

Numerical Analysis of Convex Splitting Schemes for Cahn-Hilliard and Coupled Cahn-Hilliard-Fluid-Flow Equations

A Dissertation Presented for the
Doctor of Philosophy
Degree
The University of Tennessee, Knoxville

Amanda Emily Diegel

May 2015

© by Amanda Emily Diegel, 2015
All Rights Reserved.

I dedicate this dissertation to my parents Charles Kevin Diegel and Anne O'Dell McHargue Diegel. These two people are truly the reason I am the person I am today.

I have often told people “when I think about my education, I think about my parents”. Every memory of learning begins with them. Whether it be reading, writing, arithmetic, or life, they were, and still remain my teachers and my inspiration. Love and support don't even begin to capture all they have given me. To my parents...I only hope to work as hard, show as much love, and aspire to be as amazing as you continue to be every day.

Acknowledgements

I would like to thank my adviser Dr. Steven Wise for his guidance over the last six years and for providing the opportunity to work on truly interesting problems. I would also like to thank him for allowing me to develop mathematically in a way true to myself. I could not have asked for a more suited adviser. A much overdue thank you goes out to my good friend Pam Armentrout for all the invaluable support and advice she has given me over the last six years. To my Aunt Katie and brother and sister-in-law, Alex and Denise, thank you for your support, understanding, and patience during this process. Finally, although a ‘thank you’ doesn’t seem enough, I would like to thank my lifelong friend Amanda Mohny who not only cooked me countless dinners but spent hours listening, empathizing, and finding ways to brighten my days. You are a special person and I’m not sure I could have done this without you.

Abstract

This dissertation investigates numerical schemes for the Cahn-Hilliard equation and the Cahn-Hilliard equation coupled with a Darcy-Stokes flow. Considered independently, the Cahn-Hilliard equation is a model for spinodal decomposition and domain coarsening. When coupled with a Darcy-Stokes flow, the resulting system describes the flow of a very viscous block copolymer fluid. Challenges in creating numerical schemes for these equations arise due to the nonlinear nature and high derivative order of the Cahn-Hilliard equation. Further challenges arise during the coupling process as the coupling terms tend to be nonlinear as well. The numerical schemes presented herein preserve the energy dissipative structure of the Cahn-Hilliard equation while maintaining unique solvability and optimal error bounds.

Specifically, we devise and analyze two mixed finite element schemes: a first order in time numerical scheme for a modified Cahn-Hilliard equation coupled with a non-steady Darcy-Stokes flow and a second order in time numerical scheme for the Cahn-Hilliard equation in two and three dimensions. The time discretizations are based on a convex splitting of the energy of the systems. We prove that our schemes are unconditionally energy stable with respect to a spatially discrete analogue of the continuous free energies and unconditionally uniquely solvable. For each system, we prove that the discrete phase variable is essentially bounded in both time and space with respect to the Lebesgue integral and the discrete chemical potential is Lebesgue square integrable in space and essentially bounded in time. We show these bounds are completely independent of the time and space step sizes in two and three

dimensions. We subsequently prove that these variables converge with optimal rates in the appropriate energy norms. The analyses included in this dissertation will provide a bridge to the development of stable, efficient, and optimally convergent numerical schemes for more robust and descriptive coupled Cahn-Hilliard-Fluid-Flow systems.

Table of Contents

1	Introduction	1
1.1	Summary of this Dissertation	8
2	Mathematical Preliminaries	10
2.1	Notation	10
2.2	Definitions, Lemmas, and Theorems	13
3	The Numerical Analysis of a First-Order Convex Splitting Scheme for the Cahn-Hilliard-Darcy-Stokes System	25
3.1	A Weak Formulation of the Cahn-Hilliard-Darcy-Stokes System . . .	26
3.2	The State-of-the-Art on Numerical Schemes for Coupled Cahn-Hilliard- Fluid-Flow Equations	28
3.3	A Mixed Finite Element Convex Splitting Scheme	30
3.3.1	Definition of the Scheme	30
3.3.2	Unconditional Solvability	33
3.3.3	Unconditional Energy Stability	39
3.4	Error Estimates for the Fully Discrete Convex Splitting Scheme . . .	48
3.5	Numerical Experiments	63
4	The Numerical Analysis of a Second-Order Convex Splitting Scheme for the Cahn-Hilliard Equation	66

4.1	A Weak Formulation of the Cahn-Hilliard Equation	67
4.2	The State-of-the-Art on Second-Order Numerical Schemes for the Cahn-Hilliard Equation	68
4.3	A Mixed Finite Element Splitting Scheme	70
4.3.1	Definition of the Scheme	70
4.3.2	Unconditional Energy Stability	71
4.4	Error Estimates for the Fully Discrete Convex Splitting Scheme . . .	88
4.5	Numerical Experiments	107
5	Future Directions	110
5.1	Global-in-Time Estimates	110
5.2	The Cahn-Hilliard-Navier-Stokes Equations	111
5.3	Variable Parameters and Mobilities	113
5.4	Fast Solvers	114
	Bibliography	115
	Vita	124

List of Tables

- 3.1 H^1 Cauchy convergence test. The final time is $T = 4.0 \times 10^{-1}$, and the refinement path is taken to be $\tau = .001\sqrt{2}h$. The other parameters are $\varepsilon = 6.25 \times 10^{-2}$; $\Omega = (0, 1)^2$. The Cauchy difference is defined via $\delta_\phi := \phi_{h_f} - \phi_{h_c}$, where the approximations are evaluated at time $t = T$, and analogously for δ_μ , and δ_p . Since $q = 1$, *i.e.*, we use $\mathcal{P}_1$ elements for these variables, the norm of the Cauchy difference at T is expected to be $\mathcal{O}(\tau_f) + \mathcal{O}(h_f) = \mathcal{O}(h_f)$ 65
- 4.1 H^1 Cauchy convergence test. The final time is $T = 4.0 \times 10^{-1}$, and the refinement path is taken to be $\tau = .001\sqrt{2}h$ with $\varepsilon = 6.25 \times 10^{-2}$. The Cauchy difference is defined via $\delta_\phi := \phi_{h_f} - \phi_{h_c}$, where the approximations are evaluated at time $t = T$, and analogously for δ_μ . Since $q = 2$, *i.e.*, we use $\mathcal{P}_2$ elements for these variables, the norm of the Cauchy difference at T is expected to be $\mathcal{O}(\tau_f^2) + \mathcal{O}(h_f^2) = \mathcal{O}(h_f^2)$. 109

List of Figures

1.1	[61] Simulation snapshots of phase separation by which two fluids decompose.	2
1.2	Demonstration of the bistable property exhibited by the Cahn-Hilliard energy. Energy density is measured along the y-axis and the phase parameter is measured along the x-axis.	3
1.3	(a) A 2D dumbbell-shaped droplet described by a diffuse interface in a time snapshot from a Cahn-Hilliard simulation. Where $\phi \approx +1$ (resp., -1), we have fluid phase A (resp., B). (b) As ε is decreased, the diffuse interface describing a hypothetical 1D particle becomes thinner. The limit as $\varepsilon \rightarrow 0$ is a characteristic function, which represents the “sharp” interface profile.	4

1.4	[13] Phase separation of a two-dimensional (very viscous) block-copolymer fluid in shear flow. The parameters are $\Omega = (0, 8) \times (0, 4)$, $\epsilon = 0.02$, $\gamma = 0.4$, $\theta = 15000$, $\omega = 0$, $\eta = 0$, $\bar{\phi}_0 = -0.1$. The shear velocity on the top and bottom is ∓ 2.0 , respectively. Periodic boundary conditions are assumed in the x -direction. The time unit referenced above is $\tau = 0.02$. The long-range θ term suppresses phase separation and coarsening, relative to the case $\theta = 0$, and relatively long and thin phase domains emerge. Note that $\phi_{\min} \approx -0.75$ and $\phi_{\max} \approx 0.75$. These simulation results are comparable to other studies [66, 67] that use a different dynamic density functional approach. With a slightly larger value of θ , the phase domains remain as dots and can form into hexagonal patterns, as in [67].	6
3.1	Energy dissipation for the first order numerical scheme for the Cahn-Hilliard-Darcy-Stokes problem. All parameters are as listed in Table 3.1 and we have taken $h = \frac{\sqrt{2}}{64}$	65
4.1	Energy dissipation for the second order numerical scheme for the Cahn-Hilliard problem. All parameters are as listed in Table 4.1 and we have taken $h = \frac{\sqrt{2}}{32}$	109
4.2	Energy dissipation for the second order numerical scheme for the Cahn-Hilliard problem. If we zoom in on the first four time steps, we are able to see the difference between the modified energy $F(\phi)$ and the Cahn-Hilliard energy $E(\phi)$. All parameters are as listed in Table 4.1 and we have taken $h = \frac{\sqrt{2}}{32}$	109

Chapter 1

Introduction

Consider a binary fluid in a closed container consisting of two distinct atomic or molecular components, oil and water for example. Suppose, for the sake of illustration, that one is colored white (say the A atoms), and the other is colored black (say the B atoms). Further suppose that at high temperatures, the fluid is perfectly and uniformly mixed. The fluid would then appear grey in color, due to the uniform distribution of volume fractions throughout the container. But, when the mixture is suddenly cooled below a certain temperature, the fluid separates into two distinguishable phases with one nearly perfectly white (A -rich phase), and another nearly perfectly black (B -rich phase). Following this, on a very slow timescale, some of the white and black phase regions grow while others shrink, in a process called *coarsening*. The total volumes of the white and black fluid phases must remain essentially constant because the number of white and black atoms (or molecules) in the system is fixed. This phenomenon, depicted in Figure 1.1, is termed *spinodal decomposition* [49], and it occurs in both solid and fluid binary systems. The theory for spinodal decomposition was developed by Cahn and Hilliard [6, 7] as a way to describe certain phase transformations in solid-state alloys during quenching (rapid temperature reduction). The model they derived is known as the Cahn-Hilliard (CH) equation and is defined below.

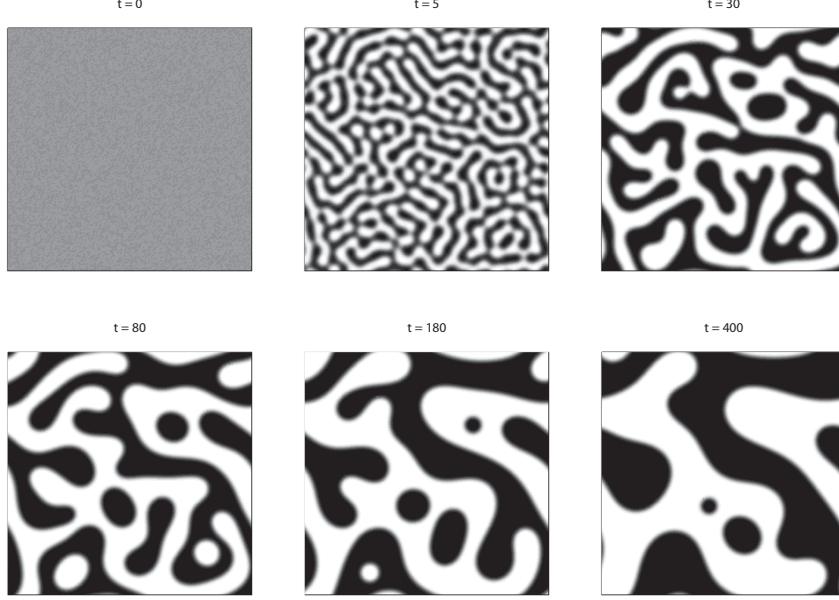


Figure 1.1: [61] Simulation snapshots of phase separation by which two fluids decompose.

Let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, be an open domain and let $\phi : \Omega \rightarrow \mathbb{R}$ indicate the fluid states described above. For a subdomain $\Omega_1 \subseteq \Omega$ which is comprised entirely of A atoms, $\phi(\mathbf{x}) = +1$ for all $\mathbf{x} \in \Omega_1$. Likewise, $\phi(\mathbf{x}) = -1$ for all $\mathbf{x} \in \Omega_2 \subseteq \Omega$ means the subdomain Ω_2 is comprised entirely of B atoms and the state $\phi = 0$ represents a perfect 50-50 mixture of A and B , *et cetera*. Now suppose the fluid has an energy that depends upon ϕ as follows [7]:

$$E(\phi) = \int_{\Omega} \left\{ \frac{1}{\varepsilon} f(\phi) + \frac{\varepsilon}{2} |\nabla \phi|^2 \right\} d\mathbf{x}, \quad f(\phi) = \frac{1}{4} (\phi^2 - 1)^2, \quad (1.1)$$

where ε is a positive constant and f is the homogeneous energy density. The Cahn-Hilliard equation is a bistable (time-dependent) gradient flow with respect to the total energy E [6, 7]:

$$\partial_t \phi = \varepsilon \Delta \mu, \quad \text{in } \Omega_T, \quad (1.2a)$$

$$\mu := \delta_{\phi} E = \varepsilon^{-1} (\phi^3 - \phi) - \varepsilon \Delta \phi, \quad \text{in } \Omega_T, \quad (1.2b)$$

$$\partial_n \phi = \partial_n \mu = 0, \quad \text{on } \partial\Omega \times (0, T), \quad (1.2c)$$

where μ is the chemical potential, $\delta_\phi E$ denotes the variational derivative of E with respect to ϕ , and the total energy E represents a competition between f , which is minimized by the spatially uniform states $\phi = \pm 1$, and the gradient energy density, $\frac{\varepsilon}{2}|\nabla\phi|^2$, which penalizes any derivatives of ϕ , allowing interfacial energy to be modeled. By bistable, we mean that the energy is composed of a convex piece and a concave piece. (See Figure 1.2). The boundary conditions represent local thermodynamic equilibrium ($\partial_n\phi = 0$) and no-mass-flux ($\partial_n\mu = 0$). The equation is mass conservative, $d_t \int_\Omega \phi(\mathbf{x}, t) d\mathbf{x} = 0$ – which reflects the fact that the total numbers of the components remain fixed – and energy dissipative, $d_t E = -\epsilon \|\nabla\mu\|_{L^2}^2 \leq 0$.

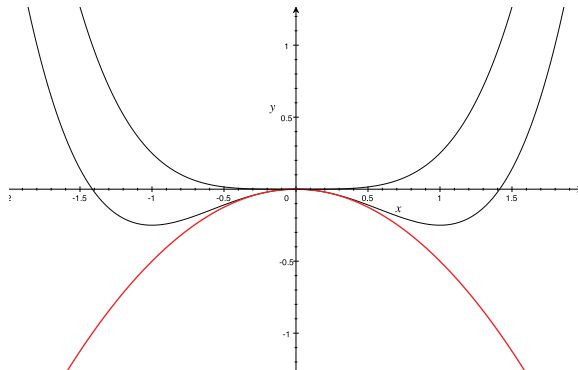


Figure 1.2: Demonstration of the bistable property exhibited by the Cahn-Hilliard energy. Energy density is measured along the y-axis and the phase parameter is measured along the x-axis.

At later times, *i.e.*, in the coarsening regime mentioned above, solutions of the *CH* equation have the following diffuse interface structure (see Figure 1.3): pure phase *A* regions are separated from pure phase *B* regions by diffuse interfaces of thicknesses $\sim \varepsilon$, such that the indicator function is essentially a hyperbolic tangent in the direction perpendicular to the interface. Indeed, for a hypothetical one-dimensional system, non-trivial energy minimizers of E are (essentially) given as $\phi(x) = \pm \tanh\left(\frac{(x-x_0)}{(\sqrt{2\varepsilon})}\right)$, which represents a “diffuse” interface between fluids *A* (+1) and *B* (−1) of thickness $\mathcal{O}(\varepsilon)$. This concept, where a material interface is described by the continuous variation of an indicator function, precedes the work of Cahn and Hilliard, dating back to van der Waals and Lord Rayleigh [53, 54, 60] and is commonly referred to as diffuse interface theory.

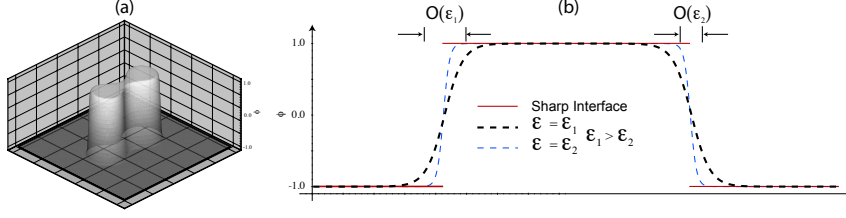


Figure 1.3: (a) A 2D dumbbell-shaped droplet described by a diffuse interface in a time snapshot from a Cahn-Hilliard simulation. Where $\phi \approx +1$ (resp., -1), we have fluid phase A (resp., B). (b) As ε is decreased, the diffuse interface describing a hypothetical 1D particle becomes thinner. The limit as $\varepsilon \rightarrow 0$ is a characteristic function, which represents the “sharp” interface profile.

Besides describing the process of spinodal decomposition, the Cahn-Hilliard equation is commonly paired with other models – generally through nonlinear coupling terms – that describe important multi-phase, multi-physics processes. Prominent examples of these multi-physics models include the Cahn-Hilliard-Navier-Stokes equation, describing two-phase flow [1, 21, 29, 30, 40, 41, 46, 48, 56], the Cahn-Hilliard-Hele-Shaw equation [44, 45, 62] which describes spinodal decomposition of a binary fluid in a Hele-Shaw cell, and the Cahn-Larché equation [25, 28, 42, 64] describing solid-state, binary phase transformations involving coherent, linear-elastic misfit. The role the Cahn-Hilliard equation plays in the pairing is to provide a diffuse interface-type description of the boundary separating the phases. The advantage is that explicit tracking of the motion of interfaces in the system is not required as the motion is captured by the indicator function. It is important to note that as the interfacial width parameter, ε , goes to zero, the diffuse interface profile approaches a sharp interface profile as demonstrated in Figure 1.3. Chapter 3 of this dissertation will focus on the pairing of a modified Cahn-Hilliard equation with a Darcy-Stokes equation which can be used to describe the flow of a very viscous block copolymer fluid [11, 10, 51, 52, 66, 67]. The Cahn-Hilliard equation is modified by adding a “growth” term shown here in the definition of the chemical potential:

$$\partial_t \phi = \varepsilon \Delta \mu, \quad \mu := \delta_\phi E = \frac{1}{\varepsilon} (\phi^3 - \phi) - \varepsilon \Delta \phi - \theta \Delta^{-1} (\phi - \bar{\phi}_0), \quad \partial_n \phi = \partial_n \mu = 0, \quad (1.3)$$

where Δ^{-1} is the inverse laplacian operator relative to the natural boundary conditions and $\bar{\phi}_0 = \frac{1}{|\Omega|} \int_{\Omega} \phi_0(\mathbf{x}) d\mathbf{x}$. Hence, the modified Cahn-Hilliard-Darcy-Stokes problem with natural and no-flux/no-flow boundary conditions may be written as:

$$\partial_t \phi = \varepsilon \Delta \mu - \nabla \cdot (\mathbf{u} \phi) \quad \text{in } \Omega_T, \quad (1.4a)$$

$$\mu = \varepsilon^{-1} (\phi^3 - \phi) - \varepsilon \Delta \phi + \xi \quad \text{in } \Omega_T, \quad (1.4b)$$

$$-\Delta \xi = \theta (\phi - \bar{\phi}_0) \quad \text{in } \Omega_T, \quad (1.4c)$$

$$\omega \partial_t \mathbf{u} - \lambda \Delta \mathbf{u} + \eta \mathbf{u} + \nabla p = \gamma \mu \nabla \phi \quad \text{in } \Omega_T, \quad (1.4d)$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega_T, \quad (1.4e)$$

$$\partial_n \phi = \partial_n \mu = \partial_n \xi = 0, \quad \mathbf{u} = \mathbf{0} \quad \text{on } \partial\Omega \times (0, T). \quad (1.4f)$$

Here ϕ represents the polymer concentration, $\bar{\phi}_0$ is the initial mass average over the domain Ω , and $\mathbf{u}$ and p represent the fluid velocity and pressure, respectively. We assume that the dimensionless model parameters satisfy $\varepsilon, \gamma, \lambda > 0$ and $\eta, \omega, \theta \geq 0$. The parameters are understood such that, ε is the interfacial thickness, λ is the fluid viscosity, η is the Darcy drag parameter, and γ is a surface tension. Furthermore, the term ξ represents a non-local interaction that can suppress or enhance separation according to the sign of θ which represents the non-local interaction strength. The multi-physics coupling terms, $\gamma \mu \nabla \phi$ in the flow equation and $\nabla \cdot (\mathbf{u} \phi)$ in the diffusion equation, essentially represent the surface tension-flow interaction. The parameter ω is used to indicate whether or not the flow may be taken as steady and takes on only the values $\omega = 0$ for steady flow and $\omega = 1$ for non-steady flow. We remark that it is possible to replace the right-hand-side of Equation (1.4d), the excess forcing due to surface tension, by the term $-\gamma \phi \nabla \mu$. The equivalence of the resulting PDE model with that above can be seen by redefining the pressure appropriately.

For the coupled system we consider an energy which is closely related to (1.1):

$$E(\mathbf{u}, \phi) = \int_{\Omega} \left\{ \frac{\omega}{2\gamma} |\mathbf{u}|^2 + \frac{1}{\varepsilon} (\phi^2 - 1)^2 + \frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{\theta}{2} \left| \nabla (\Delta^{-1}(\phi - \bar{\phi}_0)) \right|^2 \right\} d\mathbf{x}. \quad (1.5)$$

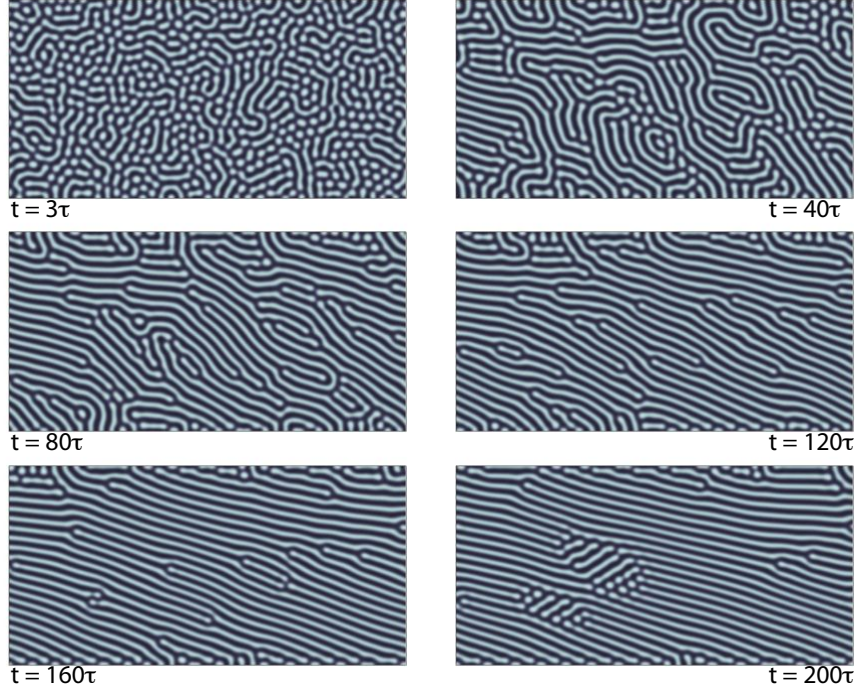


Figure 1.4: [13] Phase separation of a two-dimensional (very viscous) block-copolymer fluid in shear flow. The parameters are $\Omega = (0, 8) \times (0, 4)$, $\epsilon = 0.02$, $\gamma = 0.4$, $\theta = 15000$, $\omega = 0$, $\eta = 0$, $\bar{\phi}_0 = -0.1$. The shear velocity on the top and bottom is ∓ 2.0 , respectively. Periodic boundary conditions are assumed in the x -direction. The time unit referenced above is $\tau = 0.02$. The long-range θ term suppresses phase separation and coarsening, relative to the case $\theta = 0$, and relatively long and thin phase domains emerge. Note that $\phi_{\min} \approx -0.75$ and $\phi_{\max} \approx 0.75$. These simulation results are comparable to other studies [66, 67] that use a different dynamic density functional approach. With a slightly larger value of θ , the phase domains remain as dots and can form into hexagonal patterns, as in [67].

As with (1.1), this energy typically “prefers” the fluid phase states $\phi \approx \pm 1$ (the pure phases) separated by a diffuse interface of (small) thickness ϵ . However, the long-range energy described by the last term can change this picture [3, 10, 11, 51]. Specifically, when $\theta > 0$, the energy term $\frac{\theta}{2} \|\nabla (\Delta^{-1}(\phi - \bar{\phi}_0))\|_{L^2}^2$ in (1.5) is convex and stabilizing, and this energy tends to stabilize (or suppress) both the phase separation and the coarsening processes. This is observed in Figure 1.4 where we show simulation snapshots using the equations to describe the phase separation of a block-copolymer in shear flow. The parameters are given in the caption. If $\theta < 0$ the term is concave and destabilizing. In this case, the process of phase separation will be enhanced. Throughout this dissertation we assume that $\theta \geq 0$.

Due to the extensive use of the Cahn-Hilliard equation in multi-physics modeling, there is a need to develop stable, efficient, and convergent numerical schemes for the equation. This is a challenge because the Cahn-Hilliard equation is highly nonlinear and of high (derivative) order. For instance, defining τ and h to be the time and space steps sizes, respectively, if naive explicit time stepping strategies are used, a restrictive stability constraint of the order $\tau \leq Ch^4$ (CFL condition) must be enforced [59]. The goal in creating numerical schemes for the Cahn-Hilliard equation and equations such as the modified Cahn-Hilliard-Darcy-Stokes equation is to preserve the energy dissipative structure of the equations at the time-discrete level. As an added benefit, one would also hope that the schemes are uniquely solvable, given any time step size. The first property is called *unconditional* energy stability and the second is *unconditional* unique solvability. It is also important, if possible, to prove that one's method is convergent, with optimal error bounds.

The numerical schemes presented in this dissertation utilize an energy splitting approach similar to the convex splitting technique popularized by Eyre [20]. The standard convex splitting technique of Eyre is first-order accurate in time and uses the fact that the energy (1.1) may be represented as the difference between two purely convex energies:

$$E(\phi) = E_c(\phi) - E_e(\phi), \quad E_c(\phi) = \frac{1}{4\varepsilon} \|\phi\|_{L^4}^4 + \frac{\varepsilon}{2} \|\nabla \phi\|_{L^2}^2 + \frac{|\Omega|}{4\varepsilon}, \quad E_e(\phi) = \frac{1}{2\varepsilon} \|\phi\|_{L^2}^2. \quad (1.6)$$

The principal idea is to treat the variation of E_c implicitly and that of E_e , explicitly. The concept can be extended to coupled systems such as the modified Cahn-Hilliard-Darcy-Stokes as will be demonstrated in Chapter 3, and with slight modification, to second-order accuracy in time, as was shown originally in [37] and as will be exhibited in Chapter 4. The main advantages of the convex splitting approach are that the resulting schemes are unconditionally energy stable and unconditionally uniquely solvable. An added advantage is that optimal-order error estimates are often obtainable in this framework with fewer time and space step parameter constraints.

Furthermore, the numerical schemes presented in Chapters 3 and 4 retain the mass conservation properties and dissipative structure observed in the both the Cahn-Hilliard equation and the Cahn-Hilliard-Darcy-Stokes system.

1.1 Summary of this Dissertation

The importance of the work presented by this dissertation is reflected in the growing popularity in the use of diffuse interface models in multi-physics applications. As such, there is a need to develop stable, efficient, and convergent numerical schemes for the Cahn-Hilliard equation and couple Cahn-Hilliard-fluid-flow systems and extensive research has been conducted in this area, in particular for first order (in time) schemes, see [3, 8, 16, 17, 18, 21, 23, 26, 34, 31, 39, 40, 41, 62] and the references therein. The analyses presented on numerical schemes for coupled Cahn-Hilliard-fluid-flow systems focus on two types of limited convergence results: (i) error estimates and convergence rates for the semi-discrete setting (time continuous) and/or (ii) abstract convergence results with no convergence rates. *Optimal error estimates in the energy norms for the fully discrete schemes of coupled Cahn-Hilliard-fluid-flow systems are lacking in the literature.* Furthermore, second order (in time) schemes are less commonly investigated due to the additional challenges these schemes present. However, we do note the recent works [4, 8, 14, 15, 26, 57, 55, 65].

The work presented in this dissertation is unique in the following sense. We are able to prove unconditional unique solvability, unconditional energy stability, and optimal error estimates for both a first order (in time) fully discrete finite element scheme in three dimensions for a modified Cahn-Hilliard-Darcy-Stokes system and a second order (in time) fully discrete finite element scheme in three dimensions for the Cahn-Hilliard equation. Specifically, the stability and solvability statements we prove are *completely unconditional with respect to the time and space step sizes*. In fact, all of our *a priori* stability estimates hold completely independently of the time and space step sizes. We use a bootstrapping technique to leverage the energy stabilities

to achieve unconditional $L^\infty(0, T; L^\infty(\Omega))$ stability for the phase field variable ϕ_h and unconditional $L^\infty(0, T; L^2(\Omega))$ stability for the chemical potential μ_h . Obtaining these stabilities unlocks a convergence analysis where we are able to prove optimal error estimates for the phase field variable ϕ_h and chemical potential μ_h in the appropriate energy norms.

The remainder of this dissertation proceeds as follows. In Chapter 2, we define our notation and introduce several useful definitions, lemmas, and theorems. In Chapter 3, we provide solvability, stability, and error analyses for a first order mixed finite element scheme for the modified Cahn-Hilliard-Darcy-Stokes system (1.4a)–(1.4f). The chapter begins with a weak formulation of the system to be analyzed and presents the state-of-the art on numerical schemes for coupled Cahn-Hilliard fluid flow problems. We then introduce the mixed finite element scheme. Once the scheme is defined, a detailed analysis for unique solvability and unconditional stability is presented. The chapter continues with an error analysis which demonstrates that the mixed finite element scheme converges optimally in the appropriate energy norm with certain regularity assumptions on weak solutions of the Cahn-Hilliard-Darcy-Stokes equation (1.4a)–(1.4f). To conclude the chapter, we show the results of some numerical experiments which confirm the results of the analyses presented. Chapter 4 mimics the structure of Chapter 3 for the second-order-accurate-in-time, fully discrete, mixed finite element scheme for the Cahn-Hilliard problem (1.2a)–(1.2c). Finally, in Chapter 5 we present plans for future research.

Chapter 2

Mathematical Preliminaries

This dissertation employs standard and non-standard mathematical notation. That notation which will be used frequently throughout the dissertation is defined here.

2.1 Notation

Let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, be an open polygonal or polyhedral domain and assume this to be true for the remainder of the dissertation. We use the standard notation for Lebesgue measurable functions, $L^p(\Omega) := \{u : \|u\|_{L^p} < \infty\}$ where

$$\|u\|_{L^p} := \left(\int_{\Omega} |u(x)|^p dx \right)^{\frac{1}{p}} \text{ for } 1 \leq p < \infty \quad \text{and} \quad \|u\|_{L^\infty} := \text{ess sup} \{|u(x)| : x \in \Omega\}.$$

The notation $(\cdot, \cdot)$ will be used to denote the standard L^2 -inner product defined for all $u, v \in L^2(\Omega)$ as

$$(u, v) := \int_{\Omega} uv \, dx.$$

Additionally, this dissertation employs the frequent use of three non-standard inner products prefaced by a , b , and c :

$$a(u, v) := (\nabla u, \nabla v), \quad b(\psi, \mathbf{v}, \nu) := (\nabla \psi \cdot \mathbf{v}, \nu), \quad \text{and } c(\mathbf{v}, q) := (\nabla \cdot \mathbf{v}, q). \quad (2.1)$$

A bold-faced font is used to denote a vector or vector valued function, $\mathbf{v} \in \mathbb{R}^n$. The symbol $\nabla \psi$ is standard notation representing the gradient of the function ψ and $\nabla \cdot \psi$ is standard notation representing the divergence of the function ψ .

Using the notion of a weak derivative, the Sobolev space, $W^{k,p}$, defined as

$$W^{k,p} := \{u : D^\alpha u \in L^p(\Omega), \forall 0 \leq |\alpha| \leq k\},$$

has norm

$$\|u\|_{W^{k,p}} = \left\{ \sum_{0 \leq |\alpha| \leq k} \|D^\alpha u\|_{L^p}^p \right\}^{\frac{1}{p}},$$

for any non-negative integer k . We furthermore adopt the notations $H^k = W^{k,2}$, H_0^1 for H^1 functions which are zero on the boundary, $\partial\Omega$, and $\mathbf{H}_0^1(\Omega) := [H_0^1(\Omega)]^d$ as the vector valued space with dimension d of H^1 functions which are zero on $\partial\Omega$. We define a non-standard notation $H^{-1}(\Omega) := (H^1(\Omega))^*$ to represent the dual space of $H^1(\Omega)$ and $\mathbf{H}^{-1}(\Omega) := (\mathbf{H}_0^1(\Omega))^*$ to represent the dual space of $\mathbf{H}_0^1(\Omega)$. A duality pairing between $H^{-1}(\Omega)$ and $H^1(\Omega)$ in the first instance and a duality pairing between $\mathbf{H}^{-1}(\Omega)$ and $(\mathbf{H}_0^1(\Omega))^*$ in the second is denoted by $\langle \cdot, \cdot \rangle$. Additional spaces which

will be used throughout this dissertation are defined as follows:

$$H_N^2(\Omega) := \{v \in H^2(\Omega) \mid \partial_n v = 0 \text{ on } \partial\Omega\}; \quad (2.2)$$

$$L_0^2(\Omega) := \{v \in L^2(\Omega) \mid (v, 1) = 0\}; \quad (2.3)$$

$$\mathring{H}^1(\Omega) := H^1(\Omega) \cap L_0^2(\Omega); \quad (2.4)$$

$$\mathring{H}^{-1}(\Omega) := \{v \in H^{-1}(\Omega) \mid \langle v, 1 \rangle = 0\}; \quad (2.5)$$

$$\mathbf{V} := \{\mathbf{v} \in \mathbf{H}_0^1(\Omega) \mid (\nabla \cdot \mathbf{v}, q) = 0, \forall q \in L_0^2(\Omega)\}. \quad (2.6)$$

Furthermore, we note that the notation $\Phi(t) := \Phi(\cdot, t) \in X$ views a spatiotemporal function as a map from the time interval $[0, T]$ into an appropriate Banach space, X . Therefore, the Lebesgue space $L^p(0, T; X)$ consists of all those functions $\Phi(t)$ that take values in X for almost every $t \in [0, T]$, such that the $L^p([0, T])$ norm of $\|\Phi(t)\|_X$ is finite.

In order to define the finite element spaces, let M be a positive integer and $0 = t_0 < t_1 < \dots < t_M = T$ be a uniform partition of $[0, T]$, with $\tau = t_i - t_{i-1}$, $i = 1, \dots, M$. Suppose $\mathcal{T}_h = \{K\}$ is a conforming, shape-regular, quasi-uniform family of triangulations of Ω . With r representing a positive integer, we define the sets $\mathcal{M}_r^h$ and $\mathcal{M}_{r,0}^h$ such that $\mathcal{M}_r^h := \{v \in C^0(\Omega) \mid v|_K \in \mathcal{P}_r(K), \forall K \in \mathcal{T}_h\} \subset H^1(\Omega)$ and $\mathcal{M}_{r,0}^h := \mathcal{M}_r^h \cap H_0^1(\Omega)$. Then, for a given positive integer q , we define the following finite element spaces:

$$S_h := \mathcal{M}_q^h; \quad (2.7)$$

$$\mathring{S}_h := S_h \cap L_0^2(\Omega); \quad (2.8)$$

$$\mathbf{X}_h := \left\{ \mathbf{v} \in [C^0(\Omega)]^d \mid v_i \in \mathcal{M}_{q+1,0}^h, i = 1, \dots, d \right\}; \quad (2.9)$$

$$\mathbf{V}_h := \left\{ \mathbf{v} \in \mathbf{X}_h \mid (\nabla \cdot \mathbf{v}, w) = 0, \forall w \in \mathring{S}_h \right\}. \quad (2.10)$$

Note that $\mathbf{V}_h \not\subset \mathbf{V}$, in general.

2.2 Definitions, Lemmas, and Theorems

In this section, we list several definitions, lemmas, and theorems which will be useful throughout this dissertation. Most of the lemmas and theorems listed below are commonly found in mathematical literature and are therefore presented without proof. Those which are not commonly found are either supported with proof or referenced.

Lemma 2.2.1. Young's Inequality: *If $a, b \geq 0$ and $1 < p, q < \infty$ with $\frac{1}{p} + \frac{1}{q} = 1$, then*

$$ab \leq \epsilon a^p + C(\epsilon)b^q, \quad (2.11)$$

where $C(\epsilon) = (\epsilon p)^{-\frac{q}{p}} q^{-1}$.

Lemma 2.2.2. Hölder's Inequality: *Let $1 \leq p, q \leq \infty$ with $\frac{1}{p} + \frac{1}{q} = 1$ and suppose that $f \in L^p(\Omega)$ and $g \in L^q(\Omega)$. Then $fg \in L^1(\Omega)$ with*

$$\int |fg| dx = \|fg\|_{L^1} \leq \|f\|_{L^p} \|g\|_{L^q}. \quad (2.12)$$

Lemma 2.2.3. Poincaré's Inequality: *Suppose $1 \leq p \leq \infty$ and that $\Omega \subset \mathbb{R}^n$ is bounded, connected, and open with a Lipschitz boundary. Then there exists a constant C , depending only on Ω and p , such that for every function u in the Sobolev space $W^{1,p}(\Omega)$,*

$$\|u - \bar{u}\|_{L^p} \leq C \|\nabla u\|_{L^p}, \quad (2.13)$$

where

$$\bar{u} = \frac{1}{|\Omega|} \int_{\Omega} u(x) dx$$

is the average value of u over Ω , with $|\Omega|$ standing for the Lebesgue measure of the domain Ω .

