_0' \theta_1' + f'(\varphi_0)\theta_1 \varphi_0''] d\rho \\
&= \int_{\mathbb{R}} f''(\varphi_0)(\varphi_0')^2 \theta_1 d\rho.
\end{aligned}$$

It follows that the function θ_1 satisfies

$$\int_{\mathbb{R}} f''(\varphi_0)(\varphi_0')^2 \theta_1 d\rho = 0. \quad (\text{A1.32})$$

By integrating the equations (A1.26) and (A1.27), we get

$$K_0 \partial_\rho T_1 = -Lv_0 \varphi_0 + C_1(t, s) \quad (\text{A1.33})$$

$$D_0 \partial_\rho \mu_1 = -Mv_0 \varphi_0 + C_2(t, s) \quad (\text{A1.34})$$

We differentiate the matching condition (A1.17) with respect to ρ and obtain

$$\lim_{\rho \rightarrow \pm\infty} \partial_\rho T_1 = \nabla U_0 \cdot n|_{\Gamma_\pm}.$$

This implies that

$$K_0 \nabla U_0 \cdot n|_{\Gamma_\pm} = \mp Lv_0 + C_1(t, s). \quad (\text{A1.35})$$

The difference between the (+) and (-) parts of this equation gives us the latent heat condition

$$[K_0 \nabla U_0 \cdot n]_\Gamma = -2Lv_0. \quad (\text{A1.36})$$

If T_0 is known, this condition combined with the continuity of U_0 that follows from (A1.22) supplement equation (A1.11) and may determine U_0 in the zero-th order outer problem considered with appropriate initial conditions. Similar condition as (A1.36) can be derived for V_0 and supplement equation (A1.12) alongwith (A1.23) (provided that μ_0 is known). Once U_0, V_0 are known, they can be used to determine $C_1(t, s), C_2(t, s)$ from (A1.35) and the analogous equation $D_0 \nabla V_0 \cdot n|_{\Gamma_\pm} = \mp Mv_0 + C_2(t, s)$. Then we can also get Φ_1 from (A1.13) considered with a behaviour at large ρ derived from the matching condition (A1.17). Similarly, one can proceed with the other equations of the second order and also with the terms of higher order.

Remark. For the spectrum estimates (Section 3.3) a certain regularity condition is assumed for the second order remainder of the inner expansions. The assumption can be justified by a more rigorous analysis. For the Cahn-Hilliard equation which is closely related to the phase field equation, it is shown in [2] that it is possible to construct a family of approximate solutions satisfying the assumption and the spectrum estimates.

Bibliography

- [1] M. Ainsworth, J.T. Oden. A posteriori error estimation in finite element analysis. *Comput. Methods Appl. Mech. Engrg.*, 142, 1-88, 1997.
- [2] Nicholas D. Alikakos, Peter W. Bates and Xinfu Chen. Convergence of the Cahn-Hilliard Equation to the Hele-Shaw Model. *Arch. Rational Mech. Anal.*, 128, 165–205, 1994.
- [3] J. Bergh, J. Löfström. *Interpolation Spaces, an Introduction*. Springer, Berlin, 1976.
- [4] O. Besov, V.P. Il'yin, S.M. Nikolskii. *Integral Transformations of Functions and Embedding Theorems*. Vol. II, V.H. Winston & Sons, Washington D.C., 1979.
- [5] R.J. Braun, G.B. McFadden, S.R. Coriell. Morphological instability in phase-field models of solidification. *Physical Review E*, 49(5), 4336–4352, 1994.
- [6] S. C. Brenner, L. R. Scott. *The Mathematical Theory of Finite Element Methods*. Springer, 1996.
- [7] G. Caginalp. An analysis of a Phase Field Model of a Free Boundary. *Arch. Rational. Mech. Anal.*, 92, 205–242, 1986.
- [8] G. Caginalp, Mathematical models of phase boundaries. In *Material Instabilities in Continuum Mechanics and Related Mathematical Problems* (ed. J. Ball), 35–52, Oxford Science Publications, 1988.
- [9] G. Caginalp. Stefan and Hele-Shaw type models as asymptotic limits of the phase field equations. *Physical Review A*, 39(11), 5887–5896, 1989.
- [10] G. Caginalp, P.C. Fife. Dynamics of layered interfaces arising from phase boundaries. *SIAM J. Appl. Math.*, 48(3), 1988.
- [11] G. Caginalp, J.T. Lin. A Numerical Analysis of an Anisotropic Phase Field Model. *IMA J. Appl. Math.*, 39, 51–66, 1987.