Theorem 2.2.4. Riesz Representation Theorem. *Any continuous linear functional L on a Hilbert space H can be represented uniquely as*

$$L(v) = (u, v) \quad (2.14)$$

for some $u \in H$. Furthermore, we have

$$\|L\|_{H'} = \|u\|_H \quad (2.15)$$

where $\|L\|_{H'} = \sup_{0 \neq v \in H} \frac{|L(v)|}{\|v\|_H}$.

Remark 2.2.5. *It is important to note that the notation $\langle \rho, v \rangle$ may additionally be interpreted as the action of the linear functional ρ on the test function v .*

Definition 2.2.6. The Linear Operator T : *The linear operator $\mathsf{T} : \mathring{H}^{-1}(\Omega) \rightarrow \mathring{H}^1(\Omega)$ is defined via the following variational problem: given $\zeta \in \mathring{H}^{-1}(\Omega)$, find $\mathsf{T}(\zeta) \in \mathring{H}^1(\Omega)$ such that*

$$a(\mathsf{T}(\zeta), \chi) = \langle \zeta, \chi \rangle \quad \forall \chi \in \mathring{H}^1(\Omega). \quad (2.16)$$

Remark 2.2.7. *The operator T is well-defined, as is guaranteed by the Riesz Representation Theorem.*

Lemma 2.2.8. *Let $\zeta, \xi \in \mathring{H}^{-1}(\Omega)$ and, for such functions, set*

$$(\zeta, \xi)_{H^{-1}} := a(\mathsf{T}(\zeta), \mathsf{T}(\xi)) = (\zeta, \mathsf{T}(\xi)) = (\mathsf{T}(\zeta), \xi). \quad (2.17)$$

$(\cdot, \cdot)_{H^{-1}}$ defines an inner product on $\mathring{H}^{-1}(\Omega)$, and the induced norm is equal to the operator norm:

$$\|\zeta\|_{H^{-1}} := \sqrt{(\zeta, \zeta)_{H^{-1}}} = \sup_{0 \neq \chi \in \mathring{H}^1} \frac{|\langle \zeta, \chi \rangle|}{\|\nabla \chi\|_{L^2}}. \quad (2.18)$$

Consequently, for all $\chi \in H^1(\Omega)$ and all $\zeta \in \mathring{H}^{-1}(\Omega)$,

$$|\langle \zeta, \chi \rangle| \leq \|\zeta\|_{H^{-1}} \|\nabla \chi\|_{L^2}. \quad (2.19)$$

Furthermore, for all $\zeta \in L_0^2(\Omega)$, we have the Poincaré type inequality

$$\|\zeta\|_{H^{-1}} \leq C \|\zeta\|_{L^2}, \quad (2.20)$$

where $C > 0$ is the usual Poincaré constant.

Proof. We begin by showing $(\cdot, \cdot)_{H^{-1}}$ defines an inner product on $\mathring{H}^{-1}(\Omega)$. Let $\zeta, \psi, \xi \in \mathring{H}^{-1}(\Omega)$ with $\lambda, \mu \in \mathbb{R}$. By definition (2.17),

$$\begin{aligned} (\lambda\zeta + \mu\psi, \xi)_{H^{-1}} &= (\lambda\zeta + \mu\psi, \mathsf{T}(\xi)) = \lambda(\zeta, \mathsf{T}(\xi)) + \mu(\psi, \mathsf{T}(\xi)) \\ &= \lambda(\zeta, \xi)_{H^{-1}} + \mu(\psi, \xi)_{H^{-1}}, \\ (\zeta, \xi)_{H^{-1}} &= a(\mathsf{T}(\zeta), \mathsf{T}(\xi)) = a(\mathsf{T}(\xi), \mathsf{T}(\zeta)) = (\xi, \zeta)_{H^{-1}}, \\ (\zeta, \zeta)_{H^{-1}} &= a(\mathsf{T}(\zeta), \mathsf{T}(\zeta)) \geq 0 \end{aligned}$$

with equality if and only if $\zeta = 0$. The equivalence of the induced norm and the operator norm follows from the definition of the inner product and the Cauchy Schwartz inequality,

$$\begin{aligned} \sqrt{(\zeta, \zeta)_{H^{-1}}} &= \|\nabla \mathsf{T}(\zeta)\|_{L^2} = \frac{a(\mathsf{T}(\zeta), \mathsf{T}(\zeta))}{\|\nabla \mathsf{T}(\zeta)\|_{L^2}} = \frac{|\langle \zeta, \mathsf{T}(\zeta) \rangle|}{\|\nabla \mathsf{T}(\zeta)\|_{L^2}} \\ &\leq \sup_{0 \neq \chi \in H^1} \frac{|\langle \zeta, \chi \rangle|}{\|\nabla \chi\|_{L^2}} = \sup_{0 \neq \chi \in H^1} \frac{|a(\mathsf{T}(\zeta), \chi)|}{\|\nabla \chi\|_{L^2}} \\ &\leq \sup_{0 \neq \chi \in H^1} \frac{\|\nabla \mathsf{T}(\zeta)\|_{L^2} \|\nabla \chi\|_{L^2}}{\|\nabla \chi\|_{L^2}} = \|\nabla \mathsf{T}(\zeta)\|_{L^2} = \sqrt{(\zeta, \zeta)_{H^{-1}}}. \end{aligned}$$

Inequality (2.19) easily follows from the definition of the operator norm,

$$\|\zeta\|_{H^{-1}} = \sup_{0 \neq \chi \in H^1} \frac{|\langle \zeta, \chi \rangle|}{\|\nabla \chi\|_{L^2}} \geq \frac{|\langle \zeta, \chi \rangle|}{\|\nabla \chi\|_{L^2}}.$$

Finally, we use definitions (2.17) and (2.18) and the Poicarè inequality to obtain

$$\|\zeta\|_{H^{-1}}^2 = (\mathsf{T}(\zeta), \zeta) \leq \|\mathsf{T}(\zeta)\|_{L^2} \|\zeta\|_{L^2} \leq C \|\nabla \mathsf{T}(\zeta)\|_{L^2} \|\zeta\|_{L^2} = C \|\zeta\|_{H^{-1}} \|\zeta\|_{L^2}$$

where $C > 0$ is the usual Poincaré constant. □

Lemma 2.2.9. Elliptic Regularity [5]: *Let Ω be bounded. Then,*

$$\|u\|_{W^{2,p}} \leq \|\Delta u\|_{L^p}, \quad 1 < p < \mu,$$

where μ depends on the smoothness of $\partial\Omega$.

Definition 2.2.10. The Ritz Projection: *The operator $R_h : H^1(\Omega) \rightarrow S_h$ is the referred to as the Ritz projection for the Neumann problem and is defined by:*

$$a(R_h\phi - \phi, \chi) = 0, \quad \forall \chi \in S_h, \quad (2.21)$$

with

$$(R_h\phi - \phi, 1) = 0.$$

Theorem 2.2.11. An Approximation Theorem [5]: *Suppose we have a family of subspaces $S_h \subset H^m(\Omega)$ with the property that, for all $\phi \in H^k(\Omega)$ and $0 < h \leq 1$,*

$$\inf_{\chi \in S_h} \|\phi - \chi\|_{H^m} \leq Ch^{k-m} \|\phi\|_{H^k}. \quad (2.22)$$

and let $s < m$ and $m \leq r \leq k$. Then there is a constant C such that

$$\inf_{\chi \in S_h} (h^s \|\phi - \chi\|_{H^s} + h^m \|\phi - \chi\|_{H^m}) \leq Ch^r \|\phi\|_{H^r}$$

provided $\phi \in H^r(\Omega)$.

Remark 2.2.12. *The construction of the finite element spaces used throughout this dissertation satisfy assumption (2.22) in Theorem 2.2.11.*

Theorem 2.2.13. Ritz Projection Error [5, 59]: *The Ritz Projection for the Neumann problem satisfies the following for any $\phi \in H^q(\Omega)$,*

$$\|\phi - R_h\phi\|_{L^2} + h \|\nabla(\phi - R_h\phi)\|_{L^2} \leq Ch^q \|\phi\|_{H^q}.$$

Proof. We follow the proofs provided in both [5] and [59]. We start with the estimate for the error in the gradient. By the error estimate above,

$$\|\nabla(R_h\phi - \phi)\|_{L^2}^2 \leq \inf_{\chi \in S_h} \|\nabla(\phi - \chi)\|_{L^2}^2 \leq Ch^{q-1} \|\phi\|_{H^q}.$$

For the error bound in the L^2 -norm, we use a duality argument. Let $\xi \in L^2(\Omega)$ be arbitrary and take $\psi \in H^2(\Omega)$ as the solution of

$$-\Delta\psi = \xi \quad \text{in } \Omega, \quad \text{with } \partial_n\psi = 0 \quad \text{on } \partial\Omega.$$

Then for $R_h\psi \in S_h$, we have

$$\begin{aligned} (R_h\phi - \phi, \xi) &= -(R_h\phi - \phi, \Delta\psi) \\ &= (\nabla(R_h\phi - \phi), \nabla\psi) \\ &= (\nabla(R_h\phi - \phi), \nabla(\psi - R_h\psi)) \\ &\leq \|\nabla(R_h\phi - \phi)\|_{L^2} \|\nabla(\psi - R_h\psi)\|_{L^2}, \end{aligned}$$

where we have used the definition of the Ritz projection for the Neumann problem and the Cauchy-Schwarz inequality. Hence, using elliptic regularity and assumption (2.22),

$$(R_h\phi - \phi, \xi) \leq Ch^{q-1} \|\phi\|_{H^q} Ch \|\psi\|_{H^2} \leq Ch^q \|\phi\|_{H^q} \|\Delta\psi\|_{L^2} \leq Ch^q \|\phi\|_{H^q} \|\xi\|_{L^2}.$$

Choose $\xi = R_h\phi - \phi$ to conclude the proof. $\square$

Definition 2.2.14. The Darcy-Stokes Projection: *The operator $(\mathbf{P}_h, P_h) : \mathbf{V} \times L_0^2 \rightarrow \mathbf{V}_h \times \mathring{S}_h$ is referred to as the Darcy-Stokes projection and is defined by:*

$$\lambda a(\mathbf{P}_h\mathbf{u} - \mathbf{u}, \mathbf{v}) + \eta(\mathbf{P}_h\mathbf{u} - \mathbf{u}, \mathbf{v}) - c(\mathbf{v}, P_h p - p) = 0, \quad \forall \mathbf{v} \in \mathbf{X}_h, \quad (2.23)$$

$$c(\mathbf{P}_h\mathbf{u} - \mathbf{u}, q) = 0, \quad \forall q \in \mathring{S}_h. \quad (2.24)$$

Theorem 2.2.15. Darcy-Stokes Projection Error [5]: *The Darcy-Stokes Projection above satisfies*

$$\|\mathbf{P}_h \mathbf{u} - \mathbf{u}\|_{H^1} + \|P_h p - p\|_{L^2} \leq Ch^q (|\mathbf{u}|_{H^{q+1}} + |p|_{H^q}),$$

for any $\mathbf{u} \in H^{q+1}(\Omega)$ and $p \in H^q(\Omega)$.

Definition 2.2.16. The Discrete Laplacian: *We define the discrete Laplacian, $\Delta_h : S_h \rightarrow \mathring{S}_h$, as follows: for any $v_h \in S_h$, $\Delta_h v_h \in \mathring{S}_h$ denotes the unique solution to the problem*

$$(\Delta_h v_h, \chi) = -a(v_h, \chi), \quad \forall \chi \in S_h. \quad (2.25)$$

In particular, setting $\chi = \Delta_h v_h$ in (2.25), we obtain

$$\|\Delta_h v_h\|_{L^2}^2 = -a(v_h, \Delta_h v_h).$$

Theorem 2.2.17. A Local Inverse Inequality [5]: *Let $(K, \mathcal{P}, \mathcal{N})$ be a reference finite element such that $\rho h \leq \text{diam } K \leq h$ and $\mathcal{P}$ is a finite-dimensional subspace of $W^{l,p}(K) \cap W^{m,q}(K)$, where $1 \leq p, q \leq \infty$ and $0 \leq m \leq l$. Then there exists $C = C(\hat{\mathcal{P}}, \hat{K}, l, p, q, \rho)$ such that for all $v \in \mathcal{P}$, we have*

$$\|v\|_{W^{l,p}(K)} \leq Ch^{m-l+n/p-n/q} \|v\|_{W^{m,q}(K)},$$

where $(\hat{K}, \hat{\mathcal{P}}, \hat{\mathcal{N}})$ is the affine-equivalent finite element to the reference finite-element.

Lemma 2.2.18. An Inverse Inequality [5]: *Let $\{\mathcal{T}_h\}$, $0 < h \leq 1$ be a conforming, quasi-uniform triangulation of a polygonal or polyhedral domain $\Omega \subset \mathbf{R}^n$. Let $(K, \mathcal{P}, \mathcal{N})$ be a reference finite element such that $\rho h \leq \text{diam } K \leq h$ and $\mathcal{P}$ is a finite-dimensional subspace of $W^{l,p}(K) \cap W^{m,q}(K)$, where $1 \leq p, q \leq \infty$ and $0 \leq m \leq l$. Then there exists $C = C(l, p, q, \rho)$ such that for all $v \in S_h$, we have*

$$\|v\|_{W^{l,p}(\Omega)} \leq Ch^{m-l+\min(0, n/p-n/q)} \|v\|_{W^{m,q}(\Omega)}.$$

Definition 2.2.19. The Linear Operator T_h : *The invertible linear operator $\mathsf{T}_h : \mathring{S}_h \rightarrow \mathring{S}_h$ is defined via the variational problem: given $\zeta \in \mathring{S}_h$, find $\mathsf{T}_h(\zeta) \in \mathring{S}_h$ such that*

$$a(\mathsf{T}_h(\zeta), \chi) = (\zeta, \chi) \quad \forall \chi \in \mathring{S}_h. \quad (2.26)$$

Remark 2.2.20. *The variational problem used to define the linear operator T_h clearly has a unique solution because $a(\cdot, \cdot)$ is an inner product on $\mathring{S}_h$.*

Lemma 2.2.21. *Let $\zeta, \xi \in \mathring{S}_h$ and set*

$$(\zeta, \xi)_{-1,h} := a(\mathsf{T}_h(\zeta), \mathsf{T}_h(\xi)) = (\zeta, \mathsf{T}_h(\xi)) = (\mathsf{T}_h(\zeta), \xi). \quad (2.27)$$

$(\cdot, \cdot)_{-1,h}$ defines an inner product on $\mathring{S}_h$, and the induced negative norm satisfies

$$\|\zeta\|_{-1,h} := \sqrt{(\zeta, \zeta)_{-1,h}} = \sup_{0 \neq \chi \in \mathring{S}_h} \frac{(\zeta, \chi)}{\|\nabla \chi\|_{L^2}}. \quad (2.28)$$

Consequently, for all $\chi \in S_h$ and all $\zeta \in \mathring{S}_h$,

$$|(\zeta, \chi)| \leq \|\zeta\|_{-1,h} \|\nabla \chi\|_{L^2}. \quad (2.29)$$

The following Poincaré-type estimate holds:

$$\|\zeta\|_{-1,h} \leq C \|\zeta\|_{L^2}, \quad \forall \zeta \in \mathring{S}_h, \quad (2.30)$$

for some $C > 0$ that is independent of h . Finally, if $\mathcal{T}_h$ is globally quasi-uniform, then the following inverse estimate holds:

$$\|\zeta\|_{L^2} \leq Ch^{-1} \|\zeta\|_{-1,h}, \quad \forall \zeta \in \mathring{S}_h, \quad (2.31)$$

for some $C > 0$ that is independent of h .

Proof. The proof follows similarly to Lemma 2.2.8 with the inverse inequality remaining. Set $\chi = \zeta$ in (2.29). Then by the inverse inequality (2.2.18), we have

$$\|\zeta\|_{L^2}^2 \leq \|\zeta\|_{-1,h} \|\nabla \zeta\|_{L^2} \leq Ch^{-1} \|\zeta\|_{-1,h} \|\zeta\|_{L^2}.$$

□

Lemma 2.2.22. *Suppose $g \in H^1(\Omega)$, and $v \in \mathring{S}_h$. Then*

$$|(g, v)| \leq C \|\nabla g\|_{L^2} \|v\|_{-1,h}, \quad (2.32)$$

for some $C > 0$ that is independent of h .

Proof. If $g \in S_h$, we can apply Lemma 2.2.21 directly. Otherwise, using the triangle inequality, the Cauchy-Schwarz inequality, and Lemma 2.2.21,

$$|(g, v)| \leq |(g - R_h g, v)| + |(R_h g, v)| \leq \|g - R_h g\|_{L^2} \|v\|_{L^2} + \|\nabla R_h g\|_{L^2} \|v\|_{-1,h}. \quad (2.33)$$

Using the Ritz projection estimate,

$$\|g - R_h g\|_{L^2} \leq C \|\nabla(g - R_h g)\|_{L^2} \leq Ch \|\nabla g\|_{L^2}, \quad (2.34)$$

we have

$$|(g, v)| \leq Ch \|\nabla g\|_{L^2} \|v\|_{L^2} + \|\nabla R_h g\|_{L^2} \|v\|_{-1,h}. \quad (2.35)$$

Finally, using the (uniform) inverse estimate $h \|v\|_{L^2} \leq C \|v\|_{-1,h}$ from Lemma 2.2.21, and the stability of the elliptic projection, $\|\nabla R_h g\|_{L^2} \leq C \|\nabla g\|_{L^2}$, we have the result. □

Theorem 2.2.23. The Sobolev Embedding Theorem [2]: *Let $\Omega \subset \mathbb{R}^n$ be an n -dimensional bounded Lipschitz domain, let $m \geq 1$ be an integer, and let p be a real number in the range $1 \leq p < \infty$.*

Case 1. If either $mp > n$ or $m = n$ and $p = 1$, then for $n \geq 1$

$$W^{m,p}(\Omega) \hookrightarrow L^q(\Omega) \quad \text{for } p \leq q < \infty.$$

Case 2. If $n \geq 1$ and $mp = n$, then

$$W^{m,p}(\Omega) \hookrightarrow L^q(\Omega) \quad \text{for } p \leq q < \infty.$$

Case 3. If $mp < n$ and either $n - mp \leq n$ or $p = 1$ and $n - m < n$, then

$$W^{m,p}(\Omega) \hookrightarrow L^q(\Omega) \quad \text{for } p \leq q \leq \frac{np}{n - mp}.$$

The embedding constants for the embeddings above depend only on n, m, p, q and the dimensions of the Lipschitz condition on the domain.

Lemma 2.2.24. Gagliardo-Nirenberg Interpolation Inequality [50, 9]: Let $\Omega \subset \mathbf{R}^d$ be a bounded, connected, open set with Lipschitz boundary, $1 \leq q, r \leq \infty$, $\frac{j}{m} \leq \theta \leq 1$ and

$$\frac{1}{p} - \frac{j}{d} = \left(\frac{1}{r} - \frac{m}{d} \right) \theta + \frac{1 - \theta}{q}.$$

Suppose that $u \in L^q\Omega$ with $\partial^\alpha u \in L^r(\Omega)$ for all $|\alpha| = m$. Then $\partial^\beta u \in L^p(\Omega)$ for all $|\beta| = j$, and there exists a constant $C = C(d, j, m, p, q, r, \Omega) > 0$ such that

$$|u|_{W^{j,p}} \leq C \left(|u|_{W^{j,r}}^\theta \|u\|_{L^q}^{1-\theta} + \|u\|_{L^q} \right).$$

Lemma 2.2.25. Discrete Gagliardo-Nirenberg Inequality [9, 63]: Suppose $\mathcal{T}_h$ is a conforming mesh (no hanging nodes) that is globally quasi-uniform and Ω is a convex polygonal domain. For all $u \in S_h$, there is a constant $C > 0$ such that for $d = 2, 3$,

$$\|u_h\|_{L^\infty} \leq C \|\Delta_h u_h\|_{L^2}^{\frac{d}{2(6-d)}} \|u_h\|_{L^6}^{\frac{3(4-d)}{2(6-d)}} + C \|u_h\|_{L^6}, \quad (2.36)$$

where Δ_h is the discrete Laplacian defined in 2.2.16.

Proof. Let $\mathcal{I}_h : H^2(\Omega) \rightarrow S_h$ denote the $C^0(\Omega)$ nodal interpolation operator. From Brenner and Scott [5] for any $u \in H^2(\Omega)$,

$$\|u - \mathcal{I}_h u\|_{L^\infty} \leq Ch^{2-\frac{d}{2}} |u|_{H^2(\Omega)}, \quad (2.37)$$

for some constant $C > 0$. Then, by approximation properties, the inverse inequality 2.2.18, and elliptic regularity, we have

$$\begin{aligned} \|u - u_h\|_{L^6} &\leq \|u_h - \mathcal{I}_h u\|_{L^6} + \|\mathcal{I}_h u - u\|_{L^6} \\ &\leq Ch^{-\frac{d}{3}} \|u_h - \mathcal{I}_h u\|_{L^2} + Ch^{\frac{d}{6}} \|\mathcal{I}_h u - u\|_{L^\infty} \\ &\leq Ch^{-\frac{d}{3}} \|u_h - \mathcal{I}_h u\|_{L^2} + Ch^{2-\frac{d}{3}} |u|_{H^2(\Omega)} \\ &\leq Ch^{-\frac{d}{3}} \|u_h - u\|_{L^2} + Ch^{-\frac{d}{3}} \|u - \mathcal{I}_h u\|_{L^2} + Ch^{2-\frac{d}{3}} |u|_{H^2(\Omega)} \\ &\leq Ch^{2-\frac{d}{3}} |u|_{H^2(\Omega)} \leq Ch^{2-\frac{d}{3}} \|\Delta u\|_{L^2} = Ch^{2-\frac{d}{3}} \|\Delta_h u\|_{L^2}. \end{aligned}$$

Using the triangle inequality,

$$\|u\|_{L^6} \leq \|u_h\|_{L^6} + Ch^{2-\frac{d}{3}} \|\Delta_h u\|_{L^2}. \quad (2.38)$$

Note from [5], we have the inverse inequality

$$\|\nabla u_h\|_{L^2} \leq Ch^{-1+\frac{d}{3}} \|u_h\|_{L^6}. \quad (2.39)$$

Hence, it follows that

$$\|\Delta_h u\|_{L^2} \leq Ch^{-2+\frac{d}{3}} \|u_h\|_{L^6}. \quad (2.40)$$

Now, using the Gagliardo-Nirenberg inequality 2.2.24, elliptic regularity, and repeatedly using inverse inequalities and the approximation properties above,

$$\begin{aligned}
\|u_h\|_{L^\infty} &\leq \|u_h - \mathcal{I}_h u\|_{L^\infty} + \|\mathcal{I}_h u - u\|_{L^\infty} + \|u\|_{L^\infty} \\
&\leq Ch^{-\frac{d}{2}} \|u_h - \mathcal{I}_h u\|_{L^2} + Ch^{2-\frac{d}{2}} \|u\|_{H^2} + \|u\|_{L^\infty} \\
&\leq Ch^{-\frac{d}{2}} \|u_h - u\|_{L^2} + Ch^{-\frac{d}{2}} \|u - \mathcal{I}_h u\|_{L^2} + Ch^{2-\frac{d}{2}} \|\Delta u\|_{L^2} + \|u\|_{L^\infty} \\
&\leq Ch^{2-\frac{d}{2}} \|\Delta u\|_{L^2} + \|u\|_{L^\infty} \\
&\leq Ch^{2-\frac{d}{2}} \|\Delta u\|_{L^2} + \|u\|_{L^6}^{\frac{3(4-d)}{2(6-d)}} \|\Delta u\|_{L^2}^{\frac{d}{2(6-d)}} + C \|u\|_{L^6} \\
&= Ch^{2-\frac{d}{2}} \|\Delta_h u\|_{L^2} + \|u\|_{L^6}^{\frac{3(4-d)}{2(6-d)}} \|\Delta_h u\|_{L^2}^{\frac{d}{2(6-d)}} + C \|u\|_{L^6} \\
&\leq Ch^{2-\frac{d}{2}} \|\Delta_h u\|_{L^2} + C \left(\|u_h\|_{L^6} + Ch^{2-\frac{d}{3}} \|\Delta_h u_h\|_{L^2} \right)^{\frac{3(4-d)}{2(6-d)}} \|\Delta_h u\|_{L^2}^{\frac{d}{2(6-d)}} \\
&\quad + C \|u_h\|_{L^6} + Ch^{2-\frac{d}{3}} \|\Delta_h u_h\|_{L^2} \\
&\leq Ch^{2-\frac{d}{2}} \|\Delta_h u\|_{L^2} + C \left(\|u_h\|_{L^6}^{\frac{3(4-d)}{2(6-d)}} + Ch^{2-\frac{d}{2}} \|\Delta_h u_h\|_{L^2}^{\frac{3(4-d)}{2(6-d)}} \right) \|\Delta_h u\|_{L^2}^{\frac{d}{2(6-d)}} \\
&\quad + C \|u_h\|_{L^6} \\
&\leq Ch^{2-\frac{d}{2}} \|\Delta_h u\|_{L^2} + C \|u_h\|_{L^6}^{\frac{3(4-d)}{2(6-d)}} \|\Delta_h u\|_{L^2}^{\frac{d}{2(6-d)}} + C \|u_h\|_{L^6} \\
&= Ch^{2-\frac{d}{2}} \|\Delta_h u\|_{L^2}^{\frac{3(4-d)}{2(6-d)}} \|\Delta_h u\|_{L^2}^{\frac{d}{2(6-d)}} + C \|u_h\|_{L^6}^{\frac{3(4-d)}{2(6-d)}} \|\Delta_h u\|_{L^2}^{\frac{d}{2(6-d)}} + C \|u_h\|_{L^6} \\
&\leq Ch^{2-\frac{d}{2}} \left(h^{-2+\frac{d}{3}} \|u_h\|_{L^6} \right)^{\frac{3(4-d)}{2(6-d)}} \|\Delta_h u\|_{L^2}^{\frac{d}{2(6-d)}} + C \|u_h\|_{L^6}^{\frac{3(4-d)}{2(6-d)}} \|\Delta_h u\|_{L^2}^{\frac{d}{2(6-d)}} \\
&\quad + C \|u_h\|_{L^6} \\
&\leq C \|u_h\|_{L^6}^{\frac{3(4-d)}{2(6-d)}} \|\Delta_h u\|_{L^2}^{\frac{d}{2(6-d)}} + C \|u_h\|_{L^6} .
\end{aligned}$$

□

Lemma 2.2.26. The Discrete Gronwall Inequality [35, 43]: Fix $T > 0$, and suppose $\{a^m\}_{m=1}^M$, $\{b^m\}_{m=1}^M$ and $\{c^m\}_{m=1}^{M-1}$ are non-negative sequences such that $\tau \sum_{m=1}^{M-1} c^m \leq C_1$, where C_1 is independent of τ and M , and $M\tau = T$. Suppose that, for all $\tau > 0$,

$$a^M + \tau \sum_{m=1}^M b^m \leq C_2 + \tau \sum_{m=1}^{M-1} a^m c^m, \quad (2.41)$$

where $C_2 > 0$ is a constant independent of τ and M . Then, for all $\tau > 0$,

$$a^M + \tau \sum_{m=1}^M b^m \leq C_2 \exp \left(\tau \sum_{m=1}^{M-1} c^m \right) \leq C_2 \exp(C_1). \quad (2.42)$$

Note that the sum on the right-hand-side of (2.41) must be explicit.

Theorem 2.2.27. Taylor's Theorem. If $f \in C^{n+1}([a, b])$, then for any points $x, x_0 \in [a, b]$,

$$f(x) = \sum_{k=0}^n \frac{1}{k!} f^{(k)}(x_0) \cdot (x - x_0)^k + R_n(x), \quad (2.43)$$

where

$$R_n(x) = \frac{1}{n!} \int_{x_0}^x f^{(n+1)}(s) (x - s)^n ds. \quad (2.44)$$

Chapter 3

The Numerical Analysis of a First-Order Convex Splitting Scheme for the Cahn-Hilliard-Darcy-Stokes System

Chapter 3 is devoted to the development and analysis of a first order in time convex splitting numerical scheme for the Cahn-Hilliard-Darcy-Stokes problem. We will begin by setting up a weak formulation of the problem (1.4a) – (1.4f) and presenting the recent developments on numerical schemes related to this problem. We then introduce our new mixed methods numerical scheme and prove that the scheme is uniquely solvable. We furthermore show that the scheme is unconditionally stable and optimally convergent and back up these findings with the results from a few numerical experiments.

3.1 A Weak Formulation of the Cahn-Hilliard-Darcy-Stokes System

A weak formulation of (1.4a) – (1.4f) may be written as follows: find $(\phi, \mu, \xi, \mathbf{u}, p)$ such that

$$\phi \in L^\infty(0, T; H^1(\Omega)) \cap L^4(0, T; L^\infty(\Omega)), \quad (3.1a)$$

$$\partial_t \phi \in L^2(0, T; H^{-1}(\Omega)), \quad (3.1b)$$

$$\mu \in L^2(0, T; H^1(\Omega)), \quad (3.1c)$$

$$\mathbf{u} \in L^2(0, T; \mathbf{H}_0^1(\Omega)) \cap L^\infty(0, T; \mathbf{L}^2(\Omega)), \quad (3.1d)$$

$$\partial_t \mathbf{u} \in L^2(0, T; \mathbf{H}^{-1}(\Omega)), \quad (3.1e)$$

$$p \in L^2(0, T; L_0^2(\Omega)), \quad (3.1f)$$

and there hold for almost all $t \in (0, T)$

$$\langle \partial_t \phi, \nu \rangle + \varepsilon a(\mu, \nu) + b(\phi, \mathbf{u}, \nu) = 0 \quad \forall \nu \in H^1(\Omega), \quad (3.2a)$$

$$(\mu, \psi) - \varepsilon a(\phi, \psi) - \varepsilon^{-1}(\phi^3 - \phi, \psi) - (\xi, \psi) = 0 \quad \forall \psi \in H^1(\Omega), \quad (3.2b)$$

$$a(\xi, \zeta) - \theta(\phi - \bar{\phi}_0, \zeta) = 0 \quad \forall \zeta \in H^1(\Omega), \quad (3.2c)$$

$$\omega \langle \partial_t \mathbf{u}, \mathbf{v} \rangle + \lambda a(\mathbf{u}, \mathbf{v}) + \eta(\mathbf{u}, \mathbf{v}) - c(\mathbf{v}, p) - \gamma b(\phi, \mathbf{v}, \mu) = 0 \quad \forall \mathbf{v} \in \mathbf{H}_0^1(\Omega), \quad (3.2d)$$

$$c(\mathbf{u}, q) = 0 \quad \forall q \in L_0^2(\Omega), \quad (3.2e)$$

with the “compatible” initial data

$$\phi(0) = \phi_0 \in H_N^2(\Omega), \quad \mathbf{u}(0) = \mathbf{u}_0 \in \mathbf{V}. \quad (3.3)$$

The system (3.2a) – (3.2e) is mass conservative: for almost every $t \in [0, T]$, $(\phi(t) - \phi_0, 1) = 0$. This observation rests on the fact that $b(\phi, \mathbf{u}, 1) = 0$, for all $\phi \in L^2(\Omega)$ and all $\mathbf{u} \in \mathbf{V}$. Observe that the homogeneous Neumann boundary

conditions associated with the phase variables ϕ , μ , and ξ are natural in this mixed weak formulation of the problem. The existence of weak solutions is a straightforward exercise using the compactness/energy method. See, for example, [24]. Furthermore, in [9], it was shown that global-in-time strong solutions exist for a Cahn-Hilliard-Stokes equation similar to the problem (1.4a)–(1.4f), with sufficiently smooth initial data.

Now consider the energy

$$\begin{aligned} E(\mathbf{u}, \phi) &= \frac{\omega}{2\gamma} \|\mathbf{u}\|_{L^2}^2 + \frac{1}{4\varepsilon} \|\phi^2 - 1\|_{L^2}^2 + \frac{\varepsilon}{2} \|\nabla \phi\|_{L^2}^2 + \frac{\theta}{2} \|\phi - \bar{\phi}_0\|_{H^{-1}}^2 \\ &= \frac{\omega}{2\gamma} \|\mathbf{u}\|_{L^2}^2 + \frac{1}{4\varepsilon} \|\phi\|_{L^4}^4 - \frac{1}{2\varepsilon} \|\phi\|_{L^2}^2 + \frac{|\Omega|}{4\varepsilon} + \frac{\varepsilon}{2} \|\nabla \phi\|_{L^2}^2 + \frac{\theta}{2} \|\phi - \bar{\phi}_0\|_{H^{-1}}^2, \end{aligned} \quad (3.4)$$

which is defined for all $\mathbf{u} \in \mathbf{L}^2(\Omega)$ and $\phi \in \mathcal{A} := \{\phi \in H^1(\Omega) \mid (\phi - \bar{\phi}_0, 1) = 0\}$. Clearly, if $\theta \geq 0$, then $E(\mathbf{u}, \phi) \geq 0$ for all $\mathbf{u} \in \mathbf{L}^2(\Omega)$ and $\phi \in \mathcal{A}$. For arbitrary $\theta \in \mathbb{R}$, $\varepsilon > 0$, $\mathbf{u} \in \mathbf{L}^2(\Omega)$, and $\phi \in \mathcal{A}$, there exist positive constants $M_1 = M_1(\varepsilon, \theta)$ and $M_2 = M_2(\varepsilon, \theta)$ such that

$$0 < M_1 (\|\mathbf{u}\|_{L^2}^2 + \|\phi\|_{H^1}^2) \leq E(\mathbf{u}, \phi) + M_2. \quad (3.5)$$

It is straightforward to show that weak solutions of (3.2a) – (3.2e) dissipate the energy (3.4). In other words, (1.4a) – (1.4f) is a conserved gradient flow with respect to the energy (3.4). Precisely, for any $t \in [0, T]$, we have the energy law

$$E(\mathbf{u}(t), \phi(t)) + \int_0^t \left(\frac{\lambda}{\gamma} \|\nabla \mathbf{u}(s)\|_{L^2}^2 + \frac{\eta}{\gamma} \|\mathbf{u}(s)\|_{L^2}^2 + \varepsilon \|\nabla \mu(s)\|_{L^2}^2 \right) ds = E(\mathbf{u}_0, \phi_0). \quad (3.6)$$

Formally, one can also easily demonstrate that μ in (1.4b) is the variational derivative of E with respect to ϕ . In symbols, $\mu = \delta_\phi E$. In Section 3.3, we present a numerical scheme which follows a similar energy law making rigorous mathematical proofs for unconditional unique solvability and unconditional energy stability possible.

3.2 The State-of-the-Art on Numerical Schemes for Coupled Cahn-Hilliard-Fluid-Flow Equations

Galerkin numerical methods for the Cahn-Hilliard-Navier-Stokes (*CHNS*) and the Allen-Cahn-Navier-Stokes equations have been investigated in the recent papers [1, 21, 22, 24, 38, 40, 29, 30, 57, 56]. The rigorous analyses of numerical schemes – mostly for the matched-density *CHNS* system – can be found in [21, 22, 24, 38, 40, 29, 57, 56]. Specifically, there have been convergence proofs for these schemes, but all of these analyses focus on two types of limited convergence results: (i) error estimates and convergence rates for the semi-discrete setting (time continuous) [22, 38] and/or (ii) abstract convergence results with no convergence rates [22, 24, 29, 38]. *Optimal error estimates in the energy norms for the fully discrete schemes of CHNS-type systems are lacking in the literature.*

Kay *et al.* develop both a semi-discrete and a fully discrete mixed finite element method for the Cahn-Hilliard-Navier-Stokes system of equations. For the semi-discrete model, they were able to show unconditional stabilities resulting from the discrete energy law. For the fully discrete model, they use a first order implicit-explicit Euler method to discretize time and were able to show conditional energy stability, with a restriction on the time step. They were able to obtain optimal error (convergence) rates for the semi-discrete model, but only an abstract convergence for the fully discrete model. In [29], Grün proves the abstract convergence of a fully discrete finite element scheme for a diffuse interface model for two-phase flow of incompressible, viscous fluids with different mass densities. No convergence rates were presented in his paper. Feng [21] presented a fully discrete mixed finite element method for the Cahn-Hilliard-Navier-Stokes system of equations. The time discretization used is a first order implicit Euler with the exception of a stabilization term which is treated explicitly. Conditional stability for the basic energy law is

developed along with abstract convergence of the finite element model to the PDE model. However, no additional stability estimates are presented beyond the estimates achieved from the energy law. Additionally, Feng *et al.* [22] develop both a semi-discrete and fully discrete finite element method model for the Non-steady-Stokes-Allen-Cahn system of equations. For both the semi-discrete and fully discrete models, conditional energy stability is developed. Optimal error estimates are obtained for the semi-discrete scheme (time-continuous) while abstract convergence is proven for the fully discrete model.

In the case that $\mathbf{u} \equiv 0$ – which occurs if $\gamma = 0$ – the model (1.4a)–(1.4f) reduces to the modified Cahn-Hilliard equation [11, 10] which was analyzed by Aristotelous *et al.* [3]. Their scheme was comprised of a convex splitting method for time discretization and a discontinuous galerkin finite element method for space discretization. They showed that their mixed, fully discrete scheme was unconditionally energy stable, unconditionally uniquely solvable, and optimally convergent in the energy norm in two-dimensions. Finally, Collins *et al.* [12] used a convex splitting method in time and a finite difference method in space to devise an energy stable method for a system similar to (1.2a)–(1.2c), though they did not prove convergence or error estimates.

The work presented in Chapter 3 on the modified Cahn-Hilliard-Darcy-Stokes system is unique in the following sense. We are able to prove unconditional unique solvability, unconditional energy stability, and optimal error estimates for a fully discrete finite element scheme in three dimensions. Specifically, the stability and solvability statements we prove are *completely unconditional with respect to the time and space step sizes*. The phase field parameter ϕ_h is bounded unconditionally (with respect to the time and space step sizes, τ and h) in $L^\infty(0, T; L^\infty(\Omega))$ and the chemical potential μ_h is bounded unconditionally in $L^\infty(0, T; L^2(\Omega))$. With these stabilities in hand we are able to prove optimal error estimates for ϕ_h and μ_h in the appropriate energy norms.

3.3 A Mixed Finite Element Convex Splitting Scheme

3.3.1 Definition of the Scheme

Considering the finite element spaces defined in Chapter 2, our mixed convex splitting scheme is defined as follows: for any $1 \leq m \leq M$, given $\phi_h^{m-1} \in S_h$, $\mathbf{u}_h^{m-1} \in \mathbf{X}_h$, find $\phi_h^m, \mu_h^m \in S_h$, $\xi_h^m, p_h^m \in \dot{S}_h$, and $\mathbf{u}_h^m \in \mathbf{X}_h$, such that

$$(\delta_\tau \phi_h^m, \nu) + \varepsilon a(\mu_h^m, \nu) + b(\phi_h^{m-1}, \mathbf{u}_h^m, \nu) = 0 \quad \forall \nu \in S_h, \quad (3.7a)$$

$$\varepsilon^{-1} ((\phi_h^m)^3 - \phi_h^{m-1}, \psi) + \varepsilon a(\phi_h^m, \psi) - (\mu_h^m, \psi) + (\xi_h^m, \psi) = 0 \quad \forall \psi \in S_h, \quad (3.7b)$$

$$a(\xi_h^m, \zeta) - \theta(\phi_h^m - \bar{\phi}_0, \zeta) = 0 \quad \forall \zeta \in S_h, \quad (3.7c)$$

$$\begin{aligned} (\delta_\tau \mathbf{u}_h^m, \mathbf{v}) + \lambda a(\mathbf{u}_h^m, \mathbf{v}) + \eta(\mathbf{u}_h^m, \mathbf{v}) - c(\mathbf{v}, p_h^m) \\ - \gamma b(\phi_h^{m-1}, \mathbf{v}, \mu_h^m) = 0 \quad \forall \mathbf{v} \in \mathbf{X}_h, \end{aligned} \quad (3.7d)$$

$$c(\mathbf{u}_h^m, q) = 0 \quad \forall q \in \dot{S}_h, \quad (3.7e)$$

where

$$\delta_\tau \phi_h^m := \frac{\phi_h^m - \phi_h^{m-1}}{\tau}, \quad \phi_h^0 := R_h \phi_0, \quad \mathbf{u}_h^0 := \mathbf{P}_h \mathbf{u}_0. \quad (3.8)$$

Remark 3.3.1. To shorten the presentation, we have set $\omega = 1$ (appearing in (1.4d)). With some slight modifications here and there, the singular limit case, $\omega = 0$, can be covered in the analysis that follows. In this setting, one loses the stability $\mathbf{u}_h \in L^\infty(0, T; L^2(\Omega))$, but this is not crucial for us. For perspective, the analysis of Feng et al. [22] requires $\mathbf{u}_h \in L^\infty(0, T; L^2(\Omega))$.

Remark 3.3.2. Note that $(\phi_h^0 - \bar{\phi}_0, 1) = 0$, where $\bar{\phi}_0$ is the initial mass average, which in the typical case, satisfies $|\bar{\phi}_0| \leq 1$. We also point out that, appealing to (3.7a) and (3.7e), we have $(\phi_h^m - \bar{\phi}_0, 1) = 0$, for all $m = 1, \dots, M$, which follows because $a(\mu, 1) = 0$, for all $\mu \in S_h$, and $b(\phi_h, \mathbf{u}, 1) = 0$, for all $\phi \in S_h$ and all $\mathbf{u} \in \mathbf{V}_h$.

Remark 3.3.3. *The elliptic projections are used in the initialization for simplicity in the forthcoming analysis. We can use other (simpler) projections in the initialization step, as long as they have good approximation properties.*

Remark 3.3.4. *Note that it is not necessary for solvability and some basic energy stabilities that the μ -space and the ϕ -space be equal. However, the proofs of the higher-order stability estimates, in particular those in Lemma 3.3.14, do require the equivalence of these spaces. Mass conservation of the scheme requires some compatibility of the p -space with that of the ϕ -space, to obtain $b(\phi_h, \mathbf{u}, 1) = 0$. For the flow problem, we have chosen the inf-sup-stable Taylor-Hood element. One can also use the simpler MINI element. Recall that the stability of the Taylor-Hood element typically requires that the family of meshes $\mathcal{T}_h$ has the property that no tetrahedron/triangle in the mesh has more than one face/edge on the boundary [5].*

In order to prove unique solvability, we define a scheme that is equivalent to (3.7a) - (3.7e) above. For any $1 \leq m \leq M$, given $\varphi_h^{m-1} \in S_h$, $\mathbf{u}_h^{m-1} \in \mathbf{X}_h$, find $\varphi_h^m, \mu_h^m \in S_h$, $\xi_h^m \in \dot{S}_h$, $\mathbf{u}_h^{m,0}, \mathbf{u}_h^{m,1} \in \mathbf{X}_h$, $p_h^{m,0}, p_h^{m,1} \in \dot{S}_h$, such that

$$\lambda a(\mathbf{u}_h^{m,0}, \mathbf{v}) + \left(\eta + \frac{1}{\tau} \right) (\mathbf{u}_h^{m,0}, \mathbf{v}) - c(\mathbf{v}, p_h^{m,0}) - \frac{1}{\tau} (\mathbf{u}_h^{m-1}, \mathbf{v}) = 0 \quad \forall \mathbf{v} \in \mathbf{X}_h, \quad (3.9a)$$

$$c(\mathbf{u}_h^{m,0}, q) = 0 \quad \forall q \in \dot{S}_h, \quad (3.9b)$$

and

$$\left(\frac{\varphi_h^m - \varphi_{h,\star}^{m-1}}{\tau}, \nu \right) + \varepsilon a(\mu_h^m, \nu) + b(\varphi_h^{m-1}, \mathbf{u}_h^{m,1}, \nu) = 0 \quad \forall \nu \in S_h, \quad (3.10a)$$

$$\begin{aligned} \varepsilon^{-1} \left((\varphi_h^m + \bar{\phi}_0)^3 - \varphi_h^{m-1} - \bar{\phi}_0, \psi \right) + \varepsilon a(\varphi_h^m, \psi) \\ - (\mu_h^m, \psi) + (\xi_h^m, \psi) = 0 \quad \forall \psi \in S_h, \end{aligned} \quad (3.10b)$$

$$a(\xi_h^m, \zeta) - \theta(\varphi_h^m, \zeta) = 0 \quad \forall \zeta \in S_h, \quad (3.10c)$$

$$\begin{aligned} \lambda a(\mathbf{u}_h^{m,1}, \mathbf{v}) + \left(\eta + \frac{1}{\tau} \right) (\mathbf{u}_h^{m,1}, \mathbf{v}) - c(\mathbf{v}, p_h^{m,1}) \\ - \gamma b(\varphi_h^{m-1}, \mathbf{v}, \mu_h^m) = 0 \quad \forall \mathbf{v} \in \mathbf{X}_h, \end{aligned} \quad (3.10d)$$

$$c(\mathbf{u}_h^{m,1}, q) = 0 \quad \forall q \in \mathring{S}_h, \quad (3.10e)$$

where

$$\varphi_{h,\star}^{m-1} := \varphi_h^{m-1} - \tau \mathcal{Q}_h(\nabla \varphi_h^{m-1} \cdot \mathbf{u}_h^{m,0}) \in S_h, \quad (3.11)$$

and $\mathcal{Q}_h : L^2(\Omega) \rightarrow S_h$ is the L^2 projection, *i.e.*, $(\mathcal{Q}_h \nu - \nu, \chi) = 0$, for all $\chi \in S_h$. For the initial data, we set

$$\varphi_h^0 := R_h \phi_0 - \bar{\phi}_0, \quad \mathbf{u}_h^0 := \mathbf{P}_h \mathbf{u}_0. \quad (3.12)$$

Hence, $(\varphi_h^0, 1) = 0$. By setting $\nu \equiv 1$ in (3.7a) and (3.10a) and observing that $a(\varphi, 1) = 0$ for all $\varphi \in S_h$, one finds that, provided solutions for the two schemes exist, they are related via

$$\varphi_h^m + \bar{\phi}_0 = \phi_h^m, \quad \varphi_h^m \in \mathring{S}_h, \quad \mathbf{u}_h^m = \mathbf{u}_h^{m,0} + \mathbf{u}_h^{m,1} \in \mathbf{X}_h, \quad p_h^m = p_h^{m,0} + p_h^{m,1} \in \mathring{S}_h \quad (3.13)$$

for all $1 \leq m \leq M$. The variables μ_h^m and ξ_h^m are the same as before. Note that the average mass of μ_h^m will change with the time step m , *i.e.*, $(\mu_h^m, 1) \neq (\mu_h^{m-1}, 1)$, in general.

Remark 3.3.5. *The utility of this new, equivalent formulation is that we can straightforwardly show its unconditional unique solvability by convex optimization methods. Our arguments require that the velocity $\mathbf{u}_h^{m,1}$ is a linear function of μ_h^m , as is the case in (3.10d). (See Lemma 3.3.6.) This was not the case in (3.7d), where $\mathbf{u}_h^m$ is an affine function of μ_h^m .*

3.3.2 Unconditional Solvability

In this subsection, we show that our schemes are unconditionally uniquely solvable. We begin by building some machinery.

Lemma 3.3.6. *Given $\varphi_h^{m-1} \in \mathring{S}_h$ define the bilinear form $\ell_h^m : \mathring{S}_h \times \mathring{S}_h \rightarrow \mathbb{R}$ via*

$$\ell_h^m(\mu, \nu) := \varepsilon a(\mu, \nu) + b(\varphi_h^{m-1}, \mathbf{u}, \nu), \quad (3.14)$$

where, for each fixed $\mu \in \mathring{S}_h$, $\mathbf{u} = \mathbf{u}(\mu) \in \mathbf{X}_h$ and $p = p(\mu) \in \mathring{S}_h$ solve

$$\lambda a(\mathbf{u}, \mathbf{v}) + \left(\eta + \frac{1}{\tau} \right) (\mathbf{u}, \mathbf{v}) - c(\mathbf{v}, p) - \gamma b(\varphi_h^{m-1}, \mathbf{v}, \mu) = 0 \quad \forall \mathbf{v} \in \mathbf{X}_h, \quad (3.15a)$$

$$c(\mathbf{u}, q) = 0 \quad \forall q \in \mathring{S}_h. \quad (3.15b)$$

Then $\ell_h^m(\cdot, \cdot)$ is a coercive, symmetric bilinear form, and therefore, an inner product on $\mathring{S}_h$.

Proof. The solvability and stability of the flow problem follows from the fact that $(\mathbf{X}_h, \mathring{S}_h)$ form a stable pair for the Darcy-Stokes problem. Now, let $\mu_i \in \mathring{S}_h$, $i = 1, 2$. Set $\mathbf{u}_i = \mathbf{u}(\mu_i) \in \mathbf{X}_h$ and $p_i = p(\mu_i) \in \mathring{S}_h$, $i = 1, 2$, with $\mathbf{u}$ and p defined in (3.15a) and (3.15b) above. Then with $\alpha, \beta \in \{1, 2\}$,

$$\lambda a(\mathbf{u}_\alpha, \mathbf{u}_\beta) + \left(\eta + \frac{1}{\tau} \right) (\mathbf{u}_\alpha, \mathbf{u}_\beta) - c(\mathbf{u}_\beta, p_\alpha) - \gamma b(\varphi_h^{m-1}, \mathbf{u}_\beta, \mu_\alpha) = 0, \quad (3.16a)$$

$$c(\mathbf{u}_\beta, p_\alpha) = 0, \quad (3.16b)$$

and setting $\alpha = 2$, $\beta = 1$ in the last two equations, we have

$$\begin{aligned}\ell_h^m(\mu_1, \mu_2) &= \varepsilon a(\mu_1, \mu_2) + b(\varphi_h^{m-1}, \mathbf{u}_1, \mu_2) \\ &= \varepsilon a(\mu_1, \mu_2) + \frac{\lambda}{\gamma} a(\mathbf{u}_2, \mathbf{u}_1) + \frac{\eta + \frac{1}{\tau}}{\gamma} (\mathbf{u}_2, \mathbf{u}_1).\end{aligned}\quad (3.17)$$

It is now clear that $\ell_h^m(\cdot, \cdot)$ is a coercive, symmetric bilinear form on $\mathring{S}_h$. $\square$

Owing to the last result, we can define an invertible linear operator $\mathcal{L}_{h,m} : \mathring{S}_h \rightarrow \mathring{S}_h$ via the following problem: given $\zeta \in \mathring{S}_h$, find $\mu \in \mathring{S}_h$ such that

$$\ell_h^m(\mu, \nu) = -(\zeta, \nu) \quad \forall \nu \in \mathring{S}_h. \quad (3.18)$$

This clearly has a unique solution because $\ell_h^m(\cdot, \cdot)$ is an inner product on $\mathring{S}_h$. We write $\mathcal{L}_{h,m}(\mu) = -\zeta$, or, equivalently, $\mu = -\mathcal{L}_{h,m}^{-1}(\zeta)$.

We now wish to define another discrete negative norm.

Lemma 3.3.7. *Let $\zeta, \xi \in \mathring{S}_h$ and suppose $\mu_\zeta, \mu_\xi \in \mathring{S}_h$ are the unique weak solutions to $\mathcal{L}_{h,m}(\mu_\zeta) = -\zeta$ and $\mathcal{L}_{h,m}(\mu_\xi) = -\xi$. Define*

$$(\zeta, \xi)_{\mathcal{L}_{h,m}^{-1}} := \ell_h^m(\mu_\zeta, \mu_\xi) = -(\zeta, \mu_\xi) = -(\mu_\zeta, \xi). \quad (3.19)$$

$(\cdot, \cdot)_{\mathcal{L}_{h,m}^{-1}}$ defines an inner product on $\mathring{S}_h$. The induced norm is

$$\|\zeta\|_{\mathcal{L}_{h,m}^{-1}} = \sqrt{(\zeta, \zeta)_{\mathcal{L}_{h,m}^{-1}}}, \quad \forall \zeta \in \mathring{S}_h. \quad (3.20)$$

Proof. Let $\zeta, \psi, \xi \in \mathring{S}_h$ with $\alpha, \beta \in \mathbb{R}$. By definition (3.19)

$$\begin{aligned}
(\alpha\zeta + \beta\psi, \xi)_{\mathcal{L}_{h,m}^{-1}} &= -(\alpha\zeta + \beta\psi, \mu_\xi) = -\alpha(\zeta, \mu_\xi) - \beta(\psi, \mu_\xi) \\
&= \alpha(\zeta, \xi)_{\mathcal{L}_{h,m}^{-1}} + \beta(\psi, \xi)_{\mathcal{L}_{h,m}^{-1}}, \\
(\zeta, \xi)_{\mathcal{L}_{h,m}^{-1}} &= \ell_h^m(\mu_\zeta, \mu_\xi) = \ell_h^m(\mu_\xi, \mu_\zeta) = (\xi, \zeta)_{\mathcal{L}_{h,m}^{-1}}, \\
(\zeta, \zeta)_{\mathcal{L}_{h,m}^{-1}} &= \ell_h^m(\mu_\zeta, \mu_\zeta) \geq 0
\end{aligned}$$

with equality if and only if $\mu_\zeta = 0$ since $\ell_h^m(\cdot, \cdot)$ defines an inner product on $\mathring{S}_h$. By definition, $\mu_\zeta = 0$ if and only if $\zeta = 0$. $\square$

Using our discrete negative norm we can define a variational problem closely related to our fully discrete scheme.

Lemma 3.3.8. *Let $\varphi_h^{m-1} \in \mathring{S}_h$ be given. Take $\varphi_{h,\star}^{m-1}$ as in (3.11). For all $\varphi_h \in \mathring{S}_h$, define the nonlinear functional*

$$\begin{aligned}
G_h(\varphi_h) &:= \frac{\tau}{2} \left\| \frac{\varphi_h - \varphi_{h,\star}^{m-1}}{\tau} \right\|_{\mathcal{L}_{h,m}^{-1}}^2 + \frac{1}{4\varepsilon} \|\varphi_h + \bar{\phi}_0\|_{L^4}^4 + \frac{\varepsilon}{2} \|\nabla \varphi_h\|_{L^2}^2 \\
&\quad - \frac{1}{\varepsilon} (\varphi_h^{m-1} + \bar{\phi}_0, \varphi_h) + \frac{\theta}{2} \|\varphi_h\|_{-1,h}^2.
\end{aligned} \tag{3.21}$$

G_h is strictly convex and coercive on the linear subspace $\mathring{S}_h$. Consequently, G_h has a unique minimizer, call it $\varphi_h^m \in \mathring{S}_h$. Moreover, $\varphi_h^m \in \mathring{S}_h$ is the unique minimizer of G_h if and only if it is the unique solution to

$$\varepsilon^{-1} \left((\varphi_h^m + \bar{\phi}_0)^3, \psi \right) + \varepsilon a(\varphi_h^m, \psi) - (\mu_{h,\star}^m, \psi) + (\xi_h^m, \psi) = \varepsilon^{-1} (\varphi_h^{m-1} + \bar{\phi}_0, \psi) \tag{3.22}$$

for all $\psi \in \mathring{S}_h$, where $\mu_{h,\star}^m, \xi_h^m \in \mathring{S}_h$ are the unique solutions to

$$\ell_h^m(\mu_{h,\star}^m, \nu) = - \left(\frac{\varphi_h^m - \varphi_{h,\star}^{m-1}}{\tau}, \nu \right) \quad \forall \nu \in \mathring{S}_h, \quad (3.23)$$

$$a(\xi_h^m, \zeta) = \theta(\varphi_h^m, \zeta) \quad \forall \zeta \in \mathring{S}_h. \quad (3.24)$$

Proof. We begin by showing G_h is strictly convex. To do so, we consider the second derivative of $G_h(\varphi_h + s\psi)$ with respect to s and set $s = 0$. Hence,

$$\begin{aligned} G_h(\varphi_h + s\psi) &= \frac{1}{2\tau} \|\varphi_h + s\psi - \varphi_{h,\star}^{m-1}\|_{\mathcal{L}_{h,m}^{-1}}^2 + \frac{1}{4\varepsilon} \|\varphi_h + s\psi + \bar{\phi}_0\|_{L^4}^4 + \frac{\varepsilon}{2} \|\nabla(\varphi_h + s\psi)\|_{L^2}^2 \\ &\quad - \frac{1}{\varepsilon} (\varphi_h^{m-1} + \bar{\phi}_0, \varphi_h + s\psi) + \frac{\theta}{2} \|\varphi_h + s\psi\|_{-1,h}^2. \end{aligned}$$

Taking the derivative with respect to s , we have

$$\begin{aligned} G'_h(\varphi_h + s\psi) &= \frac{1}{\tau} (\varphi_h + s\psi - \varphi_{h,\star}^{m-1}, \psi)_{\mathcal{L}_{h,m}^{-1}} + \frac{1}{\varepsilon} \left(\psi (\varphi_h + s\psi + \bar{\phi}_0), (\varphi_h + s\psi + \bar{\phi}_0)^2 \right) \\ &\quad + \varepsilon (\nabla(\varphi_h + s\psi), \nabla\psi) - \frac{1}{\varepsilon} (\varphi_h^{m-1} + \bar{\phi}_0, \psi) + \theta (\varphi_h + s\psi, \psi)_{-1,h}. \end{aligned} \quad (3.25)$$

Taking the second derivative with respect to s , we have

$$G''_h(\varphi_h + s\psi) = \frac{1}{\tau} \|\psi\|_{\mathcal{L}_{h,m}^{-1}}^2 + \frac{3}{\varepsilon} \left((\varphi_h + s\psi + \bar{\phi}_0)^2, \psi^2 \right) + \varepsilon \|\nabla\psi\|_{L^2}^2 + \theta \|\psi\|_{-1,h}^2.$$

Setting $s = 0$,

$$G''_h(\varphi_h) = \frac{1}{\tau} \|\psi\|_{\mathcal{L}_{h,m}^{-1}}^2 + \frac{3}{\varepsilon} \left((\varphi_h + \bar{\phi}_0)^2, \psi^2 \right) + \varepsilon \|\nabla\psi\|_{L^2}^2 + \theta \|\psi\|_{-1,h}^2 > 0$$

for all $\varphi_h \in \mathring{S}_h$. To show G_h is coercive, we need to show that there exists constants $\alpha > 0, \beta \geq 0$ such that $G_h(\varphi_h) \geq \alpha \|\varphi_h\|_{H^1} - \beta$ for all $\varphi_h \in \mathring{S}_h$. Using the Cauchy

Schwartz inequality, Young's inequality, and Poincaré's inequality,

$$G_h(\varphi_h) \geq C_0(\varepsilon) \|\nabla \varphi_h\|_{L^2}^2 - C_1(\varepsilon) \|\varphi_h^{m-1} + \bar{\phi}_0\|_{L^2}^2 - C_2(\varepsilon) \|\varphi_h\|_{L^2}^2,$$

where $C_0(\varepsilon)$ depends on the Poincaré constant and $C_2(\varepsilon)$ is chosen to be less than $C_0(\varepsilon)$. Therefore,

$$G_h(\varphi_h) \geq \alpha \|\nabla \varphi_h\|_{L^2}^2 - \beta,$$

where $\alpha = C_0(\varepsilon) - C_2(\varepsilon)$ and $\beta = C_1(\varepsilon) \|\varphi_h^{m-1} + \bar{\phi}_0\|_{L^2}^2$ do not depend on φ_h . Hence, G_h has a unique minimizer, $\varphi_h^m \in \mathring{S}_h$ which solves

$$\begin{aligned} G'_h(\varphi_h^m) &= \frac{1}{\tau} (\varphi_h^m - \varphi_{h,\star}^{m-1}, \psi)_{\mathcal{L}_{h,m}^{-1}} + \frac{1}{\varepsilon} \left((\varphi_h^m + \bar{\phi}_0)^3, \psi \right) \\ &\quad + \varepsilon (\nabla \varphi_h^m, \nabla \psi) - \frac{1}{\varepsilon} (\varphi_h^{m-1} + \bar{\phi}_0, \psi) + \theta (\varphi_h^m, \psi)_{-1,h} = 0, \end{aligned}$$

for all $\psi \in \mathring{S}_h$ where we have set $s = 0$ in (3.25). By Lemma 3.3.7 and (3.10c), we have $\varphi_h^m \in \mathring{S}_h$ is the unique minimizer of G_h if and only if it is the unique solution to

$$\varepsilon^{-1} \left((\varphi_h^m + \bar{\phi}_0)^3, \psi \right) + \varepsilon a(\varphi_h^m, \psi) - (\mu_{h,\star}^m, \psi) + (\xi_h^m, \psi) = \varepsilon^{-1} (\varphi_h^{m-1} + \bar{\phi}_0, \psi) \quad (3.26)$$

for all $\psi \in \mathring{S}_h$, where $\mu_{h,\star}^m, \xi_h^m \in \mathring{S}_h$ are the unique solutions to

$$\begin{aligned} \ell_h^m(\mu_{h,\star}^m, \nu) &= - \left(\frac{\varphi_h^m - \varphi_{h,\star}^{m-1}}{\tau}, \nu \right) \quad \forall \nu \in \mathring{S}_h, \\ a(\xi_h^m, \zeta) &= \theta (\varphi_h^m, \zeta) \quad \forall \zeta \in \mathring{S}_h. \end{aligned}$$

□

Finally, we are in the position to prove the unconditional unique solvability of our scheme.

Theorem 3.3.9. *The scheme (3.7a) – (3.7e), or, equivalently, the scheme (3.10a) – (3.10e), is uniquely solvable for any mesh parameters τ and h and for any of the model parameters.*

Proof. Suppose $(\varphi_h^{m-1}, 1) = 0$. It is clear that a necessary condition for solvability of (3.10a) – (3.10e) is that

$$(\varphi_h^m, 1) = (\varphi_h^{m-1}, 1) = 0, \quad (3.27)$$

as can be found by taking $\nu \equiv 1$ in (3.10a). Now, let $\varphi_h^m, \mu_{h,\star}^m \in \mathring{S}_h \times \mathring{S}_h$ be a solution of (3.22) – (3.24). (The other variables may be regarded as auxiliary.) Set

$$\overline{\mu_h^m} := \frac{1}{\varepsilon|\Omega|} ((\varphi_h^m + \overline{\phi}_0)^3 - (\varphi_h^m + \overline{\phi}_0), 1) = \frac{1}{\varepsilon|\Omega|} ((\varphi_h^m + \overline{\phi}_0)^3, 1) - \frac{\overline{\phi}_0}{\varepsilon}, \quad (3.28)$$

and define $\mu_h^m := \mu_{h,\star}^m + \overline{\mu_h^m}$. There is a one-to-one correspondence of the respective solution sets: $\varphi_h^m, \mu_{h,\star}^m \in \mathring{S}_h \times \mathring{S}_h$ is a solution to (3.22) – (3.24), if and only if $\varphi_h^m, \mu_h^m \in \mathring{S}_h \times S_h$ is a solution to (3.10a) – (3.10e), if and only if $\phi_h^m, \mu_h^m \in S_h \times S_h$ is a solution to (3.7a) – (3.7e), where

$$\phi_h^m = \varphi_h^m + \overline{\phi}_0, \quad \mu_h^m = \mu_{h,\star}^m + \overline{\mu_h^m}. \quad (3.29)$$

But (3.22) – (3.24) admits a unique solution, which proves that (3.7a) – (3.7e) and (3.10a) – (3.10e) are uniquely solvable. $\square$

3.3.3 Unconditional Energy Stability

We now show that the solutions to our scheme enjoy stability properties that are similar to those of the PDE solutions, and moreover, these properties hold regardless of the sizes of h and τ . To begin, we establish a few necessary identities.

Lemma 3.3.10. *Let $(\phi_h^m, \mu_h^m, \mathbf{u}_h^m) \in S_h \times S_h \times \mathbf{X}_h$ be the unique solution of (3.7a)–(3.7e), with the other variables regarded as auxiliary. Then the following identities hold for any $h, \tau > 0$:*

$$(\delta_\tau \mathbf{u}_h^m, \mathbf{u}_h^m) = \frac{1}{2} \left[\delta_\tau \|\mathbf{u}_h^m\|_{L^2}^2 + \tau \|\delta_\tau \mathbf{u}_h^m\|_{L^2}^2 \right], \quad (3.30)$$

$$a(\phi_h^m, \delta_\tau \phi_h^m) = \frac{1}{2} \left[\delta_\tau \|\nabla \phi_h^m\|_{L^2}^2 + \tau \|\nabla \delta_\tau \phi_h^m\|_{L^2}^2 \right], \quad (3.31)$$

$$\begin{aligned} ((\phi_h^m)^3 - \phi_h^{m-1}, \delta_\tau \phi_h^m) &= \frac{1}{4} \delta_\tau \|(\phi_h^m)^2 - 1\|_{L^2}^2 + \frac{\tau}{4} \left[\|\delta_\tau (\phi_h^m)^2\|_{L^2}^2 \right. \\ &\quad \left. + 2 \|\phi_h^m \delta_\tau \phi_h^m\|_{L^2}^2 + 2 \|\delta_\tau \phi_h^m\|_{L^2}^2 \right], \end{aligned} \quad (3.32)$$

$$(\phi_h^m - \bar{\phi}_0, \delta_\tau \phi_h^m)_{-1,h} = \frac{1}{2} \left[\delta_\tau \|\phi_h^m - \bar{\phi}_0\|_{-1,h}^2 + \tau \|\delta_\tau \phi_h^m\|_{-1,h}^2 \right]. \quad (3.33)$$

Proof. To prove (3.30), we use the definition of $\delta_\tau \mathbf{u}_h^m$ and expand as follows,

$$\begin{aligned} (\delta_\tau \mathbf{u}_h^m, \mathbf{u}_h^m) &= \frac{1}{\tau} \left(\mathbf{u}_h^m - \mathbf{u}_h^{m-1}, \mathbf{u}_h^m + \frac{1}{2} \mathbf{u}_h^{m-1} - \frac{1}{2} \mathbf{u}_h^{m-1} \right) \\ &= \frac{1}{2\tau} (\mathbf{u}_h^m - \mathbf{u}_h^{m-1}, \mathbf{u}_h^m + \mathbf{u}_h^{m-1} + \mathbf{u}_h^m - \mathbf{u}_h^{m-1}) \\ &= \frac{1}{2} \left[\delta_\tau \|\mathbf{u}_h^m\|_{L^2}^2 + \tau \|\delta_\tau \mathbf{u}_h^m\|_{L^2}^2 \right]. \end{aligned}$$

Identities (3.31) and (3.33) follow in a similar manner to (3.30). To prove (3.32), we use the definition of $\delta_\tau \phi_h^m$ and expand as follows,

$$\begin{aligned}
((\phi_h^m)^3 - \phi_h^{m-1}, \delta_\tau \phi_h^m) &= \frac{1}{2\tau} ((\phi_h^m)^2 (\phi_h^m + \phi_h^{m-1}) + (\phi_h^m)^2 (\phi_h^m - \phi_h^{m-1}), \phi_h^m - \phi_h^{m-1}) \\
&\quad - \frac{1}{\tau} (\phi_h^{m-1}, \phi_h^m - \phi_h^{m-1}) \\
&= \frac{1}{2\tau} \left((\phi_h^m)^2, (\phi_h^m)^2 - (\phi_h^{m-1})^2 \right) + \frac{1}{2\tau} \left((\phi_h^m)^2, (\phi_h^m - \phi_h^{m-1})^2 \right) \\
&\quad - \frac{1}{2\tau} \left(\|\phi_h^m\|_{L^2}^2 - \|\phi_h^{m-1}\|_{L^2}^2 - \|\phi_h^m - \phi_h^{m-1}\|_{L^2}^2 \right) \\
&= \frac{1}{4\tau} \left((\phi_h^m)^2 + (\phi_h^{m-1})^2 + (\phi_h^m)^2 - (\phi_h^{m-1})^2, (\phi_h^m)^2 - (\phi_h^{m-1})^2 \right) \\
&\quad + \frac{1}{2\tau} \left((\phi_h^m)^2, (\phi_h^m - \phi_h^{m-1})^2 \right) \\
&\quad - \frac{1}{2\tau} \left(\|\phi_h^m\|_{L^2}^2 - \|\phi_h^{m-1}\|_{L^2}^2 - \|\phi_h^m - \phi_h^{m-1}\|_{L^2}^2 \right) \\
&= \frac{1}{4\tau} \left(\left\| (\phi_h^m)^2 \right\|_{L^2}^2 - \left\| (\phi_h^{m-1})^2 \right\|_{L^2}^2 + \left\| (\phi_h^m)^2 - (\phi_h^{m-1})^2 \right\|_{L^2}^2 \right) \\
&\quad + \frac{1}{2\tau} (\phi_h^m (\phi_h^m - \phi_h^{m-1}), \phi_h^m (\phi_h^m - \phi_h^{m-1})) \\
&\quad - \frac{1}{2\tau} \left(\|\phi_h^m\|_{L^2}^2 - \|\phi_h^{m-1}\|_{L^2}^2 - \|\phi_h^m - \phi_h^{m-1}\|_{L^2}^2 \right) \\
&= \frac{1}{4\tau} \left(\left\| (\phi_h^m)^2 \right\|_{L^2}^2 - 2 \|\phi_h^m\|_{L^2}^2 + 1 \right) \\
&\quad - \frac{1}{4\tau} \left(\left\| (\phi_h^{m-1})^2 \right\|_{L^2}^2 - 2 \|\phi_h^{m-1}\|_{L^2}^2 + 1 \right) \\
&\quad + \frac{1}{4\tau} \left\| (\phi_h^m)^2 - (\phi_h^{m-1})^2 \right\|_{L^2}^2 + \frac{1}{2\tau} \|\phi_h^m (\phi_h^m - \phi_h^{m-1})\|_{L^2}^2 \\
&\quad + \frac{1}{2\tau} \|\phi_h^m - \phi_h^{m-1}\|_{L^2}^2 \\
&= \frac{1}{4} \delta_\tau \left\| (\phi_h^m)^2 - 1 \right\|_{L^2}^2 + \frac{\tau}{4} \left\| \delta_\tau (\phi_h^m)^2 \right\|_{L^2}^2 \\
&\quad + \frac{\tau}{2} \left[\|\phi_h^m \delta_\tau \phi_h^m\|_{L^2}^2 + \|\delta_\tau \phi_h^m\|_{L^2}^2 \right].
\end{aligned}$$

□

With these identities in hand, the unconditional energy stability follows as a direct result of the convex decomposition represented in the scheme.

Lemma 3.3.11. *Let $(\phi_h^m, \mu_h^m, \mathbf{u}_h^m) \in S_h \times S_h \times \mathbf{X}_h$ be the unique solution of (3.7a)–(3.7e), with the other variables regarded as auxiliary. Then the following energy law holds for any $h, \tau > 0$:*

$$\begin{aligned}
E(\mathbf{u}_h^\ell, \phi_h^\ell) + \tau \varepsilon \sum_{m=1}^{\ell} \|\nabla \mu_h^m\|_{L^2}^2 + \tau \frac{\lambda}{\gamma} \sum_{m=1}^{\ell} \|\nabla \mathbf{u}_h^m\|_{L^2}^2 + \tau \frac{\eta}{\gamma} \sum_{m=1}^{\ell} \|\mathbf{u}_h^m\|_{L^2}^2 \\
+ \tau^2 \sum_{m=1}^{\ell} \left\{ \frac{\varepsilon}{2} \|\nabla (\delta_\tau \phi_h^m)\|_{L^2}^2 + \frac{1}{2\gamma} \|\delta_\tau \mathbf{u}_h^m\|_{L^2}^2 + \frac{1}{4\varepsilon} \|\delta_\tau (\phi_h^m)^2\|_{L^2}^2 \right. \\
\left. + \frac{1}{2\varepsilon} \|\phi_h^m \delta_\tau \phi_h^m\|_{L^2}^2 + \frac{1}{2\varepsilon} \|\delta_\tau \phi_h^m\|_{L^2}^2 + \frac{\theta}{2} \|\delta_\tau \phi_h^m\|_{-1,h}^2 \right\} = E(\mathbf{u}_h^0, \phi_h^0),
\end{aligned} \tag{3.34}$$

for all $1 \leq \ell \leq M$.

Proof. We first set $\nu = \mu_h^m$ in (3.7a), $\psi = \delta_\tau \phi_h^m$ in (3.7b), $\zeta = -\mathbb{T}_h(\delta_\tau \phi_h^m)$ in (3.7c), $\mathbf{v} = \frac{1}{\gamma} \mathbf{u}_h^m$ in (3.7d), $q = \frac{1}{\gamma} p_h^m$ in (3.7e), to obtain

$$(\delta_\tau \phi_h^m, \mu_h^m) + \varepsilon \|\nabla \mu_h^m\|_{L^2}^2 + b(\phi_h^{m-1}, \mathbf{u}_h^m, \mu_h^m) = 0, \tag{3.35}$$

$$\frac{1}{\varepsilon} ((\phi_h^m)^3 - \phi_h^{m-1}, \delta_\tau \phi_h^m) + \varepsilon a(\phi_h^m, \delta_\tau \phi_h^m) - (\mu_h^m, \delta_\tau \phi_h^m) + (\xi_h^m, \delta_\tau \phi_h^m) = 0, \tag{3.36}$$

$$-a(\xi_h^m, \mathbb{T}_h(\delta_\tau \phi_h^m)) + \theta(\phi_h^m - \bar{\phi}_0, \mathbb{T}_h(\delta_\tau \phi_h^m)) = 0, \tag{3.37}$$

$$\frac{1}{\gamma} (\delta_\tau \mathbf{u}_h^m, \mathbf{u}_h^m) + \frac{\lambda}{\gamma} \|\nabla \mathbf{u}_h^m\|_{L^2}^2 + \frac{\eta}{\gamma} \|\mathbf{u}_h^m\|_{L^2}^2 - \frac{1}{\gamma} c(\mathbf{u}_h^m, p_h^m) - b(\phi_h^{m-1}, \mathbf{u}_h^m, \mu_h^m) = 0, \tag{3.38}$$

$$\frac{1}{\gamma} c(\mathbf{u}_h^m, p_h^m) = 0. \tag{3.39}$$

Combining (3.35) – (3.39), using the identities from Lemma 3.3.10, and applying the operator $\tau \sum_{m=1}^{\ell}$ to the combined equation, the result is obtained. $\square$

The discrete energy law immediately implies the following uniform (in h and τ) *a priori* estimates for ϕ_h^m , μ_h^m , and $\mathbf{u}_h^m$. Note that, from this point, we will not track the dependence of the estimates on the interface parameter $\varepsilon > 0$, though this may be of importance, especially if ε is made smaller.