- [12] G. Caginalp, W. Xie. Phase-field and sharp-interface alloy models. *Physical Review E*, 48(3), 1897–1909, 1993.
- [13] G. Caginalp, W. Xie. An Analysis of Phase-Field Alloys and Transition Layers. *Arch. Rational Mech. Anal.*, 142, 293–329, 1998.
- [14] G. Caginalp, X. Chen. Convergence of the phase field model to its sharp interface limits. *Euro. J. Appl. Math.*, 9, 417–445, 1998.
- [15] G. Caginalp, E. Socolovsky. Phase field computations of single-needle crystals, crystal growth, and motion by mean curvature. *SIAM J. Sci. Comp.*, 15(1), 106–126, 1994.
- [16] X. Chen. Spectrum for the Allen-Cahn, Cahn-Hilliard, and phase-field equations for generic interfaces. *Commun. Partial Differ. Equations*, 19(7-8), 1371–1395, 1994.
- [17] Z. Chen, K.-H. Hoffmann. An error estimate for a finite-element scheme for a phase field model. *IMA J. Numer. Anal.*, 14, 243–255, 1994.
- [18] P. Ciarlet. *The finite element method for elliptic problems*. North-Holland publishing company, 1978.
- [19] J. Crank. *Free and moving boundary problems*. Clarendon Press, 1987.
- [20] deal.II library, <http://www.dealii.org>
- [21] J. E. Dennis, R. B. Schnabel. *Numerical methods for unconstrained optimization and nonlinear equations*. Prentice-Hall, Englewood Cliffs, NJ, 1983.
- [22] Ch. Eck. Analysis and Homogenization of a Phase Field Model for Binary Mixtures. *Preprint-Series of the Institute for Applied Mathematics*, 288, University of Erlangen-Nürnberg, 2002.
- [23] Ch. Eck. *A Two-Scale Phase Field Model for Liquid-Solid Phase Transitions of Binary Mixtures with Dendritic Structure*. Habilitation Thesis, University of Erlangen-Nürnberg, 2004.
- [24] L. C. Evans. *Partial Differential Equations*. Graduate Studies in Mathematics, Volume 19, American Mathematical Society Providence, Rhode Island, 1998.
- [25] M. Fabbri, V. R. Voller. The Phase-Field Method in the Sharp-Interface Limit: A Comparison between Model Potentials. *J. Comp. Phys.*, 130, 256–265, 1997.

- [26] X. Feng, A. Prohl. Numerical Analysis of the Allen-Cahn equation and approximation for mean curvature flows. *Numer. Math.*, 94(1), 33–65, 2003.
- [27] X. Feng, A. Prohl. *Analysis of a fully discrete finite element method for the phase field model and approximation of its sharp interface limits*. IMA Preprint 1817, 2001.
- [28] D. Gilbarg, N.S. Trudinger. *Elliptic Partial Differential Equations of Second Order*. A Series of Comprehensive Studies in Mathematics 224, Springer-Verlag, 1977.
- [29] P. Grisvard. *Elliptic problems in nonsmooth domains*. Monographs and studies in mathematics 24, Pitman, 1985.
- [30] A. Karma, W.-J. Rappel. Quantitative phase-field modeling of dendritic growth in two and three dimensions. *Phys. Review E*, 57(4), 4323–4349, 1998.
- [31] D. Kessler, O. Krüger, J. Rappaz and J. F. Scheid. A phase-field model for the isothermal solidification process of a binary alloy. *Computer Assisted Mechanics and Engineering Sciences*, 7, 279–288, 2000.
- [32] D. Kessler and J. F. Scheid. A priori estimates of a finite element method for an isothermal phase-field model related to the solidification process of a binary alloy. *IMA J. Numer. Anal.*, 22(2), 281–305, 2002.
- [33] P. Knabner, L. Angermann. *Numerik partieller Differentialgleichungen*, Springer-Verlag, Berlin, Heidelberg, New-York, 2000.
- [34] R. Kobayashi. Modeling and numerical simulations of dendritic crystal growth. *Physica D*, 63, 410–423, 1993.
- [35] W. Kurz, D.J. Fisher. *Fundamentals of solidification*, Trans Tech Publications, 1992.
- [36] J.T. Lin. The numerical analysis of a phase field model in moving boundary problems. *SIAM J. Numer. Anal.*, 25(5), 1015–1031, 1988.
- [37] J. Nitsche. Ein Kriterium für die Quasi-Optimalität des Ritzschen Verfahrens. *Numer. Math.*, 11, 346–348, 1968.
- [38] J. T. Oden, J. N. Reddy. *An Introduction to the Mathematical Theory of Finite Elements*. John Wiley & Sons, 1976.