Lemma 3.3.12. *Let $(\phi_h^m, \mu_h^m, \mathbf{u}_h^m) \in S_h \times S_h \times \mathbf{X}_h$ be the unique solution of (3.7a)–(3.7e). Suppose that $E(\mathbf{u}_h^0, \phi_h^0) < C$, independent of h . Then the following estimates hold for any $h, \tau > 0$:*

$$\max_{0 \leq m \leq M} \left[\|\mathbf{u}_h^m\|_{L^2}^2 + \|\nabla \phi_h^m\|_{L^2}^2 + \|(\phi_h^m)^2 - 1\|_{L^2}^2 + \|\phi_h^m - \bar{\phi}_0\|_{-1,h}^2 \right] \leq C, \quad (3.40)$$

$$\max_{0 \leq m \leq M} \left[\|\phi_h^m\|_{L^4}^4 + \|\phi_h^m\|_{L^2}^2 + \|\phi_h^m\|_{H^1}^2 \right] \leq C, \quad (3.41)$$

$$\tau \sum_{m=1}^M \left[\|\nabla \mu_h^m\|_{L^2}^2 + \|\nabla \mathbf{u}_h^m\|_{L^2}^2 + \|\mathbf{u}_h^m\|_{L^2}^2 \right] \leq C, \quad (3.42)$$

$$\begin{aligned} \sum_{m=1}^M \left[\|\nabla (\phi_h^m - \phi_h^{m-1})\|_{L^2}^2 + \|\phi_h^m - \phi_h^{m-1}\|_{L^2}^2 + \|\phi_h^m (\phi_h^m - \phi_h^{m-1})\|_{L^2}^2 \right. \\ \left. + \|(\phi_h^m)^2 - (\phi_h^{m-1})^2\|_{L^2}^2 + \|\phi_h^m - \phi_h^{m-1}\|_{-1,h}^2 + \|\mathbf{u}_h^m - \mathbf{u}_h^{m-1}\|_{L^2}^2 \right] \leq C, \end{aligned} \quad (3.43)$$

for some constant $C > 0$ that is independent of h, τ , and T .

We are able to prove the next set of *a priori* stability estimates without any restrictions of h and τ .

Lemma 3.3.13. *Let $(\phi_h^m, \mu_h^m, \mathbf{u}_h^m) \in S_h \times S_h \times \mathbf{X}_h$ be the unique solution of (3.7a)–(3.7e), with the other variables regarded as auxiliary. Suppose that $E(\mathbf{u}_h^0, \phi_h^0) < C$ independent of h . The following estimates hold for any $h, \tau > 0$:*

$$\tau \sum_{m=1}^M \left[\|\delta_\tau \phi_h^m\|_{H^{-1}}^2 + \|\delta_\tau \phi_h^m\|_{-1,h}^2 + \|\Delta_h \phi_h^m\|_{L^2}^2 + \|\mu_h^m\|_{L^2}^2 + \|\phi_h^m\|_{L^\infty}^{\frac{4(6-d)}{d}} \right] \leq C(T+1), \quad (3.44)$$

for some constant $C > 0$ that is independent of h, τ , and T .

Proof. Let $\mathcal{Q}_h : L^2(\Omega) \rightarrow S_h$ be the L^2 projection, i.e., $(\mathcal{Q}_h \nu - \nu, \chi) = 0$, for all $\chi \in S_h$. Suppose $\nu \in \dot{H}^1(\Omega)$. Then, using (3.40) and Sobolev embeddings,

$$(\delta_\tau \phi_h^m, \nu) = (\delta_\tau \phi_h^m, \mathcal{Q}_h \nu) \quad (3.45)$$

$$= -\varepsilon (\nabla \mu_h^m, \nabla \mathcal{Q}_h \nu) - b(\phi_h^{m-1}, \mathbf{u}_h^m, \mathcal{Q}_h \nu) \quad (3.46)$$

$$\leq \varepsilon \|\nabla \mu_h^m\|_{L^2} \|\nabla \mathcal{Q}_h \nu\|_{L^2} + \|\nabla \phi_h^{m-1}\|_{L^2} \|\mathbf{u}_h^m\|_{L^4} \|\mathcal{Q}_h \nu\|_{L^4} \quad (3.47)$$

$$\leq C [\varepsilon \|\nabla \mu_h^m\|_{L^2} + \|\mathbf{u}_h^m\|_{H^1}] \|\nabla \mathcal{Q}_h \nu\|_{L^2} \quad (3.48)$$

$$\leq C [\varepsilon \|\nabla \mu_h^m\|_{L^2} + \|\mathbf{u}_h^m\|_{H^1}] \|\nabla \nu\|_{L^2}, \quad (3.49)$$

where we used the H^1 stability of the L^2 projection in the last step. Applying $\tau \sum_{m=1}^M$ gives (3.44.1) – which, in our notation, is the bound on the first term of the left side of (3.44). The estimate (3.44.2) follows from the inequality $\|\nu\|_{-1,h} \leq \|\nu\|_{H^{-1}}$, which holds for all $\nu \in \dot{S}_h$.

Setting $\psi_h = \Delta_h \phi_h^m$ in (3.7b) and using the definition of $\Delta_h \phi_h^m$, we get

$$\begin{aligned} \varepsilon \|\Delta_h \phi_h^m\|_{L^2}^2 &= -\varepsilon a(\phi_h^m, \Delta_h \phi_h^m) \\ &= -(\mu_h^m, \Delta_h \phi_h^m) + \varepsilon^{-1} ((\phi_h^m)^3 - \phi_h^{m-1}, \Delta_h \phi_h^m) + (\xi_h^m, \Delta_h \phi_h^m) \\ &\leq a(\mu_h^m, \phi_h^m) - a(\xi_h^m, \phi_h^m) \\ &\quad + \varepsilon^{-1} \left(\frac{\varepsilon^2}{2} \|\Delta_h \phi_h^m\|_{L^2}^2 + \frac{1}{2\varepsilon^2} \|(\phi_h^m)^3 - \phi_h^{m-1}\|_{L^2}^2 \right) \\ &\leq \frac{1}{2} \|\nabla \mu_h^m\|_{L^2}^2 + \frac{1}{2} \|\nabla \phi_h^m\|_{L^2}^2 + \frac{\varepsilon}{2} \|\Delta_h \phi_h^m\|_{L^2}^2 \\ &\quad + C \|(\phi_h^m)^3 - \phi_h^{m-1}\|_{L^2}^2 - \theta (\phi_h^m - \bar{\phi}_0, \phi_h^m) \\ &\leq \frac{1}{2} \|\nabla \mu_h^m\|_{L^2}^2 + C \|\nabla \phi_h^m\|_{L^2}^2 + \frac{\varepsilon}{2} \|\Delta_h \phi_h^m\|_{L^2}^2 \\ &\quad + C \|(\phi_h^m)^3 - \phi_h^{m-1}\|_{L^2}^2 + C \|\phi_h^m - \bar{\phi}_0\|_{-1,h}^2. \end{aligned}$$

Hence,

$$\varepsilon \|\Delta_h \phi_h^m\|_{L^2}^2 \leq \|\nabla \mu_h^m\|_{L^2}^2 + C \|\nabla \phi_h^m\|_{L^2}^2 + C \|(\phi_h^m)^3 - \phi_h^{m-1}\|_{L^2}^2 + C \|\phi_h^m - \bar{\phi}_0\|_{-1,h}^2. \quad (3.50)$$

Now using (3.41), we have

$$\begin{aligned} \|(\phi_h^m)^3 - \phi_h^{m-1}\|_{L^2}^2 &\leq 2 \left(\|\phi_h^m\|_{L^6}^6 + \|\phi_h^{m-1}\|_{L^2}^2 \right) \\ &\leq C \|\phi_h^m\|_{H^1}^6 + C \\ &\leq C, \end{aligned} \quad (3.51)$$

where we used the embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$, for $d = 2, 3$. Putting the last two inequalities together, we have

$$\varepsilon \|\Delta_h \phi_h^m\|_{L^2}^2 \leq \|\nabla \mu_h^m\|_{L^2}^2 + C. \quad (3.52)$$

Applying $\tau \sum_{m=1}^M$, estimate (3.44.3) now follows from (3.42.1).

Now, take $\psi = \mu_h^m$ in (3.7b). Then, using (3.40) and (3.51), we have

$$\begin{aligned} \|\mu_h^m\|_{L^2}^2 &\leq \varepsilon^{-1} \|(\phi_h^m)^3 - \phi_h^{m-1}\|_{L^2} \|\mu_h^m\|_{L^2} + \varepsilon \|\nabla \phi_h^m\|_{L^2} \|\nabla \mu_h^m\|_{L^2} + \|\xi_h^m\|_{L^2} \|\mu_h^m\|_{L^2} \\ &\leq \frac{1}{\varepsilon^2} \|(\phi_h^m)^3 - \phi_h^{m-1}\|_{L^2}^2 + \frac{1}{4} \|\mu_h^m\|_{L^2}^2 + \frac{\varepsilon}{2} \|\nabla \phi_h^m\|_{L^2}^2 + \frac{\varepsilon}{2} \|\nabla \mu_h^m\|_{L^2}^2 \\ &\quad + C \|\nabla \xi_h^m\|_{L^2}^2 + \frac{1}{4} \|\mu_h^m\|_{L^2}^2 \\ &\leq C + \frac{1}{2} \|\mu_h^m\|_{L^2}^2 + \frac{\varepsilon}{2} \|\nabla \mu_h^m\|_{L^2}^2 + C \|\nabla \xi_h^m\|_{L^2}^2 \\ &\leq C + \frac{1}{2} \|\mu_h^m\|_{L^2}^2 + \frac{\varepsilon}{2} \|\nabla \mu_h^m\|_{L^2}^2 + C \|\phi_h^m - \bar{\phi}_0\|_{-1,h}^2 \\ &\leq C + \frac{1}{2} \|\mu_h^m\|_{L^2}^2 + \frac{\varepsilon}{2} \|\nabla \mu_h^m\|_{L^2}^2. \end{aligned}$$

Hence

$$\|\mu_h^m\|_{L^2}^2 \leq C + \varepsilon \|\nabla \mu_h^m\|_{L^2}^2. \quad (3.53)$$

Applying $\tau \sum_{m=1}^M$, estimate (3.44.4) now follows from (3.42.1).

To prove estimate (3.44.5), we use the discrete Gagliardo-Nirenberg inequality (2.36). Applying $\tau \sum_{m=1}^M$ and using $H^1(\Omega) \hookrightarrow L^6(\Omega)$, (3.41.3) and (3.44.3), estimate (3.44.5) follows. $\square$

Lemma 3.3.14. *Let $(\phi_h^m, \mu_h^m, \mathbf{u}_h^m) \in S_h \times S_h \times \mathbf{X}_h$ be the unique solution of (3.7a)–(3.7e), with the other variables regarded as auxiliary. Suppose that $E(\mathbf{u}_h^0, \phi_h^0), \|\mu_h^0\|_{L^2}^2 < C$ independent of h , where μ_h^0 is defined below in (3.56), $d = 2, 3$. The following estimates hold for any $h, \tau > 0$:*

$$\tau \sum_{m=1}^M \|\delta_\tau \phi_h^m\|_{L^2}^2 \leq C(T+1), \quad (3.54)$$

$$\max_{1 \leq m \leq M} \left[\|\mu_h^m\|_{L^2}^2 + \|\Delta_h \phi_h^m\|_{L^2}^2 + \|\phi_h^m\|_{L^\infty}^{\frac{4(6-d)}{d}} \right] \leq C(T+1), \quad (3.55)$$

for some constant $C > 0$ that is independent of h, τ , and T .

Proof. We prove (3.54) and (3.55.1) together. To do so, we first define μ_h^0 via

$$(\mu_h^0, \psi) := \varepsilon a(\phi_h^0, \psi) + \varepsilon^{-1} \left((\phi_h^0)^3 - \phi_h^0, \psi \right) + \theta \left(\mathbb{T}_h(\phi_h^0 - \bar{\phi}_0), \psi \right), \quad (3.56)$$

for all $\psi \in S_h$, and

$$\delta_\tau \phi_h^0 := 0 \in S_h. \quad (3.57)$$

Now, we subtract (3.7b) from itself at consecutive time steps to obtain

$$\begin{aligned} \tau (\delta_\tau \mu_h^m, \psi) &= \tau \varepsilon a(\delta_\tau \phi_h^m, \psi) + \varepsilon^{-1} \left((\phi_h^m)^3 - (\phi_h^{m-1})^3, \psi \right) \\ &\quad - \tau \varepsilon^{-1} (\delta_\tau \phi_h^{m-1}, \psi) + \theta \tau \left(\mathbb{T}_h(\delta_\tau \phi_h^m), \psi \right), \end{aligned} \quad (3.58)$$

for all $\psi \in S_h$, which is well-defined for all $1 \leq m \leq M$. Taking $\psi = \mu_h^m$ in (3.58) and $\nu = -\tau \delta_\tau \phi_h^m$ in (3.7a) and adding the results yields

$$\begin{aligned}
\tau (\delta_\tau \mu_h^m, \mu_h^m) + \tau \|\delta_\tau \phi_h^m\|_{L^2}^2 &= \tau \varepsilon^{-1} \left(\delta_\tau \phi_h^m \left\{ (\phi_h^m)^2 + \phi_h^m \phi_h^{m-1} + (\phi_h^{m-1})^2 \right\}, \mu_h^m \right) \\
&\quad - \tau \varepsilon^{-1} (\delta_\tau \phi_h^{m-1}, \mu_h^m) + \theta \tau (\mathbb{T}_h (\delta_\tau \phi_h^m), \mu_h^m - \overline{\mu_h^m}) \\
&\quad - \tau b(\phi_h^{m-1}, \mathbf{u}_h^m, \delta_\tau \phi_h^m) \\
&\leq \tau \varepsilon^{-1} \left\| (\phi_h^m)^2 + \phi_h^m \phi_h^{m-1} + (\phi_h^{m-1})^2 \right\|_{L^3} \|\mu_h^m\|_{L^6} \|\delta_\tau \phi_h^m\|_{L^2} \\
&\quad + \tau \varepsilon^{-1} \|\nabla \mu_h^m\|_{L^2} \|\delta_\tau \phi_h^{m-1}\|_{-1,h} \\
&\quad + \theta \tau \|\nabla \mathbb{T}_h (\delta_\tau \phi_h^m)\|_{L^2} \|\mu_h^m - \overline{\mu_h^m}\|_{-1,h} \\
&\quad - \tau b(\phi_h^{m-1}, \mathbf{u}_h^m, \delta_\tau \phi_h^m) \\
&\leq C \tau \left\| (\phi_h^m)^2 + \phi_h^m \phi_h^{m-1} + (\phi_h^{m-1})^2 \right\|_{L^3}^2 \|\mu_h^m\|_{H^1}^2 \\
&\quad + \frac{\tau}{4} \|\delta_\tau \phi_h^m\|_{L^2}^2 + C \tau \|\nabla \mu_h^m\|_{L^2}^2 + C \tau \|\delta_\tau \phi_h^{m-1}\|_{-1,h}^2 \\
&\quad + C \tau \|\nabla \mathbb{T}_h (\delta_\tau \phi_h^m)\|_{L^2}^2 + C \tau \|\mu_h^m - \overline{\mu_h^m}\|_{-1,h}^2 \\
&\quad - \tau b(\phi_h^{m-1}, \mathbf{u}_h^m, \delta_\tau \phi_h^m) \\
&\leq C \tau \left(\|\phi_h^m\|_{L^6}^4 + \|\phi_h^{m-1}\|_{L^6}^4 \right) \|\mu_h^m\|_{H^1}^2 + \frac{\tau}{4} \|\delta_\tau \phi_h^m\|_{L^2}^2 \\
&\quad + C \tau \|\nabla \mu_h^m\|_{L^2}^2 + C \tau \|\delta_\tau \phi_h^{m-1}\|_{-1,h}^2 + C \tau \|\delta_\tau \phi_h^m\|_{-1,h}^2 \\
&\quad + C \tau \|\nabla \mu_h^m\|_{L^2}^2 - \tau b(\phi_h^{m-1}, \mathbf{u}_h^m, \delta_\tau \phi_h^m) \\
&\leq C \tau \|\mu_h^m\|_{H^1}^2 + \frac{\tau}{4} \|\delta_\tau \phi_h^m\|_{L^2}^2 + C \tau \|\delta_\tau \phi_h^{m-1}\|_{-1,h}^2 \\
&\quad + C \tau \|\delta_\tau \phi_h^m\|_{-1,h}^2 - \tau b(\phi_h^{m-1}, \mathbf{u}_h^m, \delta_\tau \phi_h^m) \tag{3.59}
\end{aligned}$$

where we have used $H^1(\Omega) \hookrightarrow L^6(\Omega)$, Young's Inequality, and (3.41).

Now we bound the trilinear form $b(\cdot, \cdot, \cdot)$. To do so, we note the discrete estimate

$$\|\nabla \nu_h\|_{L^4} \leq C (\|\nabla \nu_h\|_{L^2} + \|\Delta_h \nu_h\|_{L^2})^{\frac{d}{4}} \|\nabla \nu_h\|_{L^2}^{\frac{4-d}{4}} \quad \forall \nu_h \in S_h, \quad d = 2, 3. \tag{3.60}$$

Using Holder's inequality, (3.60), (3.40.1), and (3.40.2)

$$\begin{aligned}
|b(\phi_h^{m-1}, \mathbf{u}_h^m, \delta_\tau \phi_h^m)| &\leq \|\nabla \phi_h^{m-1}\|_{L^4} \|\mathbf{u}_h^m\|_{L^4} \|\delta_\tau \phi_h^m\|_{L^2} \\
&\leq C \|\delta_\tau \phi_h^m\|_{L^2} \|\nabla \mathbf{u}_h^m\|_{L^2} (\|\nabla \phi_h^{m-1}\|_{L^2} + \|\Delta_h \phi_h^{m-1}\|_{L^2}) \\
&\leq \frac{1}{4} \|\delta_\tau \phi_h^m\|_{L^2}^2 + C \|\nabla \mathbf{u}_h^m\|_{L^2}^2 + C \|\nabla \mathbf{u}_h^m\|_{L^2}^2 \|\Delta_h \phi_h^{m-1}\|_{L^2}^2.
\end{aligned} \tag{3.61}$$

Setting $\psi_h = \Delta_h \phi_h^m$ in (3.7b) and (3.56) and using the definition of $\Delta_h \phi_h^m$, it follows that

$$\|\Delta_h \phi_h^m\|_{L^2}^2 \leq C \|\mu_h^m\|_{L^2}^2 + C, \quad 0 \leq m \leq M, \tag{3.62}$$

so that, for $1 \leq m \leq M$,

$$|b(\phi_h^{m-1}, \mathbf{u}_h^m, \delta_\tau \phi_h^m)| \leq \frac{1}{4} \|\delta_\tau \phi_h^m\|_{L^2}^2 + C \|\nabla \mathbf{u}_h^m\|_{L^2}^2 + C \|\nabla \mathbf{u}_h^m\|_{L^2}^2 \|\mu_h^{m-1}\|_{L^2}^2. \tag{3.63}$$

Thus,

$$\begin{aligned}
\tau(\delta_\tau \mu_h^m, \mu_h^m) + \frac{\tau}{2} \|\delta_\tau \phi_h^m\|_{L^2}^2 &\leq C\tau \|\mu_h^m\|_{H^1}^2 + C\tau \|\delta_\tau \phi_h^{m-1}\|_{-1,h}^2 + C\tau \|\delta_\tau \phi_h^m\|_{-1,h}^2 \\
&\quad + C\tau \|\nabla \mathbf{u}_h^m\|_{L^2}^2 \|\mu_h^{m-1}\|_{L^2}^2 + C\tau \|\nabla \mathbf{u}_h^m\|_{L^2}^2.
\end{aligned} \tag{3.64}$$

Applying $\sum_{m=1}^\ell$, and using (3.42), (3.44), $\delta_\tau \phi_h^0 \equiv 0$, and the identity

$$\tau(\delta_\tau \mu_h^m, \mu_h^m) = (\mu_h^m - \mu_h^{m-1}, \mu_h^m) = \frac{1}{2} \|\mu_h^m\|_{L^2}^2 + \frac{1}{2} \|\mu_h^m - \mu_h^{m-1}\|_{L^2}^2 - \frac{1}{2} \|\mu_h^{m-1}\|_{L^2}^2, \tag{3.65}$$

we conclude

$$\frac{1}{2} \|\mu_h^\ell\|_{L^2}^2 - \frac{1}{2} \|\mu_h^0\|_{L^2}^2 + \frac{\tau}{2} \sum_{m=1}^\ell \|\delta_\tau \phi_h^m\|_{L^2}^2 \leq C(T+1) + C\tau \sum_{m=0}^{\ell-1} \|\nabla \mathbf{u}_h^{m+1}\|_{L^2}^2 \|\mu_h^m\|_{L^2}^2. \tag{3.66}$$

Since the estimate is explicit with respect to $\{\|\mu_h^m\|_{L^2}^2\}$ and $\tau \sum_{m=1}^M \|\nabla \mathbf{u}_h^m\|_{L^2}^2 \leq C$, we may appeal directly to the discrete Gronwall inequality in Lemma 2.2.26. Estimates

(3.54) and (3.55.1) follow immediately. Estimate (3.55.2) follows from (3.55.1) and (3.62). Estimate (3.55.3) follows from the discrete Gagliardo-Nirenberg Inequality, the embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$, (3.41.3), and (3.55.2). $\square$

Remark 3.3.15. *The idea for controlling the time-lagged $\|\Delta_h \phi_h^{m-1}\|_{L^2}^2$ term in (3.61) using the discrete Gronwall inequality was inspired by a similar technique from a recent paper by G. Grün [29], which deals with a different PDE system (as well as a different numerical method) from that examined here and is not concerned with error estimates.*

3.4 Error Estimates for the Fully Discrete Convex Splitting Scheme

For the error estimates that we pursue in this section, we shall assume that weak solutions have the additional regularities

$$\begin{aligned}
\phi &\in H^2(0, T; L^2(\Omega)) \cap L^\infty(0, T; W^{1,6}(\Omega)) \cap H^1(0, T; H^{q+1}(\Omega)), \\
\xi &\in L^2(0, T; H^{q+1}(\Omega)), \\
\mu &\in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H^{q+1}(\Omega)), \\
\mathbf{u} &\in H^2(0, T; \mathbf{L}^2(\Omega)) \cap L^\infty(0, T; \mathbf{L}^4(\Omega)) \cap H^1(0, T; \mathbf{H}^{q+1}(\Omega)), \\
p &\in L^2(0, T; H^q(\Omega) \cap L_0^2(\Omega)),
\end{aligned} \tag{3.67}$$

where $q \geq 1$. Of course, some of these regularities are redundant because of embeddings.

Weak solutions (ϕ, μ) to (3.2a) - (3.2e) with the higher regularities (3.67) solve the following variational problem:

$$(\partial_t \phi, \nu) + \varepsilon a(\mu, \nu) + b(\phi, \mathbf{u}, \nu) = 0 \quad \forall \nu \in H^1(\Omega), \quad (3.68a)$$

$$(\mu, \psi) - \varepsilon a(\phi, \psi) - \varepsilon^{-1}(\phi^3 - \phi, \psi) - (\xi, \psi) = 0 \quad \forall \psi \in H^1(\Omega), \quad (3.68b)$$

$$a(\xi, \zeta) - \theta(\phi - \bar{\phi}_0, \zeta) = 0 \quad \forall \zeta \in H^1(\Omega), \quad (3.68c)$$

$$(\partial_t \mathbf{u}, \mathbf{v}) + \lambda a(\mathbf{u}, \mathbf{v}) + \eta(\mathbf{u}, \mathbf{v}) - c(\mathbf{v}, p) - \gamma b(\phi, \mathbf{v}, \mu) = 0 \quad \forall \mathbf{v} \in \mathbf{H}_0^1(\Omega), \quad (3.68d)$$

$$c(\mathbf{u}, q) = 0 \quad \forall q \in L_0^2(\Omega). \quad (3.68e)$$

We define the following: for any *real* number $m \in [0, M]$,

$$\begin{aligned} t_m &:= m\tau, \quad \phi^m := \phi(t_m), \quad \delta_\tau \phi^m := \frac{\phi^m - \phi^{m-1}}{\tau}, \\ \mathcal{E}_a^{\phi, m} &:= \phi^m - R_h \phi^m, \quad \mathcal{E}_a^{\mu, m} := \mu^m - R_h \mu^m, \quad \mathcal{E}_a^{\mathbf{u}, m} := \mathbf{u} - \mathbf{P}_h \mathbf{u}, \quad \mathcal{E}_a^{\xi, m} := \xi - R_h \xi, \\ \sigma_1^{\phi, m} &:= \delta_\tau R_h \phi^m - \delta_\tau \phi^m, \quad \sigma_2^{\phi, m} := \delta_\tau \phi^m - \partial_t \phi^m, \\ \sigma_1^{\mathbf{u}, m} &:= \delta_\tau \mathbf{P}_h \mathbf{u}^m - \delta_\tau \mathbf{u}^m, \quad \sigma_2^{\mathbf{u}, m} := \delta_\tau \mathbf{u}^m - \partial_t \mathbf{u}^m. \end{aligned}$$

Then, for all $\nu, \psi, \zeta \in S_h$, $\mathbf{v} \in \mathbf{X}_h$, and $q \in \mathring{S}_h$,

$$(\delta_\tau R_h \phi^m, \nu) + \varepsilon a(R_h \mu^m, \nu) + b(\phi^m, \mathbf{u}^m, \nu) = \left(\sigma_1^{\phi, m} + \sigma_2^{\phi, m}, \nu \right), \quad (3.69a)$$

$$\varepsilon a(R_h \phi^m, \psi) - (R_h \mu^m, \psi) + (R_h \xi^m, \psi) = (\mathcal{E}_a^{\mu, m}, \psi) - (\mathcal{E}_a^{\xi, m}, \psi) + \frac{1}{\varepsilon} ((\phi^m)^3 - \phi^m, \psi), \quad (3.69b)$$

$$a(R_h \xi^m, \zeta) - \theta(R_h \phi^m - \bar{\phi}_0, \zeta) = \theta(\mathcal{E}_a^{\phi, m}, \zeta), \quad (3.69c)$$

$$\begin{aligned} (\delta_\tau \mathbf{P}_h \mathbf{u}^m, \mathbf{v}) + \lambda a(\mathbf{P}_h \mathbf{u}^m, \mathbf{v}) + \eta(\mathbf{P}_h \mathbf{u}^m, \mathbf{v}) - c(\mathbf{v}, P_h p^m) \\ - \gamma b(\phi^m, \mathbf{v}, \mu^m) = (\sigma_1^{\mathbf{u}, m} + \sigma_2^{\mathbf{u}, m}, \mathbf{v}), \end{aligned} \quad (3.69d)$$

$$c(\mathbf{P}_h \mathbf{u}^m, q) = 0. \quad (3.69e)$$

Restating the fully discrete convex splitting scheme (3.7a) – (3.7e), for all $\nu, \psi, \zeta \in S_h$, $\mathbf{v} \in \mathbf{X}_h$, and $q \in \mathring{S}_h$, we have

$$(\delta_\tau \phi_h^m, \nu) + \varepsilon a(\mu_h^m, \nu) + b(\phi_h^{m-1}, \mathbf{u}_h^m, \nu) = 0, \quad (3.70a)$$

$$\varepsilon a(\phi_h^m, \psi) - (\mu_h^m, \psi) + (\xi_h^m, \psi) + \varepsilon^{-1} ((\phi_h^m)^3 - \phi_h^{m-1}, \psi) = 0, \quad (3.70b)$$

$$a(\xi_h^m, \zeta) - \theta(\phi_h^m - \bar{\phi}_0, \zeta) = 0, \quad (3.70c)$$

$$(\delta_\tau \mathbf{u}_h^m, \mathbf{v}) + \lambda a(\mathbf{u}_h^m, \mathbf{v}) + \eta(\mathbf{u}_h^m, \mathbf{v}) - c(\mathbf{v}, p_h^m) - \gamma b(\phi_h^{m-1}, \mathbf{v}, \mu_h^m) = 0, \quad (3.70d)$$

$$c(\mathbf{u}_h^m, q) = 0. \quad (3.70e)$$

Now, let us define the following notation

$$\begin{aligned} \mathcal{E}_h^{\phi, m} &:= R_h \phi^m - \phi_h^m, \quad \mathcal{E}^{\phi, m} := \phi^m - \phi_h^m, \quad \mathcal{E}_h^{\mu, m} := R_h \mu^m - \mu_h^m, \\ \mathcal{E}_h^{\xi, m} &:= R_h \xi^m - \xi_h^m, \quad \mathcal{E}_h^{\mathbf{u}, m} := \mathbf{P}_h \mathbf{u}^m - \mathbf{u}_h^m, \quad \mathcal{E}_h^{p, m} := P_h p^m - p_h^m. \end{aligned}$$

Subtracting (3.70a) - (3.70e) from (3.69a) - (3.69e), we obtain the following system of equations for all $\nu, \psi, \zeta \in S_h$, $\mathbf{v} \in \mathbf{X}_h$, and $q \in \mathring{S}_h$,

$$\left(\delta_\tau \mathcal{E}_h^{\phi, m}, \nu \right) + \varepsilon a(\mathcal{E}_h^{\mu, m}, \nu) = \left(\sigma_1^{\phi, m} + \sigma_2^{\phi, m}, \nu \right) - b(\phi, \mathbf{u}, \nu) + b(\phi_h^{m-1}, \mathbf{u}_h^m, \nu), \quad (3.71a)$$

$$\begin{aligned} \varepsilon a(\mathcal{E}_h^{\phi, m}, \psi) - (\mathcal{E}_h^{\mu, m}, \psi) + (\mathcal{E}_h^{\xi, m}, \psi) &= (\mathcal{E}_a^{\mu, m}, \psi) - (\mathcal{E}_a^{\xi, m}, \psi) + \varepsilon^{-1} (\phi^m - \phi_h^{m-1}, \psi) \\ &\quad - \varepsilon^{-1} (\phi^3 - (\phi_h^m)^3, \psi), \end{aligned} \quad (3.71b)$$

$$a(\mathcal{E}_h^{\xi, m}, \zeta) - \theta(\mathcal{E}_h^{\phi, m}, \zeta) = \theta(\mathcal{E}_a^{\phi, m}, \zeta), \quad (3.71c)$$

$$\begin{aligned} (\delta_\tau \mathcal{E}_h^{\mathbf{u}, m}, \mathbf{v}) + \lambda a(\mathcal{E}_h^{\mathbf{u}, m}, \mathbf{v}) + \eta(\mathcal{E}_h^{\mathbf{u}, m}, \mathbf{v}) - c(\mathbf{v}, \mathcal{E}_h^{p, m}) &= (\sigma_1^{\mathbf{u}, m} + \sigma_2^{\mathbf{u}, m}, \mathbf{v}) + \gamma b(\phi, \mathbf{v}, \mu) \\ &\quad - \gamma b(\phi_h^{m-1}, \mathbf{v}, \mu_h^m), \end{aligned} \quad (3.71d)$$

$$c(\mathcal{E}_h^{\mathbf{u}, m}, q) = 0. \quad (3.71e)$$

Setting $\nu = \mathcal{E}_h^{\mu, m}$ in (3.71a), $\psi = \delta_\tau \mathcal{E}_h^{\phi, m}$ in (3.71b), $\zeta = -\mathbb{T}_h(\delta_\tau \mathcal{E}_h^{\phi, m})$ in (3.71c), $\mathbf{v} = \frac{1}{\gamma} \mathcal{E}_h^{\mathbf{u}, m}$ in (3.71d), and $q = \frac{1}{\gamma} \mathcal{E}_h^{p, m}$ in (3.71e) and adding the resulting equations produces the key to the error analysis:

$$\begin{aligned} &\varepsilon a(\mathcal{E}_h^{\phi, m}, \delta_\tau \mathcal{E}_h^{\phi, m}) + \theta(\mathcal{E}_h^{\phi, m}, \delta_\tau \mathcal{E}_h^{\phi, m})_{-1, h} + \frac{1}{\gamma} (\delta_\tau \mathcal{E}_h^{\mathbf{u}, m}, \mathcal{E}_h^{\mathbf{u}, m}) + \varepsilon \|\nabla \mathcal{E}_h^{\mu, m}\|_{L^2}^2 \\ &\quad + \frac{\lambda}{\gamma} \|\nabla \mathcal{E}_h^{\mathbf{u}, m}\|_{L^2}^2 + \frac{\eta}{\gamma} \|\mathcal{E}_h^{\mathbf{u}, m}\|_{L^2}^2 = \left(\sigma_1^{\phi, m} + \sigma_2^{\phi, m}, \mathcal{E}_h^{\mu, m} \right) + \frac{1}{\gamma} (\sigma_1^{\mathbf{u}, m} + \sigma_2^{\mathbf{u}, m}, \mathcal{E}_h^{\mathbf{u}, m}) \\ &\quad + \left(\mathcal{E}_a^{\mu, m}, \delta_\tau \mathcal{E}_h^{\phi, m} \right) - \varepsilon^{-1} \left((\phi^m)^3 - (\phi_h^m)^3, \delta_\tau \mathcal{E}_h^{\phi, m} \right) + \frac{\tau}{\varepsilon} \left(\delta_\tau \phi, \delta_\tau \mathcal{E}_h^{\phi, m} \right) \\ &\quad + \varepsilon^{-1} \left(\mathcal{E}_h^{\phi, m-1}, \delta_\tau \mathcal{E}_h^{\phi, m} \right) - \left(\mathcal{E}_a^{\xi, m}, \delta_\tau \mathcal{E}_h^{\phi, m} \right) - \theta \left(\mathcal{E}_a^{\phi, m}, \mathbb{T}_h(\delta_\tau \mathcal{E}_h^{\phi, m}) \right) \\ &\quad - b(\phi, \mathbf{u}, \mathcal{E}_h^{\mu, m}) + b(\phi_h^{m-1}, \mathbf{u}_h^m, \mathcal{E}_h^{\mu, m}) + b(\phi, \mathcal{E}_h^{\mathbf{u}, m}, \mu) - b(\phi_h^{m-1}, \mathcal{E}_h^{\mathbf{u}, m}, \mu_h^m). \end{aligned} \quad (3.72)$$

We now proceed to estimate the terms on the right hand side of (3.72).

Lemma 3.4.1. *Suppose that $(\phi^m, \mu^m, \mathbf{u}^m)$ is a weak solution to (3.68a) – (3.68e), with the additional regularities (3.67). Then, for any $h, \tau > 0$, there exists $C > 0$, independent of h and τ , such that*

$$\begin{aligned} \|\sigma_1^{\phi, m} + \sigma_2^{\phi, m}\|_{L^2}^2 &\leq C \frac{h^{2q+2}}{\tau} \int_{t-\tau}^t \|\partial_s \phi(s)\|_{H^{q+1}}^2 ds + \frac{\tau}{3} \int_{t-\tau}^t \|\partial_{ss} \phi(s)\|_{L^2}^2 ds, \\ \|\sigma_1^{\mathbf{u}, m} + \sigma_2^{\mathbf{u}, m}\|_{L^2}^2 &\leq C \frac{h^{2q+2}}{\tau} \int_{t-\tau}^t \|\partial_s \mathbf{u}(s)\|_{H^{q+1}}^2 ds + \frac{\tau}{3} \int_{t-\tau}^t \|\partial_{ss} \mathbf{u}(s)\|_{L^2}^2 ds, \end{aligned} \quad (3.73)$$

for all $t \in (\tau, T]$.

Proof. Using Taylor's Theorem and properties of the Ritz projection,

$$\begin{aligned} \|\sigma_1^{\phi, m}\|_{L^2}^2 &= \left\| \frac{1}{\tau} \int_{t-\tau}^t \partial_s (R_h \phi(s) - \phi(s)) ds \right\|_{L^2}^2 \\ &= \frac{1}{\tau^2} \left\| \int_{t-\tau}^t (R_h \partial_s \phi(s) - \partial_s \phi(s)) ds \right\|_{L^2}^2 \\ &\leq \frac{1}{\tau^2} \int_{\Omega} \int_{t-\tau}^t 1^2 ds \int_{t-\tau}^t (R_h \partial_s \phi(s) - \partial_s \phi(s))^2 ds d\mathbf{x} \\ &= \frac{1}{\tau} \int_{t-\tau}^t \|R_h \partial_s \phi(s) - \partial_s \phi(s)\|_{L^2}^2 ds \\ &\leq C \frac{h^{2q+2}}{\tau} \int_{t-\tau}^t \|\partial_s \phi(s)\|_{H^{q+1}}^2 ds. \end{aligned} \quad (3.74)$$

By Taylor's theorem,

$$\begin{aligned} \|\sigma_2^{\phi, m}\|_{L^2}^2 &= \left\| \frac{1}{\tau} \int_{t-\tau}^t \partial_{ss} \phi(s) (t-s) ds \right\|_{L^2}^2 \\ &\leq \frac{1}{\tau^2} \int_{\Omega} \left[\int_{t-\tau}^t (t-s)^2 ds \int_{t-\tau}^t (\partial_{ss} \phi(s))^2 ds \right] d\mathbf{x} \\ &= \frac{1}{\tau^2} \int_{t-\tau}^t (t-s)^2 ds \int_{t-\tau}^t \|\partial_{ss} \phi(s)\|_{L^2}^2 ds \\ &= \frac{\tau^3}{3\tau^2} \int_{t-\tau}^t \|\partial_{ss} \phi(s)\|_{L^2}^2 ds. \end{aligned} \quad (3.75)$$

Using the triangle inequality, the result for $\left\| \sigma_1^{\phi,m} + \sigma_2^{\phi,m} \right\|_{L^2}^2$ follows. A similar proof can be constructed for $\left\| \sigma_1^{\mathbf{u},m} + \sigma_2^{\mathbf{u},m} \right\|_{L^2}^2$. $\square$

Lemma 3.4.2. *Suppose that $(\phi^m, \mu^m, \mathbf{u}^m)$ is a weak solution to (3.68a) – (3.68e), with the additional regularities (3.67). Then, for any $h, \tau > 0$,*

$$\left\| \nabla \left((\phi^m)^3 - (\phi_h^m)^3 \right) \right\|_{L^2} \leq C \left\| \nabla \mathcal{E}^{\phi,m} \right\|_{L^2}, \quad (3.76)$$

where $\mathcal{E}^{\phi,m} := \phi^m - \phi_h^m$.

Proof. For $t \in [0, T]$,

$$\begin{aligned} \left\| \nabla \left((\phi^m)^3 - (\phi_h^m)^3 \right) \right\|_{L^2} &\leq 3 \left\| (\phi_h^m)^2 \nabla \mathcal{E}^{\phi,m} \right\|_{L^2} + 3 \left\| \nabla \phi^m (\phi^m + \phi_h^m) \mathcal{E}^{\phi,m} \right\|_{L^2} \\ &\leq 3 \left\| \phi_h^m \right\|_{L^\infty}^2 \left\| \nabla \mathcal{E}^{\phi,m} \right\|_{L^2} + 3 \left\| \nabla \phi^m \right\|_{L^6} \left\| \phi^m + \phi_h^m \right\|_{L^6} \left\| \mathcal{E}^{\phi,m} \right\|_{L^6} \\ &\leq 3 \left(\left\| \phi_h^m \right\|_{L^\infty}^2 + C \left\| \nabla \phi^m \right\|_{L^6} \left\| \phi^m + \phi_h^m \right\|_{H^1} \right) \left\| \nabla \mathcal{E}^{\phi,m} \right\|_{L^2} \\ &\leq C \left\| \nabla \mathcal{E}^{\phi,m} \right\|_{L^2}, \end{aligned} \quad (3.77)$$

where $C > 0$ is independent of $t \in [0, T]$ and where we have used the unconditional *a priori* estimates in Lemmas 3.3.13 and 3.3.14 and the assumption that $\phi \in L^\infty(0, T; W^{1,6}(\Omega))$. $\square$

Lemma 3.4.3. *Suppose that $(\phi^m, \mu^m, \mathbf{u}^m)$ is a weak solution to (3.68a) – (3.68e), with the additional regularities (3.67). Then, for any $h, \tau > 0$, and any $\alpha > 0$ there exists a constant $C = C(\alpha) > 0$, independent of h and τ , such that*

$$\begin{aligned} \frac{\varepsilon}{2} \left\| \nabla \mathcal{E}_h^{\mu,m} \right\|_{L^2}^2 + \varepsilon a \left(\mathcal{E}_h^{\phi,m}, \delta_\tau \mathcal{E}_h^{\phi,m} \right) + \theta \left(\mathcal{E}_h^{\phi,m}, \delta_\tau \mathcal{E}_h^{\phi,m} \right)_{-1,h} + (\delta_\tau \mathcal{E}_h^{\mathbf{u},m}, \mathcal{E}_h^{\mathbf{u},m}) \\ + \frac{\lambda}{2\gamma} \left\| \nabla \mathcal{E}_h^{\mathbf{u},m} \right\|_{L^2}^2 + \frac{\eta}{2\gamma} \left\| \mathcal{E}_h^{\mathbf{u},m} \right\|_{L^2}^2 \leq C \left\| \nabla \mathcal{E}_h^{\phi,m} \right\|_{L^2}^2 + C \left\| \nabla L_\tau \mathcal{E}_h^{\phi,m} \right\|_{L^2}^2 \\ + \alpha \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2 + C\mathcal{R}, \end{aligned} \quad (3.78)$$

for any $t \in (\tau, T]$, where $\mathcal{R}$ is the consistency term

$$\begin{aligned}
\mathcal{R}(t) = & \frac{h^{2q+2}}{\tau} \int_{t-\tau}^t \|\partial_s \phi(s)\|_{H^{q+1}}^2 ds + \frac{\tau}{3} \int_{t-\tau}^t \|\partial_{ss} \phi(s)\|_{L^2}^2 ds + \tau \int_{t-\tau}^t \|\nabla \partial_s \phi(s)\|_{L^2}^2 ds \\
& + \frac{h^{2q+2}}{\tau} \int_{t-\tau}^t \|\partial_s \mathbf{u}(s)\|_{H^{q+1}}^2 ds + \frac{\tau}{3} \int_{t-\tau}^t \|\partial_{ss} \mathbf{u}(s)\|_{L^2}^2 ds + h^{2q+2} |\phi^m|_{H^{q+1}}^2 \\
& + h^{2q} \left(|\mu^m|_{H^{q+1}}^2 + |\phi^m|_{H^{q+1}}^2 + |\phi^{m-1}|_{H^{q+1}}^2 + |\xi^m|_{H^{q+1}}^2 + |\mathbf{u}^m|_{H^{q+1}}^2 + |p^m|_{H^q}^2 \right).
\end{aligned} \tag{3.79}$$

Proof. Using Lemmas 3.4.1 and 2.2.22, the Cauchy-Schwarz inequality, the definition above, and the fact that $(\sigma_1^{\phi,m} + \sigma_2^{\phi,m}, 1) = 0$, we get the following estimates:

$$\begin{aligned}
\left| (\sigma_1^{\phi,m} + \sigma_2^{\phi,m}, \mathcal{E}_h^{\mu,m}) \right| & \leq \left\| \sigma_1^{\phi,m} + \sigma_2^{\phi,m} \right\|_{-1,h} \|\nabla \mathcal{E}_h^{\mu,m}\|_{L^2} \\
& \leq C \left\| \sigma_1^{\phi,m} + \sigma_2^{\phi,m} \right\|_{L^2} \|\nabla \mathcal{E}_h^{\mu,m}\|_{L^2} \\
& \leq C \left\| \sigma_1^{\phi,m} + \sigma_2^{\phi,m} \right\|_{L^2}^2 + \frac{\varepsilon}{10} \|\nabla \mathcal{E}_h^{\mu,m}\|_{L^2}^2 \\
& \leq C \left(\frac{h^{2q+2}}{\tau} \int_{t-\tau}^t \|\partial_s \phi(s)\|_{H^{q+1}}^2 ds + \frac{\tau}{3} \int_{t-\tau}^t \|\partial_{ss} \phi(s)\|_{L^2}^2 ds \right) \\
& \quad + \frac{\varepsilon}{10} \|\nabla \mathcal{E}_h^{\mu,m}\|_{L^2}^2
\end{aligned} \tag{3.80}$$

and, similarly,

$$\begin{aligned}
|(\sigma_1^{\mathbf{u},m} + \sigma_2^{\mathbf{u},m}, \mathcal{E}_h^{\mathbf{u},m})| & \leq C \left(\frac{h^{2q+2}}{\tau} \int_{t-\tau}^t \|\partial_s \mathbf{u}(s)\|_{H^{q+1}}^2 ds + \frac{\tau}{3} \int_{t-\tau}^t \|\partial_{ss} \mathbf{u}(s)\|_{L^2}^2 ds \right) \\
& \quad + \frac{\eta}{2\gamma} \|\mathcal{E}_h^{\mathbf{u},m}\|_{L^2}^2.
\end{aligned} \tag{3.81}$$

Now, from the standard finite element approximation theory

$$\|\nabla \mathcal{E}_a^{\mu,m}\|_{L^2} = \|\nabla(R_h \mu^m - \mu^m)\|_{L^2} \leq Ch^q |\mu^m|_{H^{q+1}}.$$

Applying Lemma 2.2.22 and the last estimate

$$\begin{aligned}
\left| \left(\mathcal{E}_a^{\mu,m}, \delta_\tau \mathcal{E}_h^{\phi,m} \right) \right| &\leq C \left\| \nabla \mathcal{E}_a^{\mu,m} \right\|_{L^2} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h} \\
&\leq Ch^q |\mu^m|_{H^{q+1}} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h} \\
&\leq Ch^{2q} |\mu^m|_{H^{q+1}}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2
\end{aligned} \tag{3.82}$$

and, similarly,

$$\left| \left(\mathcal{E}_a^{\xi,m}, \delta_\tau \mathcal{E}_h^{\phi,m} \right) \right| \leq Ch^{2q} |\xi^m|_{H^{q+1}}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2. \tag{3.83}$$

Now, it follows that

$$\left\| \tau \nabla \delta_\tau \phi^m \right\|_{L^2}^2 \leq \tau \int_{t-\tau}^t \left\| \nabla \partial_s \phi(s) \right\|_{L^2}^2 ds \tag{3.84}$$

and, therefore,

$$\begin{aligned}
\frac{\tau}{\varepsilon} \left| \left(\delta_\tau \phi^m, \delta_\tau \mathcal{E}_h^{\phi,m} \right) \right| &\leq \frac{1}{\varepsilon} \left\| \tau \nabla \delta_\tau \phi^m \right\|_{L^2} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h} \\
&\leq C\tau \int_{t-\tau}^t \left\| \nabla \partial_s \phi(s) \right\|_{L^2}^2 ds + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2.
\end{aligned} \tag{3.85}$$

Using Lemmas 2.2.22 and 3.4.2 , as well as $\mathcal{E}^{\phi,m} = \mathcal{E}_a^{\phi,m} + \mathcal{E}_h^{\phi,m}$ and a standard error estimate,

$$\begin{aligned}
\frac{1}{\varepsilon} \left| \left((\phi^m)^3 - (\phi_h^m)^3, \delta_\tau \mathcal{E}_h^{\phi,m} \right) \right| &\leq C \left\| \nabla \left((\phi^m)^3 - (\phi_h^m)^3 \right) \right\|_{L^2} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h} \\
&\leq C \left\| \nabla \left((\phi^m)^3 - (\phi_h^m)^3 \right) \right\|_{L^2}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2 \\
&\leq C \left\| \nabla \mathcal{E}^{\phi,m} \right\|_{L^2}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2 \\
&\leq C \left\| \nabla \mathcal{E}_a^{\phi,m} \right\|_{L^2}^2 + C \left\| \nabla \mathcal{E}_h^{\phi,m} \right\|_{L^2}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2 \\
&\leq Ch^{2q} |\phi^m|_{H^{q+1}}^2 + C \left\| \nabla \mathcal{E}_h^{\phi,m} \right\|_{L^2}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2.
\end{aligned} \tag{3.86}$$

With similar steps as in the last estimate,

$$\begin{aligned}
\frac{1}{\varepsilon} \left| \left(\mathcal{E}^{\phi,m-1}, \delta_\tau \mathcal{E}_h^{\phi,m} \right) \right| &\leq C \left\| \nabla \mathcal{E}^{\phi,m-1} \right\|_{L^2} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h} \\
&\leq Ch^{2q} |\phi^{m-1}|_{H^{q+1}}^2 + C \left\| \nabla \mathcal{E}_h^{\phi,m-1} \right\|_{L^2}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2.
\end{aligned} \tag{3.87}$$

Using the estimate

$$\left\| \mathbb{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right\|_{L^2}^2 \leq C \left\| \nabla \mathbb{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right\|_{L^2}^2 = C \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2,$$

we obtain

$$\begin{aligned}
\left| \theta \left(\mathcal{E}_a^{\phi,m}, \mathbb{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right) \right| &\leq \theta \left\| \mathcal{E}_a^{\phi,m} \right\|_{L^2} \left\| \mathbb{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right\|_{L^2} \\
&\leq Ch^{q+1} |\phi^m|_{H^{q+1}} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h} \\
&\leq Ch^{2q+2} |\phi^m|_{H^{q+1}}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2.
\end{aligned} \tag{3.88}$$

Now we consider the trilinear terms. Adding and subtracting the appropriate terms and using the triangle inequality gives

$$\begin{aligned}
& \left| -b(\phi^m, \mathbf{u}^m, \mathcal{E}_h^{\mu,m}) + b(\phi_h^{m-1}, \mathbf{u}_h^m, \mathcal{E}_h^{\mu,m}) + b(\phi^m, \mathcal{E}_h^{\mathbf{u},m}, \mu^m) - b(\phi_h^{m-1}, \mathcal{E}_h^{\mathbf{u},m}, \mu_h^m) \right| \\
& \leq |b(\mathcal{E}_a^{\phi,m}, \mathbf{u}^m, \mathcal{E}_h^{\mu,m})| + |b(\mathcal{E}_h^{\phi,m-1}, \mathbf{u}^m, \mathcal{E}_h^{\mu,m})| + |b(\tau\delta_\tau R_h \phi^m, \mathbf{u}^m, \mathcal{E}_h^{\mu,m})| \\
& + |b(\phi_h^{m-1}, \mathcal{E}_a^{\mathbf{u},m}, \mathcal{E}_h^{\mu,m})| + |b(\mathcal{E}_a^{\phi,m}, \mathcal{E}_h^{\mathbf{u},m}, \mu^m)| + |b(\mathcal{E}_h^{\phi,m-1}, \mathcal{E}_h^{\mathbf{u},m}, \mu^m)| \\
& + |b(\tau\delta_\tau R_h \phi^m, \mathcal{E}_h^{\mathbf{u},m}, \mu^m)| + |b(\phi_h^{m-1}, \mathcal{E}_h^{\mathbf{u},m}, \mathcal{E}_a^{\mu,m})|. \tag{3.89}
\end{aligned}$$

With the assumption $\mathbf{u} \in L^\infty(0, T; \mathbf{L}^4(\Omega))$ we have

$$\begin{aligned}
|b(\mathcal{E}_a^{\phi,m}, \mathbf{u}^m, \mathcal{E}_h^{\mu,m})| & \leq \|\nabla \mathcal{E}_a^{\phi,m}\|_{L^2} \|\mathbf{u}^m\|_{L^4} \|\mathcal{E}_h^{\mu,m}\|_{L^4} \\
& \leq C \|\nabla \mathcal{E}_a^{\phi,m}\|_{L^2}^2 + \frac{\varepsilon}{10} \|\nabla \mathcal{E}_h^{\mu,m}\|_{L^2}^2 \\
& \leq Ch^{2q} |\phi^m|_{H^{q+1}}^2 + \frac{\varepsilon}{10} \|\nabla \mathcal{E}_h^{\mu,m}\|_{L^2}^2, \tag{3.90}
\end{aligned}$$

as well as

$$\begin{aligned}
|b(\mathcal{E}_h^{\phi,m-1}, \mathbf{u}^m, \mathcal{E}_h^{\mu,m})| & \leq \|\nabla \mathcal{E}_h^{\phi,m-1}\|_{L^2} \|\mathbf{u}^m\|_{L^4} \|\mathcal{E}_h^{\mu,m}\|_{L^4} \\
& \leq C \|\nabla \mathcal{E}_h^{\phi,m-1}\|_{L^2}^2 + \frac{\varepsilon}{10} \|\nabla \mathcal{E}_h^{\mu,m}\|_{L^2}^2. \tag{3.91}
\end{aligned}$$

Using the stability of the elliptic projection, and reusing estimate (3.84), and $\mathbf{u} \in L^\infty(0, T; \mathbf{L}^4(\Omega))$

$$\begin{aligned}
|b(\tau\delta_\tau R_h \phi^m, \mathbf{u}^m, \mathcal{E}_h^{\mu,m})| & \leq \|\nabla \tau\delta_\tau R_h \phi^m\|_{L^2} \|\mathbf{u}^m\|_{L^4} \|\mathcal{E}_h^{\mu,m}\|_{L^4} \\
& \leq C \|\tau\nabla \delta_\tau R_h \phi^m\|_{L^2} \|\nabla \mathcal{E}_h^{\mu,m}\|_{L^2} \\
& \leq C \|\tau\nabla \delta_\tau \phi^m\|_{L^2} \|\nabla \mathcal{E}_h^{\mu,m}\|_{L^2} \\
& \leq C \|\tau\nabla \delta_\tau \phi^m\|_{L^2}^2 + \frac{\varepsilon}{10} \|\nabla \mathcal{E}_h^{\mu,m}\|_{L^2}^2 \\
& \leq C\tau \int_{t-\tau}^t \|\nabla \partial_s \phi(s)\|_{L^2}^2 ds + \frac{\varepsilon}{10} \|\nabla \mathcal{E}_h^{\mu,m}\|_{L^2}^2. \tag{3.92}
\end{aligned}$$

Using (3.55.3) and the error for the Darcy-Stokes Projection,

$$\begin{aligned}
|b(\phi_h^{m-1}, \mathcal{E}_a^{\mathbf{u},m}, \mathcal{E}_h^{\mu,m})| &\leq \|\nabla \phi_h^{m-1}\|_{L^2} \|\mathcal{E}_a^{\mathbf{u},m}\|_{L^4} \|\mathcal{E}_h^{\mu,m}\|_{L^4} \\
&\leq C \|\mathcal{E}_a^{\mathbf{u},m}\|_{H^1}^2 + \frac{\varepsilon}{10} \|\nabla \mathcal{E}_h^{\mu,m}\|_{L^2}^2 \\
&\leq Ch^{2q} (|\mathbf{u}^m|_{H^{q+1}}^2 + |p^m|_{H^q}^2) + \frac{\varepsilon}{10} \|\nabla \mathcal{E}_h^{\mu,m}\|_{L^2}^2. \tag{3.93}
\end{aligned}$$

Since we assume $\mu \in L^\infty(0, T; H^1(\Omega))$,

$$\begin{aligned}
|b(\mathcal{E}_a^{\phi,m}, \mathcal{E}_h^{\mathbf{u},m}, \mu^m)| &\leq \|\nabla \mathcal{E}_a^{\phi,m}\|_{L^2} \|\mathcal{E}_h^{\mathbf{u},m}\|_{L^4} \|\mu^m\|_{L^4} \\
&\leq C \|\nabla \mathcal{E}_a^{\phi,m}\|_{L^2} \|\nabla \mathcal{E}_h^{\mathbf{u},m}\|_{L^2} \|\mu^m\|_{H^1} \\
&\leq C \|\nabla \mathcal{E}_a^{\phi,m}\|_{L^2}^2 + \frac{\lambda}{8\gamma} \|\nabla \mathcal{E}_h^{\mathbf{u},m}\|_{L^2}^2 \\
&\leq Ch^{2q} |\phi^m|_{H^{q+1}}^2 + \frac{\lambda}{8\gamma} \|\nabla \mathcal{E}_h^{\mathbf{u},m}\|_{L^2}^2, \tag{3.94}
\end{aligned}$$

and

$$\begin{aligned}
|b(\mathcal{E}_h^{\phi,m-1}, \mathcal{E}_h^{\mathbf{u},m}, \mu^m)| &\leq \|\nabla \mathcal{E}_h^{\phi,m-1}\|_{L^2} \|\mathcal{E}_h^{\mathbf{u},m}\|_{L^4} \|\mu^m\|_{L^4} \\
&\leq C \|\nabla \mathcal{E}_h^{\phi,m-1}\|_{L^2} \|\nabla \mathcal{E}_h^{\mathbf{u},m}\|_{L^2} \|\mu^m\|_{H^1} \\
&\leq C \|\nabla \mathcal{E}_h^{\phi,m-1}\|_{L^2}^2 + \frac{\lambda}{8\gamma} \|\nabla \mathcal{E}_h^{\mathbf{u},m}\|_{L^2}^2. \tag{3.95}
\end{aligned}$$

Again, using $\mu \in L^\infty(0, T; H^1(\Omega))$, the stability of the elliptic projection, and reusing estimate (3.84)

$$\begin{aligned}
|b(\tau \delta_\tau R_h \phi^m, \mathcal{E}_h^{\mathbf{u},m}, \mu^m)| &\leq \|\nabla \tau \delta_\tau R_h \phi^m\|_{L^2} \|\mathcal{E}_h^{\mathbf{u},m}\|_{L^4} \|\mu^m\|_{H^1} \\
&\leq C \|\tau \nabla \delta_\tau R_h \phi^m\|_{L^2} \|\nabla \mathcal{E}_h^{\mathbf{u},m}\|_{L^2} \\
&\leq C \|\tau \nabla \delta_\tau \phi^m\|_{L^2} \|\nabla \mathcal{E}_h^{\mathbf{u},m}\|_{L^2} \\
&\leq C\tau \int_{t-\tau}^t \|\nabla \partial_s \phi(s)\|_{L^2}^2 ds + \frac{\lambda}{8\gamma} \|\nabla \mathcal{E}_h^{\mathbf{u},m}\|_{L^2}^2. \tag{3.96}
\end{aligned}$$

Finally,

$$\begin{aligned}
|b(\phi_h^{m-1}, \mathcal{E}_h^{\mathbf{u},m}, \mathcal{E}_a^{\mu,m})| &\leq \|\nabla \phi_h^{m-1}\|_{L^2} \|\mathcal{E}_h^{\mathbf{u},m}\|_{L^4} \|\mathcal{E}_a^{\mu,m}\|_{L^4} \\
&\leq C \|\nabla \mathcal{E}_h^{\mathbf{u},m}\|_{L^2} \|\nabla \mathcal{E}_a^{\mu,m}\|_{L^2} \\
&\leq \frac{\lambda}{8\gamma} \|\nabla \mathcal{E}_h^{\mathbf{u},m}\|_{L^2}^2 + C \|\nabla \mathcal{E}_a^{\mu,m}\|_{L^2}^2 \\
&\leq \frac{\lambda}{8\gamma} \|\nabla \mathcal{E}_h^{\mathbf{u},m}\|_{L^2}^2 + Ch^{2q} |\mu^m|_{H^{q+1}}^2. \tag{3.97}
\end{aligned}$$

Combining the estimates (3.80) – (3.97) with the error equation (3.72) and using the triangle inequality, the result follows. $\square$

Lemma 3.4.4. *Suppose that $(\phi^m, \mu^m, \mathbf{u}^m)$ is a weak solution to (3.68a) – (3.68e), with the additional regularities (3.67). Then, for any $h, \tau > 0$, there exists a constant $C > 0$, independent of h and τ , such that*

$$\left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2 \leq 7\varepsilon^2 \|\nabla \mathcal{E}_h^{\mu,m}\|_{L^2}^2 + C \left\| \nabla \mathcal{E}_h^{\phi,m-1} \right\|_{L^2}^2 + 7C_2^2 \|\nabla \mathcal{E}_h^{\mathbf{u},m}\|_{L^2}^2 + C\mathcal{R}, \tag{3.98}$$

for any $t \in (\tau, T]$, where $C_2 = C_0^2 C_1$, C_0 is the $H^1(\Omega) \hookrightarrow L^4(\Omega)$ Sobolev embedding constant, C_1 is a bound for $\max_{0 \leq t \leq T} \|\nabla \phi_h^m\|_{L^2}^2$, and $\mathcal{R}$ is the consistency term given in (3.79).

Proof. Setting $\nu = \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right)$ in (3.71a), we have

$$\begin{aligned}
\left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2 &= -\varepsilon a \left(\mathcal{E}_h^{\mu,m}, \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right) + \left(\sigma_1^{\phi,m} + \sigma_2^{\phi,m}, \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right) \\
&\quad - b \left(\phi^m, \mathbf{u}^m, \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right) + b \left(\phi_h^{m-1}, \mathbf{u}_h^m, \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right) \\
&= -\varepsilon \left(\mathcal{E}_h^{\mu,m}, \delta_\tau \mathcal{E}_h^{\phi,m} \right) + \left(\sigma_1^{\phi,m} + \sigma_2^{\phi,m}, \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right) \\
&\quad - b \left(\mathcal{E}_a^{\phi,m}, \mathbf{u}^m, \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right) - b \left(\mathcal{E}_h^{\phi,m-1}, \mathbf{u}^m, \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right) \\
&\quad - b \left(\tau \delta_\tau R_h \phi^m, \mathbf{u}^m, \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right) - b \left(\phi_h^{m-1}, \mathcal{E}_a^{\mathbf{u},m}, \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right) \\
&\quad - b \left(\phi_h^{m-1}, \mathcal{E}_h^{\mathbf{u},m}, \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right) \\
&\leq \varepsilon \left\| \nabla \mathcal{E}_h^{\mu,m} \right\|_{L^2} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h} + \left\| \sigma_1^{\phi,m} + \sigma_2^{\phi,m} \right\|_{L^2} \left\| \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right\|_{L^2} \\
&\quad + \left\| \nabla \mathcal{E}_a^{\phi,m} \right\|_{L^2} \left\| \mathbf{u}^m \right\|_{L^4} \left\| \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right\|_{L^4} \\
&\quad + \left\| \nabla \mathcal{E}_h^{\phi,m-1} \right\|_{L^2} \left\| \mathbf{u}^m \right\|_{L^4} \left\| \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right\|_{L^4} \\
&\quad + \left\| \tau \nabla \delta_\tau R_h \phi^m \right\|_{L^2} \left\| \mathbf{u}^m \right\|_{L^4} \left\| \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right\|_{L^4} \\
&\quad + \left\| \nabla \phi_h^{m-1} \right\|_{L^2} \left\| \mathcal{E}_a^{\mathbf{u},m} \right\|_{L^4} \left\| \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right\|_{L^4} \\
&\quad + \left\| \nabla \phi_h^{m-1} \right\|_{L^2} \left\| \mathcal{E}_h^{\mathbf{u},m} \right\|_{L^4} \left\| \mathsf{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi,m} \right) \right\|_{L^4} \\
&\leq \frac{7\varepsilon^2}{2} \left\| \nabla \mathcal{E}_h^{\mu,m} \right\|_{L^2}^2 + \frac{1}{14} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2 + C \left\| \sigma_1^{\phi,m} + \sigma_2^{\phi,m} \right\|_{L^2}^2 \\
&\quad + \frac{1}{14} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2 + C \left\| \nabla \mathcal{E}_a^{\phi,m} \right\|_{L^2}^2 + \frac{1}{14} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2 \\
&\quad + C \left\| \nabla \mathcal{E}_h^{\phi,m-1} \right\|_{L^2}^2 + \frac{1}{14} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2 + C\tau^2 \left\| \nabla \delta_\tau R_h \phi^m \right\|_{L^2}^2 \\
&\quad + \frac{1}{14} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2 + C \left\| \mathcal{E}_a^{\mathbf{u},m} \right\|_{L^2}^2 + \frac{1}{14} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2 \\
&\quad + \frac{7C_2^2}{2} \left\| \nabla \mathcal{E}_h^{\mathbf{u},m} \right\|_{L^2}^2 + \frac{1}{14} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2 \\
&\leq \frac{1}{2} \left\| \delta_\tau \mathcal{E}_h^{\phi,m} \right\|_{-1,h}^2 + \frac{7\varepsilon^2}{2} \left\| \nabla \mathcal{E}_h^{\mu,m} \right\|_{L^2}^2 + \frac{7C_2^2}{2} \left\| \nabla \mathcal{E}_h^{\mathbf{u},m} \right\|_{L^2}^2 \\
&\quad + C \left\| \nabla \mathcal{E}_h^{\phi,m-1} \right\|_{L^2}^2 + C\mathcal{R},
\end{aligned}$$

where we have used Lemmas 2.2.21 and 3.4.1. The result now follows. $\square$

Lemma 3.4.5. *Suppose that $(\phi^m, \mu^m, \mathbf{u}^m)$ is a weak solution to (3.68a) – (3.68e), with the additional regularities (3.67). Then, for any $h, \tau > 0$, there exists a constant $C > 0$, independent of h and τ , such that*

$$\begin{aligned} \|\nabla \mathcal{E}_h^{\mu, m}\|_{L^2}^2 + \|\mathcal{E}_h^{\mathbf{u}, m}\|_{H^1}^2 + a\left(\mathcal{E}_h^{\phi, m}, \delta_\tau \mathcal{E}_h^{\phi, m}\right) + \left(\mathcal{E}_h^{\phi, m}, \delta_\tau \mathcal{E}_h^{\phi, m}\right)_{-1, h} + (\delta_\tau \mathcal{E}_h^{\mathbf{u}, m}, \mathcal{E}_h^{\mathbf{u}, m}) \\ \leq C \left\| \nabla \mathcal{E}_h^{\phi, m} \right\|_{L^2}^2 + C \left\| \nabla \mathcal{E}_h^{\phi, m-1} \right\|_{L^2}^2 + C\mathcal{R}. \end{aligned} \quad (3.99)$$

Proof. This follows upon combining the last two lemmas and choosing α in (3.78) appropriately. $\square$

Using the last lemma, we are ready to show the main convergence result for our convex splitting scheme.

Theorem 3.4.6. *Suppose $(\phi^m, \mu^m, \mathbf{u}^m)$ is a weak solution to (3.68a) – (3.68e), with the additional regularities (3.67). Then, provided $0 < \tau < \tau_0$, for some τ_0 sufficiently small,*

$$\begin{aligned} \max_{1 \leq m \leq M} \left[\left\| \nabla \mathcal{E}_h^{\phi, m} \right\|_{L^2}^2 + \left\| \mathcal{E}_h^{\phi, m} \right\|_{-1, h}^2 + \|\mathcal{E}_h^{\mathbf{u}, m}\|_{L^2}^2 \right] \\ + \tau \sum_{m=1}^M \left[\|\nabla \mathcal{E}_h^{\mu, m}\|_{L^2}^2 + \|\mathcal{E}_h^{\mathbf{u}, m}\|_{H^1}^2 + \left\| \delta_\tau \mathcal{E}_h^{\phi, m} \right\|_{-1, h}^2 \right] \leq C(T)(\tau^2 + h^{2q}) \end{aligned} \quad (3.100)$$

for some $C(T) > 0$ that is independent of τ and h .

Proof. Setting $t = t_m$ and using Lemma 3.4.5 and the arithmetic-geometric mean inequality, we have

$$\begin{aligned} \delta_\tau \left\| \nabla \mathcal{E}_h^{\phi, m} \right\|_{L^2}^2 + \delta_\tau \left\| \mathcal{E}_h^{\phi, m} \right\|_{-1, h}^2 + \delta_\tau \|\mathcal{E}_h^{\mathbf{u}, m}\|_{L^2}^2 \\ + \|\nabla \mathcal{E}_h^{\mu, m}\|_{L^2}^2 + \|\mathcal{E}_h^{\mathbf{u}, m}\|_{H^1}^2 \leq C \left\| \nabla \mathcal{E}_h^{\phi, m} \right\|_{L^2}^2 + C \left\| \nabla \mathcal{E}_h^{\phi, m-1} \right\|_{L^2}^2 + C\mathcal{R}^m. \end{aligned}$$

Let $1 < \ell \leq M$. Applying $\tau \sum_{m=1}^{\ell}$ and using $\mathcal{E}_h^{\phi,0} \equiv 0$, $\mathcal{E}_h^{\mathbf{u},0} \equiv \mathbf{0}$,

$$\begin{aligned} & \left\| \nabla \mathcal{E}_h^{\phi,\ell} \right\|_{L^2}^2 + \left\| \mathcal{E}_h^{\phi,\ell} \right\|_{-1,h}^2 + \left\| \mathcal{E}_h^{\mathbf{u},\ell} \right\|_{L^2}^2 \\ & + \tau \sum_{m=1}^{\ell} \left[\left\| \nabla \mathcal{E}_h^{\mu,m} \right\|_{L^2}^2 + \left\| \mathcal{E}_h^{\mathbf{u},m} \right\|_{H^1}^2 \right] \leq C\tau \sum_{m=1}^{\ell} \mathcal{R}^m + C_1\tau \sum_{m=1}^{\ell} \left\| \nabla \mathcal{E}_h^{\phi,m} \right\|_{L^2}^2. \end{aligned} \quad (3.101)$$

If $0 < \tau \leq \tau_0 := \frac{1}{2C_1} < \frac{1}{C_1}$, it follows from the last estimate that

$$\begin{aligned} \left\| \nabla \mathcal{E}_h^{\phi,\ell} \right\|_{L^2}^2 & \leq C\tau \sum_{m=1}^{\ell} \mathcal{R}^m + \frac{C_1\tau}{1 - C_1\tau} \sum_{m=1}^{\ell-1} \left\| \nabla \mathcal{E}_h^{\phi,m} \right\|_{L^2}^2 \\ & \leq C(\tau^2 + h^{2q}) + C\tau \sum_{m=1}^{\ell-1} \left\| \nabla \mathcal{E}_h^{\phi,m} \right\|_{L^2}^2, \end{aligned} \quad (3.102)$$

where we have used the regularity assumptions to conclude $\tau \sum_{m=1}^M \mathcal{R}^m \leq C(\tau^2 + h^{2q})$. Appealing to the discrete Gronwall inequality (2.42), it follows that, for any $1 < \ell \leq M$,

$$\left\| \nabla \mathcal{E}_h^{\phi,\ell} \right\|_{L^2}^2 \leq C(T)(\tau^2 + h^{2q}). \quad (3.103)$$

Considering estimates (3.101) and (3.103), we get the desired result. $\square$

Remark 3.4.7. *From here it is straightforward to establish an optimal error estimate of the form*

$$\max_{1 \leq m \leq M} \left[\left\| \nabla \mathcal{E}_h^{\phi,m} \right\|_{L^2}^2 + \left\| \mathcal{E}_h^{\mathbf{u},m} \right\|_{L^2}^2 \right] + \tau \sum_{m=1}^M \left[\left\| \nabla \mathcal{E}_h^{\mu,m} \right\|_{L^2}^2 + \left\| \nabla \mathcal{E}_h^{\mathbf{u},m} \right\|_{L^2}^2 \right] \leq C(T)(\tau^2 + h^{2q}) \quad (3.104)$$

using $\mathcal{E}_h^{\phi,m} = \mathcal{E}_a^{\phi,m} + \mathcal{E}_h^{\phi,m}$, et cetera, the triangle inequality, and the standard spatial approximations. We omit the details for the sake of brevity.

3.5 Numerical Experiments

In this section, we provide some numerical experiments to gauge the accuracy and reliability of the fully discrete finite element method developed in the previous sections. We use a square domain $\Omega = (0, 1)^2 \subset \mathbb{R}^2$ and take $\mathcal{T}_h$ to be a regular triangulation of Ω consisting of right isosceles triangles. To refine the mesh, we assume that $\mathcal{T}_\ell$, $\ell = 0, 1, \dots, L$, is an hierarchy of nested triangulations of Ω where $\mathcal{T}_\ell$ is obtained by subdividing the triangles of $\mathcal{T}_{\ell-1}$ into four congruent sub-triangles. Note that $h_{\ell-1} = 2h_\ell$, $\ell = 1, \dots, L$ and that $\{\mathcal{T}_\ell\}$ is a quasi-uniform family. For the flow problem, we use the inf-sup-stable Taylor-Hood element where the $\mathcal{P}_1$ finite element space is used for the pressure and the $[\mathcal{P}_2]^2$ finite element space is used for the velocity. (We use a family of meshes $\mathcal{T}_h$ such that no triangle in the mesh has more than one edge on the boundary, as is usually required for the stability of the Taylor-Hood element [5].) We use the $\mathcal{P}_1$ finite element space for the phase field and chemical potential. In short, we take $q = 1$.

We solve the scheme (3.7a) – (3.7e) with the following parameters: $\lambda = 1$, $\eta = 1$, $\theta = 0$, and $\epsilon = 6.25 \times 10^{-2}$. The initial data for the phase field are taken to be

$$\phi_h^0 = \mathcal{I}_h \left\{ \frac{1}{2} \left(1.0 - \cos(4.0\pi x) \right) \cdot \left(1.0 - \cos(2.0\pi y) \right) - 1.0 \right\}, \quad (3.105)$$

where $\mathcal{I}_h : H^2(\Omega) \rightarrow S_h$ is the standard nodal interpolation operator. Recall that our analysis does not specifically cover the use of the operator $\mathcal{I}_h$ in the initialization step. But, since the error introduced by its use is optimal, a slight modification of the analysis show that this will lead to optimal rates of convergence overall. (See Remark 3.3.3.) The initial data for the velocity are taken as $\mathbf{u}_h^0 = \mathbf{0}$. Values of the remaining parameters are given in the caption of Table 3.1. To solve the system of equations above numerically, we are using the finite element libraries from the FEniCS Project [47]. We solve the fully coupled system by a Picard-type iteration. Namely, at a given time step we fix the velocity and pressure, then solve for ϕ_h , μ_h , and ξ_h .

With these updated, we then solve for the velocity and pressure. This is repeated until convergence.

Note that source terms are not naturally present in the system of equations (1.4a) – (1.4f). To get around the fact that we do not have possession of exact solutions, we measure error by a different means. Specifically, we compute the rate at which the Cauchy difference, $\delta_\zeta := \zeta_{h_f}^{M_f} - \zeta_{h_c}^{M_c}$, converges to zero, where $h_f = 2h_c$, $\tau_f = 2\tau_c$, and $\tau_f M_f = \tau_c M_c = T$. Then, using a linear refinement path, *i.e.*, $\tau = Ch$, and assuming $q = 1$, we have

$$\|\delta_\zeta\|_{H^1} = \left\| \zeta_{h_f}^{M_f} - \zeta_{h_c}^{M_c} \right\|_{H^1} \leq \left\| \zeta_{h_f}^{M_f} - \zeta(T) \right\|_{H^1} + \left\| \zeta_{h_c}^{M_c} - \zeta(T) \right\|_{H^1} = \mathcal{O}(h_f^q + \tau_f) = \mathcal{O}(h_f). \quad (3.106)$$

The results of the H^1 Cauchy error analysis are found in Table 3.1 and confirm first-order convergence in this case. Additionally, we have proved that (at the theoretical level) the energy is non-increasing at each time step. This is observed in our computations and shown below in Figure 3.1.