- [39] N. Provatas, N. Goldenfeld, and J. Dantzig. Adaptive Mesh Refinement Computation of Solidification Microstructures using Dynamic Data Structures. *J. Comp. Phys.*, 148, 265–290, 1999.
- [40] J. Rappaz, J.F. Scheid. Existence of Solutions to a Phase-Field Model for the Isothermal Solidification Process of a Binary Alloy. *Math. Meth. Appl. Sci.*, 23, 491–513, 2000.
- [41] Vidar Thomée. *Galerkin Finite Element Methods for Parabolic Problems*. Springer, 1997.
- [42] M. Renardy, R.C. Rogers. *An Introduction to Partial Differential Equations*. Springer-Verlag, Texts in Applied Mathematics 13, 1992.
- [43] V.A. Solonnikov. On the boundary value problem for linear parabolic systems of differential equations of general form. *Proc. Steklov Inst. Math.* 83, 1965. English transl. by Amer. Math. Soc. 1967.
- [44] S.-L. Wang, R.F. Sekerka. Computation of dendritic operating state at large supercoolings by the phase field model. *Physical Review E*, 53(4), 3760–3776, 1996.
- [45] J.A. Warren, W.J. Boettinger. Prediction of dendritic growth and microsegregation patterns in a binary alloy using a phase field method. *Acta. metall. mater.* 43, 689–703, 1995.
- [46] A. A. Wheeler, W. J. Boettinger, G. B. McFadden. Phase field model for isothermal phase transitions in binary alloys. *Phys. Rev. A*, 45(10), 7424–7439, 1992.
- [47] M. F. Wheeler. A priori error estimates for Galerkin approximations to parabolic partial differential equations. *SIAM J. Numer. Anal.*, 14(4), 723–759, 1973.

Zusammenfassung

Diese Arbeit beschäftigt sich mit einem Phasenfeldmodell für binäre Legierungen. Die Phasenfeldmodelle beschreiben Phasenübergänge zwischen flüssig und fest und haben Anwendungen in vielen Bereichen. Das Modell besteht aus Gleichungen für das Phasenfeld φ (auch Ordnungsparameter genannt), die Temperatur T und die Konzentration c einer der Komponenten der Legierung. Die Arbeit enthält sowohl theoretische als auch rechnerische Untersuchungen eines volldiskreten Finite-Elemente Verfahrens für das Modell. Phasenfeldmodelle enthalten einen kleinen Parameter ε , der etwa die Dicke der Grenzfläche zwischen flüssig und fest repräsentiert. Eine Untersuchung des numerischen Verfahrens im Zusammenhang mit dem Parameter ε ist wichtig, weil der Parameter ε sehr klein sein muss um physikalisch realistische Fälle beschreiben zu können. Die Gitter, die in numerischen Verfahren (Finite-Elemente oder Finite-Differenzen) verwendet werden, müssen fein genug für die Darstellung der dünnen Phasengrenze sein. Die Verwendung feiner Gitter ist mit entsprechend höherem Arbeitsaufwand verbunden. Die Abschätzung des numerischen Fehlers von ε ist von großem Interesse.