Table 3.1: H^1 Cauchy convergence test. The final time is $T = 4.0 \times 10^{-1}$, and the refinement path is taken to be $\tau = .001\sqrt{2}h$. The other parameters are $\varepsilon = 6.25 \times 10^{-2}$; $\Omega = (0, 1)^2$. The Cauchy difference is defined via $\delta_\phi := \phi_{h_f} - \phi_{h_c}$, where the approximations are evaluated at time $t = T$, and analogously for δ_μ , and δ_p . Since $q = 1$, *i.e.*, we use $\mathcal{P}_1$ elements for these variables, the norm of the Cauchy difference at T is expected to be $\mathcal{O}(\tau_f) + \mathcal{O}(h_f) = \mathcal{O}(h_f)$.

h_c	h_f	$\ \delta_\phi\ _{H^1}$	rate	$\ \delta_\mu\ _{H^1}$	rate	$\ \delta_p\ _{H^1}$	rate
$\sqrt{2}/8$	$\sqrt{2}/16$	1.988×10^0	—	2.705×10^0	—	3.732×10^0	—
$\sqrt{2}/16$	$\sqrt{2}/32$	9.149×10^{-1}	1.09	1.309×10^0	1.03	9.73×10^{-1}	1.92
$\sqrt{2}/32$	$\sqrt{2}/64$	4.483×10^{-1}	1.02	6.216×10^{-1}	1.05	9.417×10^{-1}	1.02
$\sqrt{2}/64$	$\sqrt{2}/128$	2.231×10^{-1}	1.00	3.056×10^{-1}	1.02	4.688×10^{-1}	1.00

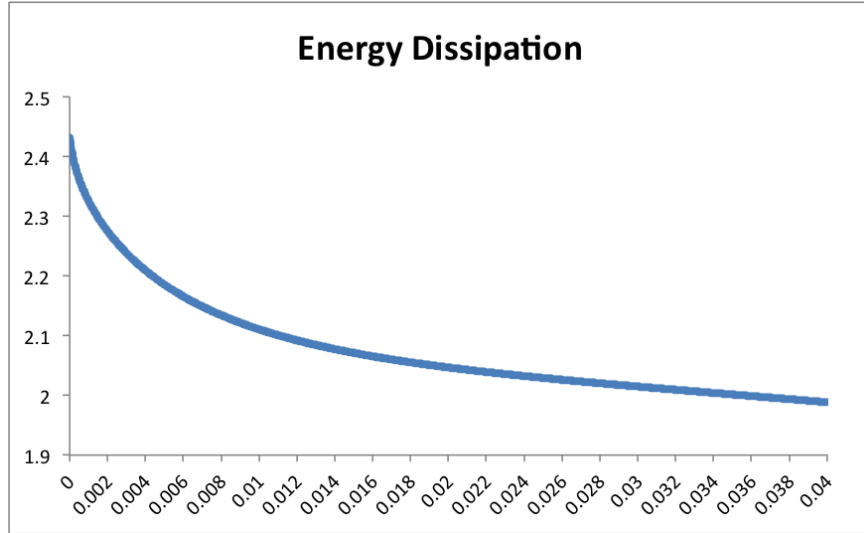


Figure 3.1: Energy dissipation for the first order numerical scheme for the Cahn-Hilliard-Darcy-Stokes problem. All parameters are as listed in Table 3.1 and we have taken $h = \frac{\sqrt{2}}{64}$.

Chapter 4

The Numerical Analysis of a Second-Order Convex Splitting Scheme for the Cahn-Hilliard Equation

In Chapter 4, we develop and analyze a second order in time convex splitting numerical scheme for the Cahn-Hilliard problem. We will begin by setting up a weak formulation of the problem (1.2a) – (1.2c) and presenting the recent developments on second order schemes related to the Cahn-Hilliard equation. We then introduce our new mixed methods numerical scheme and show that the scheme is unconditionally stable and optimally convergent. We then back up these findings with the results from a numerical experiment.

4.1 A Weak Formulation of the Cahn-Hilliard Equation

A weak formulation of (1.2a) – (1.2c) may be written as follows: find (ϕ, μ) such that

$$\phi \in L^\infty(0, T; H^1(\Omega)) \cap L^4(0, T; L^\infty(\Omega)), \quad (4.1a)$$

$$\partial_t \phi \in L^2(0, T; H^{-1}(\Omega)), \quad (4.1b)$$

$$\mu \in L^2(0, T; H^1(\Omega)), \quad (4.1c)$$

and there hold for almost all $t \in (0, T)$

$$\langle \partial_t \phi, \nu \rangle + \varepsilon a(\mu, \nu) = 0 \quad \forall \nu \in H^1(\Omega), \quad (4.2a)$$

$$(\mu, \psi) - \varepsilon a(\phi, \psi) - \varepsilon^{-1}(\phi^3 - \phi, \psi) = 0 \quad \forall \psi \in H^1(\Omega), \quad (4.2b)$$

with the “compatible” initial data

$$\phi(0) = \phi_0 \in H_N^2(\Omega) := \{v \in H^2(\Omega) \mid \partial_n v = 0 \text{ on } \partial\Omega\}. \quad (4.3)$$

We note that the system (4.2a) – (4.2b) may be recovered from the Cahn-Hilliard-Darcy-Stokes system presented in Chapter 3 by setting $\gamma, \theta = 0$. Hence, it shares those properties described in Section 3.3. Specifically, the system (4.2a)–(4.2b) is mass conservative and the homogeneous Neumann boundary conditions associated with the phase variables ϕ and μ are natural in the mixed weak formulation of the problem. Likewise, weak solutions of (4.2a) – (4.2b) dissipate the energy (1.1) and the energy law (3.34) simplifies in this setting: for any $t \in [0, T]$,

$$E(\phi(t)) + \int_0^t \varepsilon \|\nabla \mu(s)\|_{L^2}^2 ds = E(\phi_0). \quad (4.4)$$

The restriction of the equations to the Cahn-Hilliard problem does not affect the availability of the existence of weak solutions and the method by which this is proven follows a compactness/energy method shown, for example, in [19].

4.2 The State-of-the-Art on Second-Order Numerical Schemes for the Cahn-Hilliard Equation

In general, the analysis of second-order numerical schemes for nonlinear equations can be significantly more difficult than that for first-order methods [59]. As such, second order schemes for Cahn-Hilliard type equations have been less commonly investigated. Nevertheless, such work has been reported in the following articles [4, 8, 14, 15, 26, 55, 57, 65]. We mention, in particular, the secant-type algorithms described in [14, 26]. With the notation $\Psi(\phi) := \frac{1}{4}(\phi^2 - 1)^2$, the secant scheme of [14] for the Cahn-Hilliard equation may be formulated as

$$\phi^{n+1} - \phi^n = s\varepsilon \Delta \mu^{n+\frac{1}{2}}, \quad \mu^{n+\frac{1}{2}} := \varepsilon^{-1} \frac{\Psi(\phi^{n+1}) - \Psi(\phi^n)}{\phi^{n+1} - \phi^n} - \frac{\varepsilon}{2} (\Delta \phi^{n+1} - \Delta \phi^n). \quad (4.5)$$

This scheme is energy stable. However, it may not be unconditionally uniquely solvable with respect to the time step size, s . (See [14, 15, 26] for details.) Lack of unconditional solvability may be problematic as coarsening studies using the Cahn Hilliard equation may involve very large time scales, requiring potentially very large time steps for efficiency.

Chen and Shen introduce a semi-implicit Fourier-spectral method in [8] which has a couple of advantages over explicit Euler finite difference methods. In their scheme, the high-order semi-implicit treatment in time enables the use of larger time steps while maintaining higher accuracy. However, even though the time step size may be taken to be larger, the scheme's stability is still not completely independent on

the time step size. Furthermore, although they test their scheme through numerical simulations, no formal stability or convergence analyses are presented in the paper.

Wu, Zwieten, and Van Der Zee [65] introduce a semi-discrete second-order convex splitting scheme for Cahn-Hilliard-type equations with applications to diffuse-interface tumor-growth models. They are able to show unconditional energy stability relative to the energy norms, mass conservation, and a second order local truncation error for the phase field parameter. However, they do not prove second order accuracy relative to the energy norm for the phase field parameter.

In [32], Guo *et. al.* propose a new second-order-accurate-in-time, finite difference scheme for the Cahn-Hilliard equation in three dimensions. In their paper, they show their scheme is uniquely solvable and unconditionally energy stable. Boosting the basic energy stability estimates leads to a convergence analysis demonstrating that convergence of their scheme is unconditional with respect to the time and space step sizes. Following their work, we propose a fully discrete, mixed finite element scheme for the Cahn-Hilliard problem (1.2a)–(1.2c):

$$\phi_h^{n+1} - \phi_h^n = s \varepsilon \Delta_h \mu_h^{n+\frac{1}{2}}, \quad (4.6a)$$

$$\begin{aligned} \mu_h^{n+\frac{1}{2}} := & \frac{1}{4\varepsilon} (\phi_h^{n+1} + \phi_h^n) \left((\phi_h^{n+1})^2 + (\phi_h^n)^2 \right) - \frac{1}{\varepsilon} \left(\frac{3}{2} \phi_h^n - \frac{1}{2} \phi_h^{n-1} \right) \\ & - \varepsilon \Delta_h \left(\frac{3}{4} \phi_h^{n+1} + \frac{1}{4} \phi_h^{n-1} \right), \end{aligned} \quad (4.6b)$$

where Δ_h above is a finite difference stencil approximating the Laplacian, and ϕ_h and μ_h are grid variables. In our finite element version of the scheme, the stability and solvability statements we prove are *completely unconditional with respect to the time and space step sizes*. We are able to achieve unconditional $L^\infty(0, T; L^\infty(\Omega))$ stability for the phase field variable ϕ_h and unconditional $L^\infty(0, T; L^2(\Omega))$ stability for the chemical potential μ_h leading to optimal error estimates for ϕ_h and μ_h in the appropriate energy norms.

4.3 A Mixed Finite Element Splitting Scheme

4.3.1 Definition of the Scheme

Our mixed second-order splitting scheme is defined as follows: for any $1 \leq m \leq M-1$, given $\phi_h^m, \phi_h^{m-1} \in S_h$, find $\phi_h^{m+1}, \mu_h^{m+\frac{1}{2}} \in S_h$ such that

$$\left(\delta_\tau \phi_h^{m+\frac{1}{2}}, \nu \right) + \varepsilon a \left(\mu_h^{m+\frac{1}{2}}, \nu \right) = 0 \quad \forall \nu \in S_h, \quad (4.7a)$$

$$\begin{aligned} \varepsilon^{-1} \left(\chi \left(\phi_h^{m+1}, \phi_h^m \right), \psi \right) - \varepsilon^{-1} \left(\tilde{\phi}_h^{m+\frac{1}{2}}, \psi \right) \\ + \varepsilon a \left(\check{\phi}_h^{m+\frac{1}{2}}, \psi \right) - \left(\mu_h^{m+\frac{1}{2}}, \psi \right) = 0 \quad \forall \psi \in S_h, \end{aligned} \quad (4.7b)$$

where

$$\delta_\tau \phi_h^{m+\frac{1}{2}} := \frac{\phi_h^{m+1} - \phi_h^m}{\tau}, \quad \phi_h^{m+\frac{1}{2}} := \frac{1}{2} \phi_h^{m+1} + \frac{1}{2} \phi_h^m, \quad \tilde{\phi}_h^{m+\frac{1}{2}} := \frac{3}{2} \phi_h^m - \frac{1}{2} \phi_h^{m-1}, \quad (4.8)$$

$$\check{\phi}_h^{m+\frac{1}{2}} := \frac{3}{4} \phi_h^{m+1} + \frac{1}{4} \phi_h^{m-1}, \quad \chi \left(\phi_h^{m+1}, \phi_h^m \right) := \frac{1}{2} \left((\phi_h^{m+1})^2 + (\phi_h^m)^2 \right) \phi_h^{m+\frac{1}{2}}. \quad (4.9)$$

Since this is a multi-step scheme, it requires a separate initialization process. For the first step, the scheme is as follows: given $\phi_h^0 \in S_h$, find $\phi_h^1, \mu_h^{\frac{1}{2}} \in S_h$ such that

$$\left(\delta_\tau \phi_h^{\frac{1}{2}}, \nu \right) + \varepsilon a \left(\mu_h^{\frac{1}{2}}, \nu \right) = 0 \quad \forall \nu \in S_h, \quad (4.10a)$$

$$\begin{aligned} \varepsilon^{-1} \left(\chi \left(\phi_h^1, \phi_h^0 \right), \psi \right) - \varepsilon^{-1} \left(\phi_h^0, \psi \right) + \frac{\tau}{2} a \left(\mu_h^0, \psi \right) \\ + \varepsilon a \left(\phi_h^{\frac{1}{2}}, \psi \right) - \left(\mu_h^{\frac{1}{2}}, \psi \right) = 0 \quad \forall \psi \in S_h, \end{aligned} \quad (4.10b)$$

where $\phi_h^0 := R_h \phi_0$, and $\mu_h^0 := R_h \mu_0$, such that

$$\mu_0 := \varepsilon^{-1} \left(\phi_0^3 - \phi_0 \right) - \varepsilon \Delta \phi_0. \quad (4.11)$$

Remark 4.3.1. *The notation for the backwards difference operator has changed slightly from Chapter 3. The necessity of the notation change is understood through the definitions of the two schemes.*

Theorem 4.3.2. *The scheme (4.7a) – (4.7b) coupled with the initial scheme (4.10b) – (4.10b) is uniquely solvable for any mesh parameters h and τ and for any model parameters.*

Proof. The proof is based on convexity arguments and follows in a similar manner as that of Theorem 5 from reference [37]. We omit the details for brevity. $\square$

Remark 4.3.3. *Note that it is not necessary for solvability and some basic energy stabilities that the μ -space and the ϕ -space be equal. However, the proofs of the higher-order stability estimates, in particular the proof in Lemma 4.3.10, do require the equivalence of these spaces.*

Remark 4.3.4. *The elliptic projections are used in the initialization for simplicity in the forthcoming error analysis. However, other (simpler) projections may be used in the initialization step, as long as they have good approximation properties.*

4.3.2 Unconditional Energy Stability

We now show that the solutions to our scheme enjoy stability properties that are similar to those of the PDE solutions, and moreover, these properties hold regardless of the sizes of h and τ . The first property, the unconditional energy stability, is a direct result of the convex decomposition.

Lemma 4.3.5. *Let $(\phi_h^1, \mu_h^{\frac{1}{2}}) \in S_h \times S_h$ be the unique solution of the initialization scheme (4.10a) – (4.10b). Then the following first-step energy stability holds for any $h, \tau > 0$:*

$$E(\phi_h^1) + \tau\varepsilon \left\| \nabla \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 + \frac{1}{4\varepsilon} \left\| \phi_h^1 - \phi_h^0 \right\|_{L^2}^2 \leq E(\phi_h^0) + \frac{\varepsilon\tau^2}{4} \left\| \Delta_h \mu_h^0 \right\|_{L^2}^2, \quad (4.12)$$

where $E(\phi)$ is defined in (1.1).

Proof. Setting $\nu = \tau\mu_h^{\frac{1}{2}}$ in (4.10a) and $\psi = \tau\delta_\tau\phi_h^{\frac{1}{2}} = \phi_h^1 - \phi_h^0$ in (4.10b) yields the following:

$$\tau \left(\delta_\tau \phi_h^{\frac{1}{2}}, \mu_h^{\frac{1}{2}} \right) + \tau \varepsilon \left\| \nabla \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 = 0, \quad (4.13)$$

$$\begin{aligned} \varepsilon^{-1} \left(\chi(\phi_h^1, \phi_h^0), \phi_h^1 - \phi_h^0 \right) - \varepsilon^{-1} \left(\phi_h^0, \phi_h^1 - \phi_h^0 \right) + \varepsilon a \left(\phi_h^{\frac{1}{2}}, \phi_h^1 - \phi_h^0 \right) \\ + \frac{\tau}{2} a \left(\mu_h^0, \phi_h^1 - \phi_h^0 \right) - \tau \left(\mu_h^{\frac{1}{2}}, \delta_\tau \phi_h^{\frac{1}{2}} \right) = 0. \end{aligned} \quad (4.14)$$

Adding Equations (4.13) and (4.14), using Young's inequality, and the following identities

$$\left(\chi(\phi_h^1, \phi_h^0), \phi_h^1 - \phi_h^0 \right) = \frac{1}{4} \left(\left\| \phi_h^1 \right\|_{L^4}^4 - \left\| \phi_h^0 \right\|_{L^4}^4 \right), \quad (4.15)$$

$$\left(\phi_h^0, \phi_h^1 - \phi_h^0 \right) = \frac{1}{2} \left(\left\| \phi_h^1 \right\|_{L^2}^2 - \left\| \phi_h^0 \right\|_{L^2}^2 - \left\| \phi_h^1 - \phi_h^0 \right\|_{L^2}^2 \right), \quad (4.16)$$

the result is obtained. $\square$

We now define a modified energy

$$F(\phi, \psi) := E(\phi) + \frac{1}{4\varepsilon} \left\| \phi - \psi \right\|_{L^2}^2 + \frac{\varepsilon}{8} \left\| \nabla \phi - \nabla \psi \right\|_{L^2}^2, \quad (4.17)$$

where $E(\phi)$ is defined as above and present a technical lemma for use in the forthcoming stability analysis.

Lemma 4.3.6. *Let $(\phi_h^{m+1}, \mu_h^{m+\frac{1}{2}}) \in S_h \times S_h$ be the unique solution of (4.7a) – (4.7b). Then the following identities holds for any $h, \tau > 0$:*

$$\begin{aligned} \left(\chi(\phi_h^{m+1}, \phi_h^m) - \tilde{\phi}_h^{m+\frac{1}{2}}, \delta_\tau \phi_h^{m+\frac{1}{2}} \right) = \frac{1}{4\tau} \left(\left\| (\phi_h^{m+1})^2 - 1 \right\|_{L^2}^2 - \left\| (\phi_h^m)^2 - 1 \right\|_{L^2}^2 \right) \\ + \frac{1}{4\tau} \left(\left\| \phi_h^{m+1} - \phi_h^m \right\|_{L^2}^2 - \left\| \phi_h^m - \phi_h^{m-1} \right\|_{L^2}^2 \right) \\ + \frac{1}{4\tau} \left\| \phi_h^{m+1} - 2\phi_h^m + \phi_h^{m-1} \right\|_{L^2}^2 \end{aligned} \quad (4.18)$$

$$\begin{aligned}
a\left(\check{\phi}_h^{m+\frac{1}{2}}, \delta_\tau \phi_h^{m+\frac{1}{2}}\right) &= \frac{1}{2\tau} \left(\|\nabla \phi_h^{m+1}\|_{L^2}^2 - \|\nabla \phi_h^m\|_{L^2}^2 \right) \\
&\quad + \frac{1}{8\tau} \left(\|\nabla \phi_h^{m+1} - \nabla \phi_h^m\|_{L^2}^2 - \|\nabla \phi_h^m - \nabla \phi_h^{m-1}\|_{L^2}^2 \right) \\
&\quad + \frac{1}{8\tau} \|\nabla \phi_h^{m+1} - 2\nabla \phi_h^m + \nabla \phi_h^{m-1}\|_{L^2}^2. \tag{4.19}
\end{aligned}$$

Proof. To prove (4.18), we use the definitions of $\chi(\phi_h^{m+1}, \phi_h^m)$ and $\check{\phi}_h^{m+\frac{1}{2}}$ and expand as follows,

$$\begin{aligned}
&\left(\chi(\phi_h^{m+1}, \phi_h^m) - \check{\phi}_h^{m+\frac{1}{2}}, \delta_\tau \phi_h^{m+\frac{1}{2}} \right) \\
&= \frac{1}{4\tau} \left((\phi_h^{m+1})^2 + (\phi_h^m)^2, (\phi_h^{m+1})^2 - (\phi_h^m)^2 \right) - \frac{1}{\tau} \left(\frac{3}{2}\phi_h^m - \frac{1}{2}\phi_h^{m-1}, \phi_h^{m+1} - \phi_h^m \right) \\
&= \frac{1}{4\tau} \left((\phi_h^{m+1})^2 + (\phi_h^m)^2, (\phi_h^{m+1})^2 - (\phi_h^m)^2 \right) - \frac{1}{2\tau} (\phi_h^{m+1} + \phi_h^m, \phi_h^{m+1} - \phi_h^m) \\
&\quad + \frac{1}{2\tau} (\phi_h^{m+1} - 2\phi_h^m + \phi_h^{m-1}, \phi_h^{m+1} - \phi_h^m) \\
&= \frac{1}{4\tau} \left(\left\| (\phi_h^{m+1})^2 \right\|_{L^2}^2 - \left\| (\phi_h^m)^2 \right\|_{L^2}^2 \right) - \frac{1}{2\tau} \left(\|\phi_h^{m+1}\|_{L^2}^2 - \|\phi_h^m\|_{L^2}^2 \right) \\
&\quad + \frac{1}{4\tau} \left(\|\phi_h^{m+1} - \phi_h^m\|_{L^2}^2 - \|\phi_h^m - \phi_h^{m-1}\|_{L^2}^2 \right) + \frac{1}{4\tau} \|\phi_h^{m+1} - 2\phi_h^m + \phi_h^{m-1}\|_{L^2}^2 \\
&= \frac{1}{4\tau} \left[\left(\left\| (\phi_h^{m+1})^2 \right\|_{L^2}^2 - 2\|\phi_h^{m+1}\|_{L^2}^2 + 1 \right) - \left(\left\| (\phi_h^m)^2 \right\|_{L^2}^2 - 2\|\phi_h^m\|_{L^2}^2 + 1 \right) \right] \\
&\quad + \frac{1}{4\tau} \left(\|\phi_h^{m+1} - \phi_h^m\|_{L^2}^2 - \|\phi_h^m - \phi_h^{m-1}\|_{L^2}^2 \right) + \frac{1}{4\tau} \|\phi_h^{m+1} - 2\phi_h^m + \phi_h^{m-1}\|_{L^2}^2 \\
&= \frac{1}{4\tau} \left(\left\| (\phi_h^{m+1})^2 - 1 \right\|_{L^2}^2 - \left\| (\phi_h^m)^2 - 1 \right\|_{L^2}^2 \right) \\
&\quad + \frac{1}{4\tau} \left(\|\phi_h^{m+1} - \phi_h^m\|_{L^2}^2 - \|\phi_h^m - \phi_h^{m-1}\|_{L^2}^2 \right) \\
&\quad + \frac{1}{4\tau} \|\phi_h^{m+1} - 2\phi_h^m + \phi_h^{m-1}\|_{L^2}^2.
\end{aligned}$$

To prove (4.19), we use the definitions of $\check{\phi}_h^{m+\frac{1}{2}}$ and $\delta_\tau \phi_h^{m+\frac{1}{2}}$ and expand as follows,

$$\begin{aligned}
a\left(\check{\phi}_h^{m+\frac{1}{2}}, \delta_\tau \phi_h^{m+\frac{1}{2}}\right) &= \frac{1}{\tau} a\left(\frac{3}{4}\phi_h^{m+1} + \frac{1}{4}\phi_h^{m-1}, \phi_h^{m+1} - \phi_h^m\right) \\
&= \frac{1}{\tau} a\left(\frac{1}{2}\phi_h^{m+1} + \frac{1}{2}\phi_h^m + \frac{1}{4}\phi_h^{m+1} - \frac{1}{2}\phi_h^m + \frac{1}{4}\phi_h^{m-1}, \phi_h^{m+1} - \phi_h^m\right) \\
&= \frac{1}{2\tau} \left(\|\nabla \phi_h^{m+1}\|_{L^2}^2 - \|\nabla \phi_h^m\|_{L^2}^2\right) \\
&\quad + \frac{1}{4\tau} \left((\nabla \phi_h^{m+1} - \nabla \phi_h^m) - (\nabla \phi_h^m - \nabla \phi_h^{m-1}), \nabla \phi_h^{m+1} - \nabla \phi_h^m\right) \\
&= \frac{1}{2\tau} \left(\|\nabla \phi_h^{m+1}\|_{L^2}^2 - \|\nabla \phi_h^m\|_{L^2}^2\right) \\
&\quad + \frac{1}{8\tau} \left(\|\nabla \phi_h^{m+1} - \nabla \phi_h^m\|_{L^2}^2 - \|\nabla \phi_h^m - \nabla \phi_h^{m-1}\|_{L^2}^2\right) \\
&\quad + \frac{1}{8\tau} \|\nabla \phi_h^{m+1} - 2\nabla \phi_h^m + \nabla \phi_h^{m-1}\|_{L^2}^2.
\end{aligned}$$

□

We are now in position to show that our second-order (in time) mixed finite element splitting scheme is unconditionally energy stable.

Lemma 4.3.7. *Let $(\phi_h^{m+1}, \mu_h^{m+\frac{1}{2}}) \in S_h \times S_h$ be the unique solution of (4.7a) – (4.7b), and $(\phi_h^1, \mu_h^{\frac{1}{2}}) \in S_h \times S_h$, the unique solution of (4.10a) – (4.10b). Then the following energy law holds for any $h, \tau > 0$:*

$$\begin{aligned}
F(\phi_h^{\ell+1}, \phi_h^\ell) + \tau\varepsilon \sum_{m=1}^{\ell} \left\| \nabla \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + \sum_{m=1}^{\ell} \left[\frac{1}{4\varepsilon} \left\| \phi_h^{m+1} - 2\phi_h^m + \phi_h^{m-1} \right\|_{L^2}^2 \right. \\
\left. + \frac{\varepsilon}{8} \left\| \nabla \phi_h^{m+1} - 2\nabla \phi_h^m + \nabla \phi_h^{m-1} \right\|_{L^2}^2 \right] = F(\phi_h^1, \phi_h^0),
\end{aligned} \tag{4.20}$$

for all $1 \leq \ell \leq M-1$.

Proof. Setting $\nu = \mu_h^{m+\frac{1}{2}}$ in (4.7a) and $\psi = \delta_\tau \phi_h^{m+\frac{1}{2}}$ in (4.7b) gives

$$\left(\delta_\tau \phi_h^{m+\frac{1}{2}}, \mu_h^{m+\frac{1}{2}} \right) + \varepsilon \left\| \nabla \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 = 0, \quad (4.21)$$

$$\begin{aligned} \varepsilon^{-1} \left(\chi \left(\phi_h^{m+1}, \phi_h^m \right), \delta_\tau \phi_h^{m+\frac{1}{2}} \right) - \varepsilon^{-1} \left(\tilde{\phi}_h^{m+\frac{1}{2}}, \delta_\tau \phi_h^{m+\frac{1}{2}} \right) \\ + \varepsilon a \left(\check{\phi}_h^{m+\frac{1}{2}}, \delta_\tau \phi_h^{m+\frac{1}{2}} \right) - \left(\mu_h^{m+\frac{1}{2}}, \delta_\tau \phi_h^{m+\frac{1}{2}} \right) = 0. \end{aligned} \quad (4.22)$$

Combining (4.21) – (4.22), using the identities from Lemma 4.3.6, and applying the operator $\tau \sum_{m=1}^\ell$ to the combined equation, results in (4.20). $\square$

For the remainder of the chapter, we will make the following stability assumptions for the initial data:

$$E \left(\phi_h^0 \right) + \tau^2 \left\| \Delta_h \mu_h^0 \right\|_{L^2}^2 + \left\| \Delta_h \phi_h^0 \right\|_{L^2}^2 \leq C, \quad (4.23)$$

for some constant $C > 0$ that is independent of h and τ . Here we assume that $\varepsilon > 0$ is fixed. In fact, from this point in the stability and error analyses, we will not track the dependence of the estimates on the interface parameter ε , though this may be of importance, especially if ε tends to zero.

Lemma 4.3.8. *Let $(\phi_h^{m+1}, \mu_h^{m+\frac{1}{2}}) \in S_h \times S_h$ be the unique solution of (4.7a) – (4.7b), and $(\phi_h^1, \mu_h^{\frac{1}{2}}) \in S_h \times S_h$, the unique solution of (4.10a) – (4.10b). Then the following estimates hold for any $h, \tau > 0$:*

$$\max_{0 \leq m \leq M} \left[\|\nabla \phi_h^m\|_{L^2}^2 + \|(\phi_h^m)^2 - 1\|_{L^2}^2 \right] \leq C, \quad (4.24)$$

$$\max_{0 \leq m \leq M} \left[\|\phi_h^m\|_{L^4}^4 + \|\phi_h^m\|_{L^2}^2 + \|\phi_h^m\|_{H^1}^2 \right] \leq C, \quad (4.25)$$

$$\max_{1 \leq m \leq M} \left[\|\phi_h^m - \phi_h^{m-1}\|_{L^2}^2 + \|\nabla \phi_h^m - \nabla \phi_h^{m-1}\|_{L^2}^2 \right] \leq C, \quad (4.26)$$

$$\tau \sum_{m=0}^{M-1} \left\| \nabla \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq C, \quad (4.27)$$

$$\sum_{m=1}^{M-1} \left[\|\phi_h^{m+1} - 2\phi_h^m + \phi_h^{m-1}\|_{L^2}^2 + \|\nabla \phi_h^{m+1} - 2\nabla \phi_h^m + \nabla \phi_h^{m-1}\|_{L^2}^2 \right] \leq C, \quad (4.28)$$

for some constant $C > 0$ that is independent of h, τ , and T .

Proof. Starting with the stability of the initial step, inequality (4.12), and considering the stability of the initial data, inequality (4.23), we immediately have

$$\|\nabla \phi_h^1\|_{L^2}^2 + \|(\phi_h^1)^2 - 1\|_{L^2}^2 + \|\phi_h^1\|_{L^4}^4 + \|\phi_h^1\|_{L^2}^2 + \|\phi_h^1\|_{H^1}^2 + \tau \left\| \nabla \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 \leq C. \quad (4.29)$$

The triangle inequality immediately implies

$$F(\phi_h^1, \phi_h^0) = E(\phi_h^1) + \frac{1}{4\epsilon} \|\phi_h^1 - \phi_h^0\|_{L^2}^2 + \frac{\epsilon}{8} \|\nabla \phi_h^1 - \nabla \phi_h^0\|_{L^2}^2 \leq C.$$

This, together with (4.20) and the fact that $F(\phi_h^{m+1}, \phi_h^m) \geq E(\phi_h^{m+1})$, for all $0 \leq m \leq M-1$, establishes all of the inequalities. $\square$

We are able to prove the next set of *a priori* stability estimates without any restrictions on h and τ . See 2.2.21 for a definition of discrete negative norm $\|\cdot\|_{-1,h}$.

Lemma 4.3.9. *Let $(\phi_h^{m+1}, \mu_h^{m+\frac{1}{2}}) \in S_h \times S_h$ be the unique solution of (4.7a) – (4.7b), and $(\phi_h^1, \mu_h^{\frac{1}{2}}) \in S_h \times S_h$, the unique solution of (4.10a) – (4.10b). Then the following estimates hold for any $h, \tau > 0$:*

$$\tau \sum_{m=0}^{M-1} \left[\left\| \delta_\tau \phi_h^{m+\frac{1}{2}} \right\|_{H^{-1}}^2 + \left\| \delta_\tau \phi_h^{m+\frac{1}{2}} \right\|_{-1,h}^2 \right] \leq C, \quad (4.30)$$

$$\tau \sum_{m=0}^{M-1} \left\| \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq C(T+1), \quad (4.31)$$

$$\tau \sum_{m=1}^{M-1} \left[\left\| \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + \left\| \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^\infty}^{\frac{4(6-d)}{d}} \right] \leq C(T+1), \quad (4.32)$$

for some constant $C > 0$ that is independent of h, τ , and T .

Proof. Let $\mathcal{Q}_h : L^2(\Omega) \rightarrow S_h$ be the L^2 projection, i.e., $(\mathcal{Q}_h \nu - \nu, \xi) = 0$ for all $\xi \in S_h$. Suppose $\nu \in \mathring{H}^1(\Omega)$. Then, by (4.7a) and (4.10a), for all $0 < m < M-1$

$$\begin{aligned} \left(\delta_\tau \phi_h^{m+\frac{1}{2}}, \nu \right) &= \left(\delta_\tau \phi_h^{m+\frac{1}{2}}, \mathcal{Q}_h \nu \right) \\ &= -\varepsilon \left(\nabla \mu_h^{m+\frac{1}{2}}, \nabla \mathcal{Q}_h \nu \right) \\ &\leq \varepsilon \left\| \nabla \mu_h^{m+\frac{1}{2}} \right\|_{L^2} \left\| \nabla \mathcal{Q}_h \nu \right\|_{L^2} \\ &\leq C\varepsilon \left\| \nabla \mu_h^{m+\frac{1}{2}} \right\|_{L^2} \left\| \nabla \nu \right\|_{L^2}, \end{aligned} \quad (4.33)$$

where we used the H^1 stability of the L^2 projection in the last step. Applying $\tau \sum_{m=0}^{M-1}$ and using (4.27), we obtain (4.30.1) – which, in our notation, is the bound on the first term of the left side of (4.30). The estimate (4.30.2) follows from the inequality $\|\nu\|_{-1,h} \leq \|\nu\|_{H^{-1}}$, which holds for all $\nu \in \mathring{S}_h$.

To prove (4.31), for $1 \leq m \leq M-1$ we set $\psi = \mu_h^{m+\frac{1}{2}}$ in (4.7b) to obtain

$$\begin{aligned} \left\| \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 &= \varepsilon^{-1} \left(\chi(\phi_h^{m+1}, \phi_h^m), \mu_h^{m+\frac{1}{2}} \right) - \varepsilon^{-1} \left(\tilde{\phi}_h^{m+\frac{1}{2}}, \mu_h^{m+\frac{1}{2}} \right) + \varepsilon a \left(\tilde{\phi}_h^{m+\frac{1}{2}}, \mu_h^{m+\frac{1}{2}} \right) \\ &\leq C \left\| \chi(\phi_h^{m+1}, \phi_h^m) \right\|_{L^2}^2 + \frac{1}{4} \left\| \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + C \left\| \tilde{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + \frac{1}{4} \left\| \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 \\ &\quad + C \left\| \nabla \tilde{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + \frac{1}{2} \left\| \nabla \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2. \end{aligned}$$

And, similarly, setting $\psi = \mu_h^{\frac{1}{2}}$ in (4.10b), we have

$$\begin{aligned} \left\| \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 &\leq C \left\| \chi(\phi_h^1, \phi_h^0) \right\|_{L^2}^2 + \frac{1}{6} \left\| \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 + C \left\| \phi_h^0 \right\|_{L^2}^2 + \frac{1}{6} \left\| \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 + C \left\| \nabla \phi_h^{\frac{1}{2}} \right\|_{L^2}^2 \\ &\quad + \frac{1}{2} \left\| \nabla \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 + \frac{1}{6} \left\| \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 + C \tau^2 \left\| \Delta_h \mu_h^0 \right\|_{L^2}^2. \end{aligned}$$

Hence, using the triangle inequality, (4.25), and the initial stability (4.23), we have for all $0 \leq m \leq M-1$,

$$\frac{1}{2} \left\| \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq C \left\| \chi(\phi_h^{m+1}, \phi_h^m) \right\|_{L^2}^2 + \frac{1}{2} \left\| \nabla \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + C.$$

Now, using Lemma 4.3.8, we have the following bound for all $0 \leq m \leq M-1$

$$\begin{aligned} \left\| \chi(\phi_h^{m+1}, \phi_h^m) \right\|_{L^2}^2 &= \frac{1}{16} \left\| (\phi_h^{m+1})^3 + (\phi_h^{m+1})^2 \phi_h^m + \phi_h^{m+1} (\phi_h^m)^2 + (\phi_h^m)^3 \right\|_{L^2}^2 \\ &\leq C \left\| (\phi_h^{m+1})^3 \right\|_{L^2}^2 + C \left\| (\phi_h^{m+1})^2 \phi_h^m \right\|_{L^2}^2 \\ &\quad + C \left\| \phi_h^{m+1} (\phi_h^m)^2 \right\|_{L^2}^2 + C \left\| (\phi_h^m)^3 \right\|_{L^2}^2 \\ &\leq C \left\| \phi_h^{m+1} \right\|_{L^6}^6 + C \left\| \phi_h^m \right\|_{L^6}^6 \leq C \left\| \phi_h^{m+1} \right\|_{H^1}^6 + C \left\| \phi_h^m \right\|_{H^1}^6 \\ &\leq C, \end{aligned} \tag{4.34}$$

where we used Young's inequality and the embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$, for $d = 2, 3$. Hence,

$$\left\| \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq \left\| \nabla \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + C. \tag{4.35}$$

Applying $\tau \sum_{m=0}^{M-1}$, estimate (4.31) now follows from (4.27).

Setting $\psi_h = \Delta_h \check{\phi}_h^{m+\frac{1}{2}}$ in (4.7b) and using the definition of the discrete Laplacian 2.2.16, it follows that for all $1 \leq m \leq M-1$

$$\begin{aligned}
\varepsilon \left\| \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2 &= -\varepsilon a \left(\check{\phi}_h^{m+\frac{1}{2}}, \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right) \\
&= - \left(\mu_h^{m+\frac{1}{2}}, \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right) - \varepsilon^{-1} \left(\check{\phi}_h^{m+\frac{1}{2}}, \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right) \\
&\quad + \varepsilon^{-1} \left(\chi(\phi_h^{m+1}, \phi_h^m), \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right) \\
&= a \left(\mu_h^{m+\frac{1}{2}}, \check{\phi}_h^{m+\frac{1}{2}} \right) - \varepsilon^{-1} \left(\check{\phi}_h^{m+\frac{1}{2}}, \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right) \\
&\quad + \varepsilon^{-1} \left(\chi(\phi_h^{m+1}, \phi_h^m), \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right) \\
&\leq \frac{1}{2} \left\| \nabla \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + \frac{1}{2} \left\| \nabla \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + C \left\| \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + \frac{\varepsilon}{4} \left\| \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2 \\
&\quad + C \left\| \chi(\phi_h^{m+1}, \phi_h^m) \right\|_{L^2}^2 + \frac{\varepsilon}{4} \left\| \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2.
\end{aligned}$$

Using the triangle inequality, (4.25), and (4.34), we have

$$\varepsilon \left\| \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq \left\| \nabla \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + C. \tag{4.36}$$

Applying $\tau \sum_{m=1}^{M-1}$, estimate (4.32.1) now follows from (4.27).

To prove estimate (4.32.2), we use the discrete Gagliardo-Nirenberg inequality 2.2.24 to obtain,

$$\left\| \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^\infty}^{\frac{4(6-d)}{d}} \leq C \left\| \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2 \left\| \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^6}^{\frac{6(4-d)}{d}} + C \left\| \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^6}^{\frac{4(6-d)}{d}}, \text{ for } d = 2, 3. \tag{4.37}$$

Applying $\tau \sum_{m=1}^{M-1}$ and using $H^1(\Omega) \hookrightarrow L^6(\Omega)$, (4.25), and (4.32.1), estimate (4.32.2) follows. $\square$

Lemma 4.3.10. *Let $(\phi_h^{m+1}, \mu_h^{m+\frac{1}{2}}) \in S_h \times S_h$ be the unique solution of (4.7a) – (4.7b), and $(\phi_h^1, \mu_h^{\frac{1}{2}}) \in S_h \times S_h$, the unique solution of (4.10a) – (4.10b). Assume that $\|\mu_h^0\|_{L^2}^2 \leq C$, independent of h . Then the following estimates hold for any $h, \tau > 0$:*

$$\tau \sum_{m=0}^{M-1} \left\| \delta_\tau \phi_h^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq C(T+1), \quad (4.38)$$

$$\max_{0 \leq m \leq M-1} \left\| \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq C(T+1), \quad (4.39)$$

for some constant $C > 0$ that is independent of h, τ , and T .

Proof. The proof is divided into three parts.

Part 1: We first establish

$$\left\| \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 + \tau \left\| \delta_\tau \phi_h^{\frac{1}{2}} \right\|_{L^2}^2 \leq C. \quad (4.40)$$

To this end, setting $\nu = \tau \delta_\tau \phi_h^{\frac{1}{2}}$ in (4.10a) and $\psi = 2\mu_h^{\frac{1}{2}}$ in (4.10b) and adding the resulting equations, we have

$$\begin{aligned} 2 \left\| \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 + \tau \left\| \delta_\tau \phi_h^{\frac{1}{2}} \right\|_{L^2}^2 &= \frac{2}{\varepsilon} \left(\chi(\phi_h^1, \phi_h^0), \mu_h^{\frac{1}{2}} \right) - \frac{2}{\varepsilon} \left(\phi_h^0, \mu_h^{\frac{1}{2}} \right) \\ &\quad - \tau \left(\Delta_h \mu_h^0, \mu_h^{\frac{1}{2}} \right) - 2\varepsilon \left(\Delta_h \phi_h^0, \mu_h^{\frac{1}{2}} \right) \\ &\leq \left\| \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 + C \left\| \chi(\phi_h^1, \phi_h^0) \right\|_{L^2}^2 + C \left\| \phi_h^0 \right\|_{L^2}^2 \\ &\quad + C \tau^2 \left\| \Delta_h \mu_h^0 \right\|_{L^2}^2 + C \left\| \Delta_h \phi_h^0 \right\|_{L^2}^2. \end{aligned}$$

Thus,

$$\left\| \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 + \tau \left\| \delta_\tau \phi_h^{\frac{1}{2}} \right\|_{L^2}^2 \leq C, \quad (4.41)$$

considering the initial stability (4.23), (4.25), and (4.34).

Part 2: Next we prove that

$$\left\| \mu_h^{\frac{3}{2}} \right\|_{L^2}^2 + \tau \left\| \delta_\tau \phi_h^{\frac{3}{2}} \right\|_{L^2}^2 \leq C. \quad (4.42)$$

Setting $m = 1$ in (4.7b) and subtracting (4.10b), we obtain

$$\begin{aligned} \left(\mu_h^{\frac{3}{2}} - \mu_h^{\frac{1}{2}}, \psi \right) &= \varepsilon a \left(\tilde{\phi}_h^{\frac{3}{2}} - \phi_h^{\frac{1}{2}}, \psi \right) - \frac{3}{2\varepsilon} (\phi_h^1 - \phi_h^0, \psi) - \frac{\tau}{2} a (\mu_h^0, \psi) \\ &\quad + \varepsilon^{-1} (\chi(\phi_h^2, \phi_h^1) - \chi(\phi_h^1, \phi_h^0), \psi) \end{aligned} \quad (4.43)$$

$$\begin{aligned} &= \varepsilon a \left(\frac{3}{4} \tau \delta_\tau \phi_h^{\frac{3}{2}} + \frac{1}{4} \tau \delta_\tau \phi_h^{\frac{1}{2}}, \psi \right) - \frac{3}{2\varepsilon} (\phi_h^1 - \phi_h^0, \psi) - \frac{\tau}{2} a (\mu_h^0, \psi) \\ &\quad + \varepsilon^{-1} (\chi(\phi_h^2, \phi_h^1) - \chi(\phi_h^1, \phi_h^0), \psi). \end{aligned} \quad (4.44)$$

Additionally, we take a weighted average of (4.7a) with $m = 1$ and (4.10a) with the weights $\frac{3}{4}$ and $\frac{1}{4}$, respectively, to obtain,

$$\left(\frac{3}{4} \delta_\tau \phi_h^{\frac{3}{2}} + \frac{1}{4} \delta_\tau \phi_h^{\frac{1}{2}}, \nu \right) = -\varepsilon a \left(\frac{3}{4} \mu_h^{\frac{3}{2}} + \frac{1}{4} \mu_h^{\frac{1}{2}}, \nu \right), \quad \forall \nu \in S_h. \quad (4.45)$$

Taking $\psi = \frac{3}{4}\mu_h^{\frac{3}{2}} + \frac{1}{4}\mu_h^{\frac{1}{2}}$ in (4.44), $\nu = \frac{3\tau}{4}\delta_\tau\phi_h^{\frac{3}{2}} + \frac{\tau}{4}\delta_\tau\phi_h^{\frac{1}{2}}$ in (4.45), and adding the results yields

$$\begin{aligned}
& \left(\mu_h^{\frac{3}{2}} - \mu_h^{\frac{1}{2}}, \frac{3}{4}\mu_h^{\frac{3}{2}} + \frac{1}{4}\mu_h^{\frac{1}{2}} \right) + \tau \left\| \frac{3}{4}\delta_\tau\phi_h^{\frac{3}{2}} + \frac{1}{4}\delta_\tau\phi_h^{\frac{1}{2}} \right\|_{L^2}^2 \\
&= -\frac{3}{8\varepsilon} \left(\phi_h^1 - \phi_h^0, 3\mu_h^{\frac{3}{2}} + \mu_h^{\frac{1}{2}} \right) - \frac{\tau}{8\varepsilon} a \left(\mu_h^0, 3\mu_h^{\frac{3}{2}} + \mu_h^{\frac{1}{2}} \right) \\
&\quad + \frac{1}{4\varepsilon} \left(\chi(\phi_h^2, \phi_h^1) - \chi(\phi_h^1, \phi_h^0), 3\mu_h^{\frac{3}{2}} + \mu_h^{\frac{1}{2}} \right) \\
&= -\frac{3}{8\varepsilon} \left(\phi_h^1 - \phi_h^0, 3\mu_h^{\frac{3}{2}} + \mu_h^{\frac{1}{2}} \right) + \frac{\tau}{8\varepsilon} \left(\Delta_h \mu_h^0, 3\mu_h^{\frac{3}{2}} + \mu_h^{\frac{1}{2}} \right) \\
&\quad + \frac{1}{4\varepsilon} \left(\chi(\phi_h^2, \phi_h^1) - \chi(\phi_h^1, \phi_h^0), 3\mu_h^{\frac{3}{2}} + \mu_h^{\frac{1}{2}} \right) \\
&\leq \frac{1}{4} \left\| \mu_h^{\frac{3}{2}} \right\|_{L^2}^2 + C \left\| \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 + C \left\| \phi_h^1 \right\|_{L^2}^2 + C \left\| \phi_h^0 \right\|_{L^2}^2 \\
&\quad + C\tau^2 \left\| \Delta_h \mu_h^0 \right\|_{L^2}^2 + C \left\| \chi(\phi_h^2, \phi_h^1) \right\|_{L^2}^2 + C \left\| \chi(\phi_h^1, \phi_h^0) \right\|_{L^2}^2 \\
&\leq \frac{1}{4} \left\| \mu_h^{\frac{3}{2}} \right\|_{L^2}^2 + C \left\| \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 + C,
\end{aligned}$$

where we have used Young's inequality, (4.23), (4.25), and (4.34). Considering Part 1 and the inequalities

$$\begin{aligned}
\left\| \frac{3}{4}\delta_\tau\phi_h^{\frac{3}{2}} + \frac{1}{4}\delta_\tau\phi_h^{\frac{1}{2}} \right\|_{L^2}^2 &= \frac{9}{16} \left\| \delta_\tau\phi_h^{\frac{3}{2}} \right\|_{L^2}^2 + \frac{3}{8} \left(\delta_\tau\phi_h^{\frac{3}{2}}, \delta_\tau\phi_h^{\frac{1}{2}} \right) + \frac{1}{16} \left\| \delta_\tau\phi_h^{\frac{1}{2}} \right\|_{L^2}^2 \\
&\geq \frac{9}{16} \left\| \delta_\tau\phi_h^{\frac{3}{2}} \right\|_{L^2}^2 - \frac{3}{8} \left\| \delta_\tau\phi_h^{\frac{3}{2}} \right\|_{L^2} \left\| \delta_\tau\phi_h^{\frac{1}{2}} \right\|_{L^2} + \frac{1}{16} \left\| \delta_\tau\phi_h^{\frac{1}{2}} \right\|_{L^2}^2 \\
&\geq \frac{3}{8} \left\| \delta_\tau\phi_h^{\frac{3}{2}} \right\|_{L^2}^2 - \frac{1}{8} \left\| \delta_\tau\phi_h^{\frac{1}{2}} \right\|_{L^2}^2,
\end{aligned}$$

and

$$\begin{aligned}
\left(\mu_h^{\frac{3}{2}} - \mu_h^{\frac{1}{2}}, \frac{3}{4}\mu_h^{\frac{3}{2}} + \frac{1}{4}\mu_h^{\frac{1}{2}} \right) &= \frac{3}{4} \left\| \mu_h^{\frac{3}{2}} \right\|_{L^2}^2 - \frac{1}{2} \left(\mu_h^{\frac{3}{2}}, \mu_h^{\frac{1}{2}} \right) - \frac{1}{4} \left\| \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 \\
&\geq \frac{1}{2} \left\| \mu_h^{\frac{3}{2}} \right\|_{L^2}^2 - \frac{1}{2} \left\| \mu_h^{\frac{1}{2}} \right\|_{L^2}^2,
\end{aligned}$$

we have,

$$\frac{1}{4} \left\| \mu_h^{\frac{3}{2}} \right\|_{L^2}^2 + \frac{3\tau}{8} \left\| \delta_\tau \phi_h^{\frac{3}{2}} \right\|_{L^2}^2 \leq C \left\| \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 + \frac{\tau}{8} \left\| \delta_\tau \phi_h^{\frac{1}{2}} \right\|_{L^2}^2 + C \leq C. \quad (4.46)$$

Part 3: Finally, we will establish

$$\left\| \mu_h^{\ell+\frac{1}{2}} \right\|_{L^2}^2 + \frac{\tau}{8} \sum_{m=2}^{\ell} \left\| \delta_\tau \phi_h^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq C(T+1). \quad (4.47)$$

For $2 \leq m \leq M-1$, we subtract (4.7b) from itself at consecutive time steps to obtain

$$\begin{aligned} \left(\mu_h^{m+\frac{1}{2}} - \mu_h^{m-\frac{1}{2}}, \psi \right) &= \varepsilon a \left(\check{\phi}_h^{m+\frac{1}{2}} - \check{\phi}_h^{m-\frac{1}{2}}, \psi \right) - \varepsilon^{-1} \left(\tilde{\phi}_h^{m+\frac{1}{2}} - \tilde{\phi}_h^{m-\frac{1}{2}}, \psi \right) \\ &\quad + \varepsilon^{-1} \left(\chi \left(\phi_h^{m+1}, \phi_h^m \right) - \chi \left(\phi_h^m, \phi_h^{m-1} \right), \psi \right) \\ &= \varepsilon a \left(\frac{3}{4} \tau \delta_\tau \phi_h^{m+\frac{1}{2}} + \frac{1}{4} \tau \delta_\tau \phi_h^{m-\frac{3}{2}}, \psi \right) \\ &\quad - \varepsilon^{-1} \left(\frac{3}{2} \tau \delta_\tau \phi_h^{m-\frac{1}{2}} - \frac{1}{2} \tau \delta_\tau \phi_h^{m-\frac{3}{2}}, \psi \right) \\ &\quad + \frac{1}{4\varepsilon} \left(\omega_h^m \left(\phi_h^{m+1} - \phi_h^{m-1} \right), \psi \right), \end{aligned} \quad (4.48)$$

for all $\psi \in S_h$, where $\omega_h^m := \omega \left(\phi_h^{m+1}, \phi_h^m, \phi_h^{m-1} \right)$ and

$$\omega(a, b, c) := a^2 + b^2 + c^2 + ab + bc + ac.$$

Additionally, we take a weighted average of the $m + \frac{1}{2}$ and $m - \frac{3}{2}$ time steps with the weights $\frac{3}{4}$ and $\frac{1}{4}$, respectively, of (4.7a) to obtain,

$$\left(\frac{3}{4} \delta_\tau \phi_h^{m+\frac{1}{2}} + \frac{1}{4} \delta_\tau \phi_h^{m-\frac{3}{2}}, \nu \right) = -\varepsilon a \left(\frac{3}{4} \mu_h^{m+\frac{1}{2}} + \frac{1}{4} \mu_h^{m-\frac{3}{2}}, \nu \right), \quad (4.49)$$

for all $\nu \in S_h$, which is well-defined for all $2 \leq m \leq M-1$. Taking $\psi = \frac{3}{4}\mu_h^{m+\frac{1}{2}} + \frac{1}{4}\mu_h^{m-\frac{3}{2}}$ in (4.48), $\nu = \tau \left(\frac{3}{4}\delta_\tau \phi_h^{m+\frac{1}{2}} + \frac{1}{4}\delta_\tau \phi_h^{m-\frac{3}{2}} \right)$ in (4.49), and adding the results yields

$$\begin{aligned}
& \left(\mu_h^{m+\frac{1}{2}} - \mu_h^{m-\frac{1}{2}}, \frac{3}{4}\mu_h^{m+\frac{1}{2}} + \frac{1}{4}\mu_h^{m-\frac{3}{2}} \right) + \tau \left\| \frac{3}{4}\delta_\tau \phi_h^{m+\frac{1}{2}} + \frac{1}{4}\delta_\tau \phi_h^{m-\frac{3}{2}} \right\|_{L^2}^2 \\
&= -\frac{\tau}{\varepsilon} \left(\frac{3}{2}\delta_\tau \phi_h^{m-\frac{1}{2}} - \frac{1}{2}\delta_\tau \phi_h^{m-\frac{3}{2}}, \frac{3}{4}\mu_h^{m+\frac{1}{2}} + \frac{1}{4}\mu_h^{m-\frac{3}{2}} \right) \\
&\quad + \frac{1}{4\varepsilon} \left(\omega_h^m (\phi_h^{m+1} - \phi_h^{m-1}), \frac{3}{4}\mu_h^{m+\frac{1}{2}} + \frac{1}{4}\mu_h^{m-\frac{3}{2}} \right) \\
&= -\frac{\tau}{\varepsilon} \left(\frac{3}{2}\delta_\tau \phi_h^{m-\frac{1}{2}} - \frac{1}{2}\delta_\tau \phi_h^{m-\frac{3}{2}}, \frac{3}{4}\mu_h^{m+\frac{1}{2}} + \frac{1}{4}\mu_h^{m-\frac{3}{2}} \right) \\
&\quad + \frac{\tau}{4\varepsilon} \left(\omega_h^m \delta_\tau \phi_h^{m+\frac{1}{2}}, \frac{3}{4}\mu_h^{m+\frac{1}{2}} + \frac{1}{4}\mu_h^{m-\frac{3}{2}} \right) \\
&\quad + \frac{\tau}{4\varepsilon} \left(\omega_h^m \delta_\tau \phi_h^{m-\frac{1}{2}}, \frac{3}{4}\mu_h^{m+\frac{1}{2}} + \frac{1}{4}\mu_h^{m-\frac{3}{2}} \right) \\
&\leq \frac{3\tau}{8\varepsilon} \left\| \delta_\tau \phi_h^{m-\frac{1}{2}} \right\|_{L^2} \left\| 3\mu_h^{m+\frac{1}{2}} + \mu_h^{m-\frac{3}{2}} \right\|_{L^2} \\
&\quad + \frac{\tau}{8\varepsilon} \left\| \delta_\tau \phi_h^{m-\frac{3}{2}} \right\|_{L^2} \left\| 3\mu_h^{m+\frac{1}{2}} + \mu_h^{m-\frac{3}{2}} \right\|_{L^2} \\
&\quad + \frac{\tau}{16\varepsilon} \left\| \omega_h^m \right\|_{L^3} \left\| \delta_\tau \phi_h^{m+\frac{1}{2}} \right\|_{L^2} \left\| 3\mu_h^{m+\frac{1}{2}} + \mu_h^{m-\frac{3}{2}} \right\|_{L^6} \\
&\quad + \frac{\tau}{16\varepsilon} \left\| \omega_h^m \right\|_{L^3} \left\| \delta_\tau \phi_h^{m-\frac{1}{2}} \right\|_{L^2} \left\| 3\mu_h^{m+\frac{1}{2}} + \mu_h^{m-\frac{3}{2}} \right\|_{L^6}.
\end{aligned}$$

Hence,

$$\begin{aligned}
& \left(\mu_h^{m+\frac{1}{2}} - \mu_h^{m-\frac{1}{2}}, \frac{3}{4}\mu_h^{m+\frac{1}{2}} + \frac{1}{4}\mu_h^{m-\frac{3}{2}} \right) + \tau \left\| \frac{3}{4}\delta_\tau \phi_h^{m+\frac{1}{2}} + \frac{1}{4}\delta_\tau \phi_h^{m-\frac{3}{2}} \right\|_{L^2}^2 \\
&\leq \frac{\tau}{8} \left\| \delta_\tau \phi_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + \frac{\tau}{32} \left\| \delta_\tau \phi_h^{m-\frac{1}{2}} \right\|_{L^2}^2 \\
&\quad + \frac{\tau}{32} \left\| \delta_\tau \phi_h^{m-\frac{3}{2}} \right\|_{L^2}^2 + C\tau \left\| \mu_h^{m+\frac{1}{2}} \right\|_{H^1}^2 \\
&\quad + C\tau \left\| \mu_h^{m-\frac{3}{2}} \right\|_{H^1}^2,
\end{aligned}$$

where we use the $H^1(\Omega) \hookrightarrow L^6(\Omega)$ embedding to achieve following bound,

$$\begin{aligned}\|\omega_h^m\|_{L^3} &= \left\| (\phi_h^{m+1})^2 + (\phi_h^m)^2 + (\phi_h^{m-1})^2 + \phi_h^{m+1}\phi_h^m + \phi_h^{m+1}\phi_h^{m-1} + \phi_h^m\phi_h^{m-1} \right\|_{L^3} \\ &\leq C \|\phi_h^{m+1}\|_{L^6}^2 + C \|\phi_h^m\|_{L^6}^2 + C \|\phi_h^{m-1}\|_{L^6}^2 \leq C.\end{aligned}$$

Applying $\sum_{m=2}^\ell$ and using the following properties

$$\begin{aligned}\left(\mu_h^{m+\frac{1}{2}} - \mu_h^{m-\frac{1}{2}}, \frac{3}{4}\mu_h^{m+\frac{1}{2}} + \frac{1}{4}\mu_h^{m-\frac{3}{2}} \right) &= \frac{1}{2} \left(\mu_h^{m+\frac{1}{2}} - \mu_h^{m-\frac{1}{2}}, \mu_h^{m+\frac{1}{2}} + \mu_h^{m-\frac{1}{2}} \right) \\ &\quad + \frac{1}{4} \left(\mu_h^{m+\frac{1}{2}} - \mu_h^{m-\frac{1}{2}}, \mu_h^{m+\frac{1}{2}} - 2\mu_h^{m-\frac{1}{2}} + \mu_h^{m-\frac{3}{2}} \right) \\ &= \frac{1}{2} \left\| \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 - \frac{1}{2} \left\| \mu_h^{m-\frac{1}{2}} \right\|_{L^2}^2 \\ &\quad + \frac{1}{8} \left\| \mu_h^{m+\frac{1}{2}} - \mu_h^{m-\frac{1}{2}} \right\|_{L^2}^2 - \frac{1}{8} \left\| \mu_h^{m-\frac{1}{2}} - \mu_h^{m-\frac{3}{2}} \right\|_{L^2}^2 \\ &\quad + \frac{1}{8} \left\| \mu_h^{m+\frac{1}{2}} - 2\mu_h^{m-\frac{1}{2}} + \mu_h^{m-\frac{3}{2}} \right\|_{L^2}^2,\end{aligned}$$

and

$$\begin{aligned}\left\| \frac{3}{4}\delta_\tau\phi_h^{m+\frac{1}{2}} + \frac{1}{4}\delta_\tau\phi_h^{m-\frac{3}{2}} \right\|_{L^2}^2 &= \frac{9}{16} \left\| \delta_\tau\phi_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + \frac{3}{8} \left(\delta_\tau\phi_h^{m+\frac{1}{2}}, \delta_\tau\phi_h^{m-\frac{3}{2}} \right) + \frac{1}{16} \left\| \delta_\tau\phi_h^{m-\frac{3}{2}} \right\|_{L^2}^2 \\ &\geq \frac{9}{16} \left\| \delta_\tau\phi_h^{m+\frac{1}{2}} \right\|_{L^2}^2 - \frac{3}{8} \left\| \delta_\tau\phi_h^{m+\frac{1}{2}} \right\|_{L^2} \left\| \delta_\tau\phi_h^{m-\frac{3}{2}} \right\|_{L^2} \\ &\quad + \frac{1}{16} \left\| \delta_\tau\phi_h^{m-\frac{3}{2}} \right\|_{L^2}^2 \\ &\geq \frac{3}{8} \left\| \delta_\tau\phi_h^{m+\frac{1}{2}} \right\|_{L^2}^2 - \frac{1}{8} \left\| \delta_\tau\phi_h^{m-\frac{3}{2}} \right\|_{L^2}^2,\end{aligned}$$

we conclude

$$\begin{aligned}\frac{1}{2} \left\| \mu_h^{\ell+\frac{1}{2}} \right\|_{L^2}^2 + \frac{\tau}{16} \sum_{m=2}^\ell \left\| \delta_\tau\phi_h^{m+\frac{1}{2}} \right\|_{L^2}^2 &\leq \frac{1}{8} \left\| \mu_h^{\frac{3}{2}} - \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 + \frac{3\tau}{16} \left\| \delta_\tau\phi_h^{\frac{3}{2}} \right\|_{L^2}^2 + \frac{1}{2} \left\| \mu_h^{\frac{3}{2}} \right\|_{L^2}^2 \\ &\quad + \frac{5\tau}{32} \left\| \delta_\tau\phi_h^{\frac{1}{2}} \right\|_{L^2}^2 + C\tau \sum_{m=0}^\ell \left\| \mu_h^{m+\frac{1}{2}} \right\|_{H^1}^2 \leq C(T+1),\end{aligned}$$

for any $2 \leq \ell \leq M - 1$, where we have used Parts 1 and 2 and estimates (4.27) and (4.31). The proof is completed by combining all three parts. $\square$

Lemma 4.3.11. *Let $(\phi_h^{m+1}, \mu_h^{m+\frac{1}{2}}) \in S_h \times S_h$ be the unique solution of (4.7a) – (4.7b), and $(\phi_h^1, \mu_h^{\frac{1}{2}}) \in S_h \times S_h$, the unique solution of (4.10a) – (4.10b). Then the following estimates hold for any $h, \tau > 0$:*

$$\left\| \Delta_h \phi_h^{\frac{1}{2}} \right\|_{L^2}^2 + \left\| \phi_h^{\frac{1}{2}} \right\|_{L^\infty}^2 \leq C, \quad (4.50)$$

$$\max_{1 \leq m \leq M-1} \left[\left\| \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + \left\| \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^\infty}^{\frac{4(6-d)}{d}} \right] \leq C(T+1), \quad (4.51)$$

for some constant $C > 0$ that is independent of h, τ , and T .

Proof. To prove (4.50.1), set $\psi = \Delta_h \phi_h^{\frac{1}{2}}$ in (4.10b) and use the definition of the discrete Laplacian 2.2.16 to obtain

$$\begin{aligned} \varepsilon \left\| \Delta_h \phi_h^{\frac{1}{2}} \right\|_{L^2}^2 &= -\varepsilon a \left(\phi_h^{\frac{1}{2}}, \Delta_h \phi_h^{\frac{1}{2}} \right) \\ &= \varepsilon^{-1} \left(\chi(\phi_h^1, \phi_h^0) - \phi_h^0, \Delta_h \phi_h^{\frac{1}{2}} \right) - \left(\mu_h^{\frac{1}{2}}, \Delta_h \phi_h^{\frac{1}{2}} \right) + \frac{\tau}{2} a \left(\mu_h^0, \Delta_h \phi_h^{\frac{1}{2}} \right) \\ &\leq \frac{\varepsilon}{2} \left\| \Delta_h \phi_h^{\frac{1}{2}} \right\|_{L^2}^2 + C \left(\left\| \chi(\phi_h^1, \phi_h^0) \right\|_{L^2}^2 + \left\| \phi_h^0 \right\|_{L^2}^2 + \left\| \mu_h^{\frac{1}{2}} \right\|_{L^2}^2 + \tau^2 \left\| \Delta_h \mu_h^0 \right\|_{L^2}^2 \right) \\ &\leq \frac{\varepsilon}{2} \left\| \Delta_h \phi_h^{\frac{1}{2}} \right\|_{L^2}^2 + C. \end{aligned}$$

The result now follows. Estimate (4.50.2) follows from (4.37), the embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$, (4.25), and (4.50.1).

Setting $\psi = \Delta_h \check{\phi}_h^{m+\frac{1}{2}}$ in (4.7b) and using the definition of the discrete Laplacian 2.2.16, we get

$$\begin{aligned}
\varepsilon \left\| \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2 &= -\varepsilon a \left(\check{\phi}_h^{m+\frac{1}{2}}, \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right) \\
&= - \left(\mu_h^{m+\frac{1}{2}}, \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right) - \varepsilon^{-1} \left(\tilde{\phi}_h^{m+\frac{1}{2}}, \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right) \\
&\quad + \varepsilon^{-1} \left(\chi \left(\phi_h^{m+1}, \phi_h^m \right), \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right) \\
&\leq C \left\| \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + \frac{\varepsilon}{2} \left\| \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + C \left\| \tilde{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2 \\
&\quad + C \left\| \chi \left(\phi_h^{m+1}, \phi_h^m \right) \right\|_{L^2}^2 \\
&\leq C + C \left\| \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2 + \frac{\varepsilon}{2} \left\| \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2,
\end{aligned}$$

where we have used the triangle inequality and (4.34). Hence, $\left\| \Delta_h \check{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq C + C \left\| \mu_h^{m+\frac{1}{2}} \right\|_{L^2}^2$, for $1 \leq m \leq M-1$, and estimate (4.51.1) follows from (4.39). Estimate (4.51.2) follows from (4.37), the embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$, (4.25), and (4.51.1). $\square$

Lemma 4.3.12. *Let $(\phi_h^{m+1}, \mu_h^{m+\frac{1}{2}}) \in S_h \times S_h$ be the unique solution of (4.7a) – (4.7b), and $(\phi_h^1, \mu_h^{\frac{1}{2}}) \in S_h \times S_h$, the unique solution of (4.10a) – (4.10b). The following estimates hold for any $h, \tau > 0$:*

$$\max_{0 \leq m \leq M} \left[\left\| \Delta_h \phi_h^m \right\|_{L^2}^2 + \left\| \phi_h^m \right\|_{L^\infty}^{\frac{4(6-d)}{d}} \right] \leq C(T+1), \quad (4.52)$$

for some constant $C > 0$ that is independent of h, τ , and T .

Proof. We begin by proving the stability for the first time step. A simple application of the triangle inequality gives (4.52.1) for $m = 1$ as follows,

$$\begin{aligned}
\left\| \Delta_h \phi_h^1 \right\|_{L^2} &= \left\| \Delta_h \phi_h^1 + \Delta_h \phi_h^0 - \Delta_h \phi_h^0 \right\|_{L^2} \leq \left\| \Delta_h \phi_h^1 + \Delta_h \phi_h^0 \right\|_{L^2} + \left\| \Delta_h \phi_h^0 \right\|_{L^2} \\
&\leq 2 \left\| \Delta_h \phi_h^{\frac{1}{2}} \right\|_{L^2} + \left\| \Delta_h \phi_h^0 \right\|_{L^2} \leq C,
\end{aligned}$$

where we have used the stability of the initial data, inequality (4.23), and (4.50.1). Next, using (4.37), $H^1(\Omega) \hookrightarrow L^6(\Omega)$, (4.25), and (4.52.1), we arrive at (4.52.2) for $m = 1$. For $2 \leq m \leq M - 1$, by definition,

$$\begin{aligned}
\left\| \Delta_h \tilde{\phi}_h^{m+\frac{1}{2}} \right\|_{L^2}^2 &= \left\| \Delta_h \left(\frac{3}{4} \phi_h^{m+1} + \frac{1}{4} \phi_h^{m-1} \right) \right\|_{L^2}^2 \\
&= \frac{1}{16} \left(9 \left\| \Delta_h \phi_h^{m+1} \right\|_{L^2}^2 + 6 (\Delta_h \phi_h^{m+1}, \Delta_h \phi_h^{m-1}) + \left\| \Delta_h \phi_h^{m-1} \right\|_{L^2}^2 \right) \\
&\geq \frac{1}{16} \left(9 \left\| \Delta_h \phi_h^{m+1} \right\|_{L^2}^2 - 3 \left\| \Delta_h \phi_h^{m+1} \right\|_{L^2}^2 - 3 \left\| \Delta_h \phi_h^{m-1} \right\|_{L^2}^2 + \left\| \Delta_h \phi_h^{m-1} \right\|_{L^2}^2 \right) \\
&= \frac{3}{8} \left\| \Delta_h \phi_h^{m+1} \right\|_{L^2}^2 - \frac{1}{8} \left\| \Delta_h \phi_h^{m-1} \right\|_{L^2}^2.
\end{aligned}$$

Using induction and estimate (4.51.1), we find

$$\begin{aligned}
\left\| \Delta_h \phi_h^{2m} \right\|_{L^2}^2 &\leq \frac{8}{3} \left(1 + \frac{1}{3} + \left(\frac{1}{3} \right)^2 + \cdots + \left(\frac{1}{3} \right)^{m-1} \right) C(T+1) + \left(\frac{1}{3} \right)^m \left\| \Delta_h \phi_h^0 \right\|_{L^2}^2 \\
&\leq \frac{8}{3} \cdot \frac{3}{2} C(T+1) + \left(\frac{1}{3} \right)^m \cdot C \leq C(T+1),
\end{aligned}$$

and

$$\begin{aligned}
\left\| \Delta_h \phi_h^{2m+1} \right\|_{L^2}^2 &\leq \frac{8}{3} \left(1 + \frac{1}{3} + \left(\frac{1}{3} \right)^2 + \cdots + \left(\frac{1}{3} \right)^{m-1} \right) C(T+1) + \left(\frac{1}{3} \right)^m \left\| \Delta_h \phi_h^1 \right\|_{L^2}^2 \\
&\leq \frac{8}{3} \cdot \frac{3}{2} C(T+1) + \left(\frac{1}{3} \right)^m \cdot C \leq C(T+1),
\end{aligned}$$

and estimate (4.52.1) follows. Estimate (4.52.2) follows from (4.37), (4.52.1), and the embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$. $\square$

4.4 Error Estimates for the Fully Discrete Convex Splitting Scheme

In this section, we provide a rigorous convergence analysis for our scheme in the appropriate energy norms. We shall assume that weak solutions have the additional

regularities

$$\begin{aligned}
\phi &\in L^\infty(0, T; W^{1,6}(\Omega)) \cap H^1(0, T; H^{q+1}(\Omega)) \cap H^2(0, T; H^3(\Omega)) \cap H^3(0, T; L^2(\Omega)), \\
\phi^2 &\in H^2(0, T; H^1(\Omega)), \\
\mu &\in L^2(0, T; H^{q+1}(\Omega)),
\end{aligned} \tag{4.53}$$

where $q \geq 1$. The norm bounds associated to the assumed regularities above are not necessarily global-in-time and therefore can involve constants that depend upon the final time T . We also assume that the initial data are sufficiently regular so that the stability (4.23) holds. Weak solutions (ϕ, μ) to (4.2a) - (4.2b) with the higher regularities (4.53) solve the following variational problem: for all $t \in [0, T]$,

$$(\partial_t \phi, \nu) + \varepsilon a(\mu, \nu) = 0 \quad \forall \quad \nu \in H^1(\Omega), \tag{4.54a}$$

$$(\mu, \psi) - \varepsilon a(\phi, \psi) - \varepsilon^{-1}(\phi^3 - \phi, \psi) = 0 \quad \forall \quad \psi \in H^1(\Omega). \tag{4.54b}$$

We define the following: for any *real* number $m \in [0, M]$,

$$t_m := m \tau, \quad \phi^m := \phi(t_m), \quad \mathcal{E}_a^{\phi, m} := \phi^m - R_h \phi^m, \quad \mathcal{E}_a^{\mu, m} := \mu^m - R_h \mu^m;$$

and for any integer $0 \leq m \leq M - 1$,

$$\begin{aligned}
\delta_\tau \phi^{m+\frac{1}{2}} &:= \frac{\phi^{m+1} - \phi^m}{\tau}, \quad \sigma_1^{m+\frac{1}{2}} := \delta_\tau R_h \phi^{m+\frac{1}{2}} - \delta_\tau \phi^{m+\frac{1}{2}}, \\
\sigma_2^{m+\frac{1}{2}} &:= \delta_\tau \phi^{m+\frac{1}{2}} - \partial_t \phi^{m+\frac{1}{2}}, \quad \sigma_3^{m+\frac{1}{2}} := \frac{1}{2} \phi^{m+1} + \frac{1}{2} \phi^m - \phi^{m+\frac{1}{2}} \\
\sigma_4^{m+\frac{1}{2}} &:= \chi(\phi^{m+1}, \phi^m) - \left(\phi^{m+\frac{1}{2}}\right)^3.
\end{aligned}$$

Then the PDE solution, evaluated at the half-integer time steps $t_{m+\frac{1}{2}}$, satisfies

$$\left(\delta_\tau R_h \phi^{m+\frac{1}{2}}, \nu\right) + \varepsilon a\left(R_h \mu^{m+\frac{1}{2}}, \nu\right) = \left(\sigma_1^{m+\frac{1}{2}} + \sigma_2^{m+\frac{1}{2}}, \nu\right), \quad (4.55a)$$

$$\begin{aligned} \varepsilon a\left(\frac{1}{2}R_h \phi^{m+1} + \frac{1}{2}R_h \phi^m, \psi\right) - \left(R_h \mu^{m+\frac{1}{2}}, \psi\right) &= \left(\mathcal{E}_a^{\mu, m+\frac{1}{2}}, \psi\right) - \frac{1}{\varepsilon} \left(\chi(\phi^{m+1}, \phi^m), \psi\right) \\ &\quad + \frac{1}{\varepsilon} \left(\phi^{m+\frac{1}{2}}, \psi\right) + \varepsilon a\left(\sigma_3^{m+\frac{1}{2}}, \psi\right) \\ &\quad + \frac{1}{\varepsilon} \left(\sigma_4^{m+\frac{1}{2}}, \psi\right) \end{aligned} \quad (4.55b)$$

for all $\nu, \psi \in S_h$. Restating the fully discrete splitting scheme, Eqs. (4.7a) – (4.7b) and (4.10a) – (4.10b), we have, for all $\nu, \psi \in S_h$,

$$\left(\delta_\tau \phi_h^{\frac{1}{2}}, \nu\right) + \varepsilon a\left(\mu_h^{\frac{1}{2}}, \nu\right) = 0, \quad (4.56a)$$

$$\varepsilon a\left(\phi_h^{\frac{1}{2}}, \psi\right) - \left(\mu_h^{\frac{1}{2}}, \psi\right) = -\frac{1}{\varepsilon} \left(\chi(\phi_h^1, \phi_h^0), \psi\right) + \frac{1}{\varepsilon} \left(\phi_h^0 + \frac{\tau}{2} \partial_t \phi^0, \psi\right); \quad (4.56b)$$

and, for $1 \leq m \leq M-1$, and all $\nu, \psi \in S_h$,

$$\left(\delta_\tau \phi_h^{m+\frac{1}{2}}, \nu\right) + \varepsilon a\left(\mu_h^{m+\frac{1}{2}}, \nu\right) = 0, \quad (4.57a)$$

$$\begin{aligned} \varepsilon a\left(\phi_h^{m+\frac{1}{2}}, \psi\right) + \frac{\varepsilon}{4} a\left(\phi_h^{m+1} - 2\phi_h^m + \phi_h^{m-1}, \psi\right) - \left(\mu_h^{m+\frac{1}{2}}, \psi\right) &= -\frac{1}{\varepsilon} \left(\chi(\phi_h^{m+1}, \phi_h^m), \psi\right) \\ &\quad + \frac{1}{\varepsilon} \left(\tilde{\phi}_h^{m+\frac{1}{2}}, \psi\right). \end{aligned} \quad (4.57b)$$

Now let us define the following additional error terms: for any integers $0 \leq m \leq M$,

$$\mathcal{E}_h^{\phi, m} := R_h \phi^m - \phi_h^m, \quad \mathcal{E}^{\phi, m} := \phi^m - \phi_h^m, \quad (4.58)$$

and, for any integers $0 \leq m \leq M-1$

$$\mathcal{E}_h^{\mu, m+\frac{1}{2}} := R_h \mu^{m+\frac{1}{2}} - \mu_h^{m+\frac{1}{2}}, \quad \mathcal{E}^{\mu, m+\frac{1}{2}} := \mu^{m+\frac{1}{2}} - \mu_h^{m+\frac{1}{2}}. \quad (4.59)$$

Setting $m = 0$ in (4.55a) – (4.55b) and subtracting (4.56a) – (4.56b), we have

$$\left(\delta_\tau \mathcal{E}_h^{\phi, \frac{1}{2}}, \nu\right) + \varepsilon a\left(\mathcal{E}_h^{\mu, \frac{1}{2}}, \nu\right) = \left(\sigma_1^{\frac{1}{2}} + \sigma_2^{\frac{1}{2}}, \nu\right), \quad (4.60a)$$

$$\begin{aligned} \frac{\varepsilon}{2} a\left(\mathcal{E}_h^{\phi, 1} + \mathcal{E}_h^{\phi, 0}, \psi\right) - \left(\mathcal{E}_h^{\mu, \frac{1}{2}}, \psi\right) &= \left(\mathcal{E}_a^{\mu, \frac{1}{2}}, \psi\right) - \frac{1}{\varepsilon} \left(\chi(\phi^1, \phi^0) - \chi(\phi_h^1, \phi_h^0), \psi\right) \\ &\quad + \frac{1}{\varepsilon} \left(\phi^{\frac{1}{2}} - \phi_h^0 - \frac{\tau}{2} \partial_t \phi^0, \psi\right) + \varepsilon a\left(\sigma_3^{\frac{1}{2}}, \psi\right) \\ &\quad + \frac{1}{\varepsilon} \left(\sigma_4^{\frac{1}{2}}, \psi\right). \end{aligned} \quad (4.60b)$$

Similarly, subtracting (4.57a) – (4.57b) from (4.55a) – (4.55b), yields, for $1 \leq m \leq M - 1$,

$$\left(\delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}}, \nu\right) + \varepsilon a\left(\mathcal{E}_h^{\mu, m+\frac{1}{2}}, \nu\right) = \left(\sigma_1^{m+\frac{1}{2}} + \sigma_2^{m+\frac{1}{2}}, \nu\right), \quad (4.61a)$$

$$\begin{aligned} \frac{\varepsilon}{2} a\left(\mathcal{E}_h^{\phi, m+1} + \mathcal{E}_h^{\phi, m}, \psi\right) + \frac{\varepsilon \tau^2}{4} a\left(\delta_\tau^2 \mathcal{E}_h^{\phi, m}, \psi\right) - \left(\mathcal{E}_h^{\mu, m+\frac{1}{2}}, \psi\right) \\ = \left(\mathcal{E}_a^{\mu, m+\frac{1}{2}}, \psi\right) - \frac{1}{\varepsilon} \left(\chi(\phi^{m+1}, \phi^m) - \chi(\phi_h^{m+1}, \phi_h^m), \psi\right) \\ + \frac{1}{\varepsilon} \left(\phi^{m+\frac{1}{2}} - \tilde{\phi}_h^{m+\frac{1}{2}}, \psi\right) + \varepsilon a\left(\sigma_3^{m+\frac{1}{2}}, \psi\right) \\ + \frac{1}{\varepsilon} \left(\sigma_4^{m+\frac{1}{2}}, \psi\right) + \frac{\varepsilon \tau^2}{4} a\left(\delta_\tau^2 \phi^m, \psi\right), \end{aligned} \quad (4.61b)$$

where $\tau^2 \delta_\tau^2 \psi^m := \psi^{m+1} - 2\psi^m + \psi^{m-1}$.