In der Arbeit wird eine Finite-Elemente-Fehlerabschätzung für das Phasenfeldmodell hergeleitet, mittels derer die Abhängigkeit des Fehlers vom Parameter ε explizit angegeben wird. Die Fehlerkonstanten in der Abschätzung sind Polynome niedriger Ordnung in ε^{-1} . Die Arbeit ist in fünf Kapitel aufgeteilt. Das erste Kapitel enthält eine Einführung in die Modellierung von Phasenübergängen, einen kurzen Überblick über verwandte Publikationen und eine Zusammenfassung dieser Arbeit. Das zweite Kapitel widmet sich der Herleitung eines Phasenfeldmodells für binäre Legierungen. Hier wird auch über eine Anwendung von Phasenfeldmodellen diskutiert, die zur Simulation des Dendritenwachstums benutzt wird. Die dazu verwendete Modellgleichung wird mit Hilfe von anisotroper Oberflächenspannung hergeleitet.

Das nächste Kapitel (Kapitel 3) wurde in fünf Abschnitte aufgeteilt die zusammen zu einer Finite-Elemente-Fehlerabschätzung führen. Zuerst wurden einige bekannte Definitionen und Eigenschaften von wichtigen Funktionenräumen angegeben. Der erste Abschnitt enthält auch einige Einbettungs- und Interpolationssätze und einen Regularitätssatz aus der Theorie der lin-

earen parabolischen Gleichungen. Im nächsten Abschnitt werden einige Energieabschätzungen in verschiedenen Normen für die Lösung des Differentialgleichungssystems durchgeführt. Der darauffolgende Abschnitt enthält eine Spektralabschätzung für den sogenannten Allen-Cahn Operator, der in der Fehleranalyse eine wichtige Rolle spielt. Es folgt eine Stabilitätsabschätzung für das volldiskrete numerische Verfahren zur Lösung des Phasenfeldsystems. Es wird auch ein diskretes Analogon für die Spektralabschätzung hergeleitet. Mit Hilfe der obigen Vorbereitungen wird die eigentliche Finite-Elemente-Fehlerabschätzung im Abschnitt 3.5 vervollständigt. Im Kapitel 4 wird der Fehler des Lösungsverfahrens im Zusammenhang mit dem Parameter ε numerisch untersucht. Es wird die Methode der kleinsten Fehlerquadrate verwendet zur Identifizierung der Parameter des Fehlerfunktional. Hier werden Ergebnisse verschiedener Experimente in zwei und drei Raumdimensionen präsentiert. Die numerischen Experimente bestätigen die vorhergesagte Fehlerabhängigkeit vom Parameter ε . Im letzten Kapitel betrachten wir die Anwendung des Phasenfeldsystems zur Simulation des Dendritenwachstums. Das verwendete numerische Verfahren und einige Aspekte der Implementierung werden diskutiert. Die Ergebnisse der numerischen Simulationen mit verschiedenen Unterkühlungstemperaturen der Flüssigkeit und verschiedenen Stärken der Anisotropie werden verglichen. Wir verwenden adaptive Gitter zur Simulation des Dendritenwachstums. Im Anhang A.1 werden formale asymptotische Reihenentwicklungen der Lösung des Phasenfeldsystems in der Nähe der flüssig-fest Grenze betrachtet. Der Anhang dient als Hilfsmittel für Abschnitt 3.3.

Lebenslauf

Persönliche Daten:

Baasansuren Jadamba
geboren am 18.08.1971 in Bulgan, Mongolei

Bildungsweg:

Sep. 1978 – Juni 1988

Schule in Bulgan, Mongolei

Sep. 1988 – Juli 1993

Studium der Mathematik,
Nationale Universität der Mongolei
Abschluss: Mathematikerin und Mathematiklehrerin

Okt. 1997 – März 2000

Studium der Technomathematik,
Universität Kaiserslautern
Abschluß: Dipl.-Math. techn.
Titel der Diplomarbeit: “Numerical Methods for a
nonlinear convection diffusion
equation”

seit Okt. 2000

Promotion am Institut für Angewandte Mathematik
Lehrstuhl I der Friedrich-Alexander Universität
Erlangen-Nürnberg

Berufliche Tätigkeiten:

Sep. 1993 – Juli 1997

Lehrbeauftragte am Fachbereich Mathematik,
Technische Universität der Mongolei

seit Okt. 2000

Wissenschaftliche Mitarbeiterin, Wissenschaftliche
Hilfskraft am Institut für Angewandte Mathematik der
Friedrich-Alexander Universität Erlangen-Nürnberg