Now, define the additional error terms

$$\sigma_5^{m+\frac{1}{2}} := \chi(\phi_h^{m+1}, \phi_h^m) - \chi(\phi^{m+1}, \phi^m), \quad (4.62)$$

$$\sigma_6^{m+\frac{1}{2}} := \phi^{m+\frac{1}{2}} - \begin{cases} \phi_h^0 + \frac{\tau}{2} \partial_t \phi^0, & \text{for } m = 0 \\ \tilde{\phi}_h^{m+\frac{1}{2}}, & \text{for } 1 \leq m \leq M - 1 \end{cases}. \quad (4.63)$$

Then, setting $\nu = \mathcal{E}_h^{\mu, \frac{1}{2}}$ in (4.60a) and $\psi = \delta_\tau \mathcal{E}_h^{\phi, \frac{1}{2}}$ in (4.60b), setting $\nu = \mathcal{E}_h^{\mu, m+\frac{1}{2}}$ in (4.61a) and $\psi = \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}}$ in (4.61b), and adding the resulting equations, we have

$$\begin{aligned} & \frac{\varepsilon}{2} a \left(\mathcal{E}_h^{\phi, m+1} + \mathcal{E}_h^{\phi, m}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) + \frac{\gamma_m \varepsilon \tau^2}{4} a \left(\delta_\tau^2 \mathcal{E}_h^{\phi, m}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) + \varepsilon \left\| \nabla \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right\|_{L^2}^2 \\ &= \left(\sigma_1^{m+\frac{1}{2}} + \sigma_2^{m+\frac{1}{2}}, \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right) + \left(\mathcal{E}_a^{\mu, m+\frac{1}{2}}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) + \varepsilon a \left(\sigma_3^{m+\frac{1}{2}}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) \\ &+ \frac{1}{\varepsilon} \left(\sigma_4^{m+\frac{1}{2}} + \sigma_5^{m+\frac{1}{2}} + \sigma_6^{m+\frac{1}{2}}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) + \frac{\gamma_m \varepsilon \tau^2}{4} a \left(\delta_\tau^2 \phi^m, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right), \end{aligned} \quad (4.64)$$

for all $0 \leq m \leq M-1$, where $\gamma_m := 1 - \delta_{0,m}$ and $\delta_{k,\ell}$ is the Kronecker delta function. The terms involving γ_m are “turned on” only when $m \geq 1$. Expression (4.64) is the key error equation from which we will define our error estimates.

Lemma 4.4.1. *Suppose that (ϕ, μ) is a weak solution to (4.55a) – (4.55b), with the additional regularities (4.53). Then for all $t_m \in [0, T]$ and for any $h, \tau > 0$, there exists a constant $C > 0$, independent of h and τ and T , such that for all $0 \leq m \leq M-1$,*

$$\left\| \sigma_1^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq C \frac{h^{2q+2}}{\tau} \int_{t_m}^{t_{m+1}} \|\partial_s \phi(s)\|_{H^{q+1}}^2 ds, \quad (4.65)$$

$$\left\| \sigma_2^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq \frac{\tau^3}{640} \int_{t_m}^{t_{m+1}} \|\partial_{sss} \phi(s)\|_{L^2}^2 ds, \quad (4.66)$$

$$\left\| \nabla \Delta \sigma_3^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq \frac{\tau^3}{96} \int_{t_m}^{t_{m+1}} \|\nabla \Delta \partial_{ss} \phi(s)\|_{L^2}^2 ds, \quad (4.67)$$

$$\left\| \nabla \sigma_3^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq \frac{\tau^3}{96} \int_{t_m}^{t_{m+1}} \|\nabla \partial_{ss} \phi(s)\|_{L^2}^2 ds, \quad (4.68)$$

$$\left\| \frac{1}{2} (\phi^{m+1})^2 + \frac{1}{2} (\phi^m)^2 - \left(\phi^{m+\frac{1}{2}} \right)^2 \right\|_{H^1}^2 \leq \frac{\tau^3}{96} \int_{t_m}^{t_{m+1}} \|\partial_{ss} \phi^2(s)\|_{H^1}^2 ds, \quad (4.69)$$

and for all $1 \leq m \leq M-1$,

$$\|\tau^2 \nabla \Delta \delta_\tau^2 \phi^m\|_{L^2}^2 \leq \frac{\tau^3}{3} \int_{t_{m-1}}^{t_{m+1}} \|\nabla \Delta \partial_{ss} \phi(s)\|_{L^2}^2 ds, \quad (4.70)$$

$$\|\tau^2 \nabla \delta_\tau^2 \phi^m\|_{L^2}^2 \leq \frac{\tau^3}{3} \int_{t_{m-1}}^{t_{m+1}} \|\nabla \partial_{ss} \phi(s)\|_{L^2}^2 ds, \quad (4.71)$$

$$\left\| \nabla \left(\phi^{m+\frac{1}{2}} - \frac{3}{2} \phi^m + \frac{1}{2} \phi^{m-1} \right) \right\|_{L^2}^2 \leq \frac{\tau^3}{12} \int_{t_{m-1}}^{t_{m+1}} \|\nabla \partial_{ss} \phi(s)\|_{L^2}^2 ds, \quad (4.72)$$

and finally,

$$\left\| \nabla \left(\phi^{\frac{1}{2}} - \phi^0 - \frac{\tau}{2} \partial_t \phi^0 \right) \right\|_{L^2} \leq \frac{\tau^3}{24} \int_{t_0}^{t_{\frac{1}{2}}} \|\nabla \partial_{ss} \phi(s)\|_{L^2}^2 ds. \quad (4.73)$$

Proof. The proof of each of the inequalities above is a direct application of Taylor's Theorem with integral remainder 2.2.27 and Hölder's Inequality (2.12). Inequality (4.65) also uses the finite element approximation property for the Ritz projection,

$$\begin{aligned} \left\| \sigma_1^{m+\frac{1}{2}} \right\|_{L^2}^2 &= \left\| \delta_\tau R_h \phi^{m+\frac{1}{2}} - \delta_\tau \phi^{m+\frac{1}{2}} \right\|_{L^2}^2 \\ &= \left\| \frac{R_h \phi^{m+1} - \phi^{m+1}}{\tau} - \frac{R_h \phi^m - \phi^m}{\tau} \right\|_{L^2}^2 \\ &= \frac{1}{\tau^2} \left\| R_h (\phi^{m+1} - \phi^m) - (\phi^{m+1} - \phi^m) \right\|_{L^2}^2 \\ &= \frac{1}{\tau^2} \left\| \int_{t_m}^{t_{m+1}} R_h \partial_s \phi(s) - \partial_s \phi(s) ds \right\|_{L^2}^2 \\ &\leq \frac{1}{\tau^2} \left\| \left(\int_{t_m}^{t_{m+1}} 1 ds \right)^{\frac{1}{2}} \left(\int_{t_m}^{t_{m+1}} (R_h \partial_s \phi(s) - \partial_s \phi(s))^2 ds \right)^{\frac{1}{2}} \right\|_{L^2}^2 \\ &= \frac{1}{\tau} \int_{\Omega} \int_{t_m}^{t_{m+1}} (R_h \partial_s \phi(s) - \partial_s \phi(s))^2 ds d\mathbf{x} \\ &= \frac{1}{\tau} \int_{\Omega} \|R_h \partial_s \phi(s) - \partial_s \phi(s)\|_{L^2}^2 ds \\ &\leq \frac{1}{\tau} \int_{\Omega} (Ch^{q+1} \|\partial_s \phi(s)\|_{H^{q+1}})^2 ds \\ &= C \frac{h^{2q+2}}{\tau} \int_{t_m}^{t_{m+1}} \|\partial_s \phi(s)\|_{H^{q+1}}^2 ds. \end{aligned}$$

Inequality (4.66) proceeds as follows,

$$\begin{aligned}
\left\| \sigma_2^{m+\frac{1}{2}} \right\|_{L^2}^2 &= \left\| \delta_\tau \phi^{m+\frac{1}{2}} - \partial_t \phi^{m+\frac{1}{2}} \right\|_{L^2}^2 \\
&= \left\| \frac{1}{\tau} \left(\phi^{m+1} - \phi^{m+\frac{1}{2}} - \frac{\tau}{2} \partial_t \phi^{m+\frac{1}{2}} - \frac{1}{2} \left(\frac{\tau}{2} \right)^2 \partial_{tt} \phi^{m+\frac{1}{2}} \right) \right. \\
&\quad \left. - \frac{1}{\tau} \left(\phi^m - \phi^{m+\frac{1}{2}} - \left(-\frac{\tau}{2} \right) \partial_t \phi^{m+\frac{1}{2}} - \frac{1}{2} \left(-\frac{\tau}{2} \right)^2 \partial_{tt} \phi^{m+\frac{1}{2}} \right) \right\|_{L^2}^2 \\
&= \frac{1}{\tau^2} \left\| \frac{1}{2} \int_{t_{m+\frac{1}{2}}}^{t_{m+1}} (t_{m+1} - s)^2 \partial_{sss} \phi(s) ds - \frac{1}{2} \int_{t_{m+\frac{1}{2}}}^{t_m} (t_m - s)^2 \partial_{sss} \phi(s) ds \right\|_{L^2}^2 \\
&= \frac{1}{4\tau^2} \left\| \int_{t_{m+\frac{1}{2}}}^{t_{m+1}} (t_{m+1} - s)^2 \partial_{sss} \phi(s) ds + \int_{t_m}^{t_{m+\frac{1}{2}}} (t_m - s)^2 \partial_{sss} \phi(s) ds \right\|_{L^2}^2 \\
&\leq \frac{1}{4\tau^2} \int_{\Omega} \int_{t_{m+\frac{1}{2}}}^{t_{m+1}} (t_{m+1} - s)^4 ds \int_{t_{m+\frac{1}{2}}}^{t_{m+1}} (\partial_{sss} \phi(s))^2 ds d\mathbf{x} \\
&\quad + \frac{1}{4\tau^2} \int_{\Omega} \int_{t_m}^{t_{m+\frac{1}{2}}} (t_m - s)^4 ds \int_{t_m}^{t_{m+\frac{1}{2}}} (\partial_{sss} \phi(s))^2 ds d\mathbf{x} \\
&= \frac{1}{4\tau^2} \cdot \frac{\tau^5}{2^5 \cdot 5} \left(\int_{t_{m+\frac{1}{2}}}^{t_{m+1}} \|\partial_{sss} \phi(s)\|_{L^2}^2 ds + \int_{t_m}^{t_{m+\frac{1}{2}}} \|\partial_{sss} \phi(s)\|_{L^2}^2 ds \right) \\
&= \frac{\tau^3}{640} \int_{t_m}^{t_{m+1}} \|\partial_{sss} \phi(s)\|_{L^2}^2 ds.
\end{aligned}$$

Inequalities (4.67) and (4.68) are similar. The proof for (4.67) now follows,

$$\begin{aligned}
\left\| \nabla \Delta \sigma_3^{m+\frac{1}{2}} \right\|_{L^2}^2 &= \left\| \nabla \Delta \left(\frac{1}{2} \phi^{m+1} + \frac{1}{2} \phi^m - \phi^{m+\frac{1}{2}} \right) \right\|_{L^2}^2 \\
&= \frac{1}{4} \left\| \nabla \Delta \phi^{m+1} - \nabla \Delta \phi^{m+\frac{1}{2}} - \frac{\tau}{2} \nabla \Delta \partial_t \phi^{m+\frac{1}{2}} \right. \\
&\quad \left. + \nabla \Delta \phi^m - \nabla \Delta \phi^{m+\frac{1}{2}} - \left(-\frac{\tau}{2} \right) \nabla \Delta \partial_t \phi^{m+\frac{1}{2}} \right\|_{L^2}^2 \\
&= \frac{1}{4} \left\| \int_{t_{m+\frac{1}{2}}}^{t_{m+1}} (t_{m+1} - s) \partial_{ss} \nabla \Delta \phi(s) \, ds + \int_{t_{m+\frac{1}{2}}}^{t_m} (t_m - s) \partial_{ss} \nabla \Delta \phi(s) \, ds \right\|_{L^2}^2 \\
&\leq \frac{1}{4} \int_{\Omega} \int_{t_{m+\frac{1}{2}}}^{t_{m+1}} (t_{m+1} - s)^2 \, ds \int_{t_{m+\frac{1}{2}}}^{t_{m+1}} (\nabla \Delta \partial_{ss} \phi(s))^2 \, ds d\mathbf{x} \\
&\quad + \frac{1}{4} \int_{\Omega} \int_{t_m}^{t_{m+\frac{1}{2}}} (t_m - s)^2 \, ds \int_{t_m}^{t_{m+\frac{1}{2}}} (\nabla \Delta \partial_{ss} \phi(s))^2 \, ds d\mathbf{x} \\
&= \frac{1}{4} \cdot \frac{\tau^3}{24} \left(\int_{\Omega} \int_{t_{m+\frac{1}{2}}}^{t_{m+1}} (\nabla \Delta \partial_{ss} \phi(s))^2 \, ds + \int_{t_m}^{t_{m+\frac{1}{2}}} (\nabla \Delta \partial_{ss} \phi(s))^2 \, ds d\mathbf{x} \right) \\
&= \frac{\tau^3}{96} \int_{t_m}^{t_{m+1}} \left\| \nabla \Delta \partial_{ss} \phi(s) \right\|_{L^2}^2 \, ds.
\end{aligned}$$

Additionally, the proof for inequality (4.69) follows in the same manner as that for inequality (4.67) above. The details for inequality (4.70) immediately follow,

$$\begin{aligned}
\left\| \tau^2 \nabla \Delta \delta_{\tau}^2 \phi^m \right\|_{L^2}^2 &= \left\| \nabla \phi^{m+1} - 2 \nabla \phi^m + \nabla \phi^{m-1} \right\|_{L^2}^2 \\
&= \left\| \nabla \phi^{m+1} - \nabla \phi^m - \tau \partial_t \nabla \phi^m + \nabla \phi^{m-1} - \nabla \phi^m - (-\tau) \partial_t \nabla \phi^m \right\|_{L^2}^2 \\
&= \left\| \int_{t_m}^{t_{m+1}} (t_{m+1} - s) \nabla \partial_{ss} \phi(s) \, ds + \int_{t_m}^{t_{m-1}} (t_{m-1} - s) \nabla \partial_{ss} \phi(s) \, ds \right\|_{L^2}^2 \\
&\leq \int_{\Omega} \int_{t_m}^{t_{m+1}} (t_{m+1} - s)^2 \, ds \int_{t_m}^{t_{m+1}} (\nabla \partial_{ss} \phi(s))^2 \, ds d\mathbf{x} \\
&\quad + \int_{\Omega} \int_{t_{m-1}}^{t_m} (t_{m-1} - s)^2 \, ds \int_{t_{m-1}}^{t_m} (\nabla \partial_{ss} \phi(s))^2 \, ds d\mathbf{x} \\
&= \frac{\tau^3}{3} \int_{t_{m-1}}^{t_{m+1}} \left\| \nabla \Delta \partial_{ss} \phi(s) \right\|_{L^2}^2 \, ds.
\end{aligned}$$

Inequality (4.71) follows similarly. The final two inequalities uses similar tricks as above. The details are as follows,

$$\begin{aligned}
\left\| \nabla \left(\phi^{m+\frac{1}{2}} - \frac{3}{2}\phi^m + \frac{1}{2}\phi^{m-1} \right) \right\|_{L^2}^2 &= \left\| \frac{1}{2} (\nabla \phi^{m-1} - \nabla \phi^m - (-\tau) \partial_t \nabla \phi^m) \right. \\
&\quad \left. + \nabla \phi^{m+\frac{1}{2}} - \nabla \phi^m - \left(-\frac{\tau}{2} \right) \nabla \partial_t \phi^m \right\|_{L^2}^2 \\
&= \left\| \frac{1}{2} \int_{t_m}^{t_{m-1}} (t_{m-1} - s) \nabla \partial_{ss} \phi(s) \, ds \right. \\
&\quad \left. + \int_{t_m}^{t_{m+\frac{1}{2}}} (t_{m+\frac{1}{2}} - s) \nabla \partial_{ss} \phi(s) \, ds \right\|_{L^2}^2 \\
&\leq \frac{1}{4} \int_{\Omega} \int_{t_{m-1}}^{t_m} (t_{m-1} - s)^2 \, ds \int_{t_{m-1}}^{t_m} (\nabla \partial_{ss} \phi(s))^2 \, ds d\mathbf{x} \\
&\quad + \int_{\Omega} \int_{t_m}^{t_{m+\frac{1}{2}}} (t_{m+\frac{1}{2}} - s)^2 \, ds \int_{t_m}^{t_{m+\frac{1}{2}}} (\nabla \partial_{ss} \phi(s))^2 \, ds d\mathbf{x} \\
&= \frac{1}{4} \frac{\tau^3}{3} \int_{\Omega} \int_{t_{m-1}}^{t_m} (\nabla \partial_{ss} \phi(s))^2 \, ds d\mathbf{x} \\
&\quad + \frac{\tau^3}{2^3 \cdot 3} \int_{\Omega} \int_{t_m}^{t_{m+\frac{1}{2}}} (\nabla \partial_{ss} \phi(s))^2 \, ds d\mathbf{x} \\
&= \frac{\tau^3}{12} \int_{t_{m-1}}^{t_{m+1}} \|\nabla \partial_{ss} \phi(s)\|_{L^2}^2 \, ds.
\end{aligned}$$

And finally,

$$\begin{aligned}
\left\| \nabla \left(\phi^{\frac{1}{2}} - \phi^0 - \frac{\tau}{2} \partial_t \phi^0 \right) \right\|_{L^2} &= \left\| \int_{t_0}^{t_{\frac{1}{2}}} (t_{\frac{1}{2}} - s) \nabla \partial_{ss} \phi(s) \, ds \right\|_{L^2}^2 \\
&\leq \int_{\Omega} \int_{t_0}^{t_{\frac{1}{2}}} (t_{\frac{1}{2}} - s)^2 \, ds \int_{t_0}^{t_{\frac{1}{2}}} (\nabla \partial_{ss} \phi(s))^2 \, ds d\mathbf{x} \\
&= \frac{\tau^3}{2^3 \cdot 3} \int_{t_0}^{t_{\frac{1}{2}}} \|\nabla \partial_{ss} \phi(s)\|_{L^2}^2 \, ds \\
&= \frac{\tau^3}{24} \int_{t_0}^{t_{\frac{1}{2}}} \|\nabla \partial_{ss} \phi(s)\|_{L^2}^2 \, ds.
\end{aligned}$$

□

Lemma 4.4.2. *Suppose that (ϕ, μ) is a weak solution to (4.55a) – (4.55b), with the additional regularities (4.53). Then, there exists a constant $C > 0$ independent of h and τ – but possibly dependent upon T through the regularity estimates – such that, for any $h, \tau > 0$,*

$$\left\| \nabla \sigma_4^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq C\tau^3 \int_{t_m}^{t_{m+1}} \left\| \nabla \partial_{ss} \phi(s) \right\|_{L^2}^2 ds + C\tau^3 \int_{t_m}^{t_{m+1}} \left\| \partial_{ss} \phi^2(s) \right\|_{H^1}^2 ds. \quad (4.74)$$

Proof. We begin with the expansion

$$\begin{aligned} \nabla \sigma_4^{m+\frac{1}{2}} &= \left(\frac{1}{2} \phi^{m+1} + \frac{1}{2} \phi^m - \phi^{m+\frac{1}{2}} \right) \nabla \left(\frac{1}{2} (\phi^{m+1})^2 + \frac{1}{2} (\phi^m)^2 \right) \\ &\quad + \left(\frac{1}{2} (\phi^{m+1})^2 + \frac{1}{2} (\phi^m)^2 \right) \nabla \left(\frac{1}{2} \phi^{m+1} + \frac{1}{2} \phi^m - \phi^{m+\frac{1}{2}} \right) \\ &\quad + \phi^{m+\frac{1}{2}} \nabla \left(\frac{1}{2} (\phi^{m+1})^2 + \frac{1}{2} (\phi^m)^2 - \left(\phi^{m+\frac{1}{2}} \right)^2 \right) \\ &\quad + \left(\frac{1}{2} (\phi^{m+1})^2 + \frac{1}{2} (\phi^m)^2 - \left(\phi^{m+\frac{1}{2}} \right)^2 \right) \nabla \phi^{m+\frac{1}{2}}. \end{aligned} \quad (4.75)$$

By the triangle inequality, Young's inequality, and the embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$, we have

$$\begin{aligned}
\left\| \nabla \sigma_4^{m+\frac{1}{2}} \right\|_{L^2} &\leq \left\| \frac{1}{2} \phi^{m+1} + \frac{1}{2} \phi^m - \phi^{m+\frac{1}{2}} \right\|_{L^6} \left\| \nabla \left(\frac{1}{2} (\phi^{m+1})^2 + \frac{1}{2} (\phi^m)^2 \right) \right\|_{L^3} \\
&\quad + \left\| \frac{1}{2} (\phi^{m+1})^2 + \frac{1}{2} (\phi^m)^2 \right\|_{L^\infty} \left\| \nabla \left(\frac{1}{2} \phi^{m+1} + \frac{1}{2} \phi^m - \phi^{m+\frac{1}{2}} \right) \right\|_{L^2} \\
&\quad + \left\| \phi^{m+\frac{1}{2}} \right\|_{L^\infty} \left\| \nabla \left(\frac{1}{2} (\phi^{m+1})^2 + \frac{1}{2} (\phi^m)^2 - (\phi^{m+\frac{1}{2}})^2 \right) \right\|_{L^2} \\
&\quad + \left\| \frac{1}{2} (\phi^{m+1})^2 + \frac{1}{2} (\phi^m)^2 - (\phi^{m+\frac{1}{2}})^2 \right\|_{L^6} \left\| \nabla \phi^{m+\frac{1}{2}} \right\|_{L^3} \\
&\leq C \left\{ \left\| \phi^{m+1} \right\|_{L^\infty}^2 + \left\| \phi^m \right\|_{L^\infty}^2 + \left\| \phi^{m+1} \right\|_{L^6} \left\| \nabla \phi^{m+1} \right\|_{L^6} + \left\| \phi^m \right\|_{L^6} \left\| \nabla \phi^m \right\|_{L^6} \right\} \\
&\quad \times \left\| \nabla \left(\frac{1}{2} \phi^{m+1} + \frac{1}{2} \phi^m - \phi^{m+\frac{1}{2}} \right) \right\|_{L^2} \\
&\quad + C \left\{ \left\| \phi^{m+\frac{1}{2}} \right\|_{L^\infty} + \left\| \nabla \phi^{m+\frac{1}{2}} \right\|_{L^3} \right\} \\
&\quad \times \left\| \frac{1}{2} (\phi^{m+1})^2 + \frac{1}{2} (\phi^m)^2 - (\phi^{m+\frac{1}{2}})^2 \right\|_{H^1}.
\end{aligned} \tag{4.76}$$

Using the assumed regularities (4.53) of the PDE solution, and appealing to the truncation error estimates (4.68) and (4.69), the result follows. $\square$

Lemma 4.4.3. *Suppose that (ϕ, μ) is a weak solution to (4.55a) – (4.55b), with the additional regularities (4.53). Then, there exists a constant $C > 0$ independent of h and τ , but possibly dependent upon T , such that, for any $h, \tau > 0$,*

$$\left\| \nabla \sigma_5^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq C \left\| \nabla \mathcal{E}^{\phi, m+1} \right\|_{L^2}^2 + C \left\| \nabla \mathcal{E}^{\phi, m} \right\|_{L^2}^2, \tag{4.77}$$

where $\mathcal{E}^{\phi, m} := \phi^m - \phi_h^m$.

Proof. We begin with the detailed expansion

$$\begin{aligned}
4\nabla\sigma_5^{m+\frac{1}{2}} &= \nabla (4\chi(\phi_h^{m+1}, \phi_h^m) - \chi(\phi^{m+1}, \phi^m)) \\
&= 4\nabla \left(\chi(\phi_h^{m+1}, \phi_h^m) - \frac{1}{2}\chi(\phi_h^{m+1}, \phi^m) + \frac{1}{2}\chi(\phi_h^{m+1}, \phi^m) - \frac{1}{2}\chi(\phi^{m+1}, \phi_h^m) \right. \\
&\quad \left. + \frac{1}{2}\chi(\phi^{m+1}, \phi_h^m) - \chi(\phi^{m+1}, \phi^m) \right) \\
&= \frac{1}{2}\nabla (\omega(\phi_h^{m+1}, \phi_h^m, \phi^{m+1}) \cdot (\phi_h^{m+1} - \phi^{m+1})) \\
&\quad + \frac{1}{2}\nabla (\omega(\phi^{m+1}, \phi^m, \phi_h^{m+1}) \cdot (\phi_h^{m+1} - \phi^{m+1})) \\
&\quad + \frac{1}{2}\nabla (\omega(\phi_h^{m+1}, \phi_h^m, \phi^m) \cdot (\phi_h^m - \phi^m)) \\
&\quad + \frac{1}{2}\nabla (\omega(\phi^{m+1}, \phi^m, \phi_h^m) \cdot (\phi_h^m - \phi^m)) \\
&= \left\{ (\phi_h^{m+1})^2 + (\phi_h^m)^2 + 2\phi_h^{m+1}(\phi_h^{m+1} + \phi_h^m) \right\} \nabla(\phi_h^{m+1} - \phi^{m+1}) \\
&\quad + \left\{ (\phi_h^{m+1})^2 + (\phi_h^m)^2 + 2\phi_h^m(\phi_h^{m+1} + \phi_h^m) \right\} \nabla(\phi_h^m - \phi^m) \\
&\quad + \left\{ \nabla(\phi^{m+1} + \phi^m) \cdot (\phi_h^{m+1} + \phi^{m+1}) + 2\nabla\phi^{m+1}(\phi_h^{m+1} + \phi_h^m) \right. \\
&\quad \left. + 2\phi^{m+1}\nabla\phi^{m+1} + 2\phi^m\nabla\phi^m \right\} (\phi_h^{m+1} - \phi^{m+1}) \\
&\quad + \left\{ \nabla(\phi^{m+1} + \phi^m) \cdot (\phi_h^m + \phi^m) + 2\nabla\phi^m(\phi_h^{m+1} + \phi_h^m) \right. \\
&\quad \left. + 2\phi^{m+1}\nabla\phi^{m+1} + 2\phi^m\nabla\phi^m \right\} (\phi_h^m - \phi^m). \tag{4.78}
\end{aligned}$$

Then, using the unconditional *a priori* estimates in Lemmas 4.3.8 and 4.3.12, the assumption that $\phi \in L^\infty(0, T; W^{1,6}(\Omega))$, and the embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$ we

have, for any $0 \leq m \leq M-1$,

$$\begin{aligned}
\left\| \nabla \sigma_5^{m+\frac{1}{2}} \right\|_{L^2} &\leq C \left(\left\| \nabla \mathcal{E}^{\phi, m+1} \right\|_{L^2} + \left\| \nabla \mathcal{E}^{\phi, m} \right\|_{L^2} \right) \times \left\{ \left\| \phi_h^{m+1} \right\|_{L^\infty}^2 + \left\| \phi_h^m \right\|_{L^\infty}^2 \right\} \\
&\quad + C \left(\left\| \mathcal{E}^{\phi, m+1} \right\|_{L^6} + \left\| \mathcal{E}^{\phi, m} \right\|_{L^6} \right) \times \left\{ \left(\left\| \nabla \phi^{m+1} \right\|_{L^6} + \left\| \nabla \phi^m \right\|_{L^6} \right) \right. \\
&\quad \left. \times \left(\left\| \phi^{m+1} \right\|_{L^6} + \left\| \phi^m \right\|_{L^6} + \left\| \phi_h^{m+1} \right\|_{L^6} + \left\| \phi_h^m \right\|_{L^6} \right) \right\} \\
&\leq C \left\| \nabla \mathcal{E}^{\phi, m+1} \right\|_{L^2} + C \left\| \nabla \mathcal{E}^{\phi, m} \right\|_{L^2}. \tag{4.79}
\end{aligned}$$

□

Lemma 4.4.4. *Suppose that (ϕ, μ) is a weak solution to (4.55a) – (4.55b), with the additional regularities (4.53). Then, there exists a constant $C > 0$ independent of h and τ such that, for any $h, \tau > 0$,*

$$\begin{aligned}
\left\| \nabla \sigma_6^{m+\frac{1}{2}} \right\|_{L^2}^2 &\leq \gamma_m C \tau^3 \int_{t_{m-1}}^{t_m} \left\| \nabla \partial_{ss} \phi(s) \right\|_{L^2}^2 ds + C \tau^3 \int_{t_m}^{t_{m+1}} \left\| \nabla \partial_{ss} \phi(s) \right\|_{L^2}^2 ds \\
&\quad + C \left\| \nabla \mathcal{E}^{\phi, m} \right\|_{L^2}^2 + \gamma_m C \left\| \nabla \mathcal{E}^{\phi, m-1} \right\|_{L^2}^2 + \delta_{0,m} C h^{2q} |\phi_0|_{H^{q+1}}^2, \tag{4.80}
\end{aligned}$$

where $\mathcal{E}^{\phi, m} := \phi^m - \phi_h^m$ and $\delta_{k,\ell}$ is the Kronecker delta.

Proof. For $m = 0$, using the truncation error estimate (4.73) and a standard finite element estimate for the Ritz projection, we have

$$\begin{aligned}
\left\| \nabla \sigma_6^{\frac{1}{2}} \right\|_{L^2}^2 &\leq 2 \left\| \nabla \left(\phi^{\frac{1}{2}} - \phi_0 - \frac{\tau}{2} \partial_t \phi(0) \right) \right\|_{L^2}^2 + 2 \left\| \nabla (\phi_0 - \phi_h^0) \right\|_{L^2}^2 \\
&\leq 2 \frac{\tau^3}{24} \int_{t_0}^{t_{\frac{1}{2}}} \left\| \nabla \partial_{ss} \phi(s) \right\|_{L^2}^2 ds + C h^{2q} |\phi_0|_{H^{q+1}}^2, \tag{4.81}
\end{aligned}$$

with the observation that $\phi_h^0 := R_h \phi_0$. For $1 \leq m \leq M-1$, using the truncation error estimate (4.72), we obtain

$$\left\| \nabla \sigma_6^{m+\frac{1}{2}} \right\|_{L^2}^2 \leq 3 \frac{\tau^3}{6} \int_{t_{m-1}}^{t_{m+1}} \left\| \nabla \partial_{ss} \phi(s) \right\|_{L^2}^2 ds + \frac{27}{4} \left\| \nabla \mathcal{E}^{\phi, m} \right\|_{L^2}^2 + \frac{3}{4} \left\| \nabla \mathcal{E}^{\phi, m-1} \right\|_{L^2}^2. \tag{4.82}$$

□

We now proceed to estimate the terms on the right-hand-side of (4.64).

Lemma 4.4.5. *Suppose that (ϕ, μ) is a weak solution to (4.55a) – (4.55b), with the additional regularities (4.53). Then, for any $h, \tau > 0$ and any $\alpha > 0$ there exists a constant $C = C(\alpha, T) > 0$, independent of h and τ , such that, for $0 \leq m \leq M - 1$,*

$$\begin{aligned} & \frac{\varepsilon}{2} a \left(\mathcal{E}_h^{\phi, m+1} + \mathcal{E}_h^{\phi, m}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) + \frac{\gamma_m \varepsilon \tau^2}{4} a \left(\delta_\tau^2 \mathcal{E}_h^{\phi, m}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) + \frac{\varepsilon}{2} \left\| \nabla \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right\|_{L^2}^2 \\ & \leq C \left\| \nabla \mathcal{E}_h^{\phi, m+1} \right\|_{L^2}^2 + C \left\| \nabla \mathcal{E}_h^{\phi, m} \right\|_{L^2}^2 + \gamma_m C \left\| \nabla \mathcal{E}_h^{\phi, m-1} \right\|_{L^2}^2 + \alpha \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h}^2 \\ & \quad + C \mathcal{R}^{m+\frac{1}{2}}, \end{aligned} \tag{4.83}$$

where

$$\begin{aligned} \mathcal{R}^{m+\frac{1}{2}} &= \frac{h^{2q+2}}{\tau} \int_{t_m}^{t_{m+1}} \left\| \partial_s \phi(s) \right\|_{H^{q+1}}^2 ds + h^{2q} \left| \mu^{m+\frac{1}{2}} \right|_{H^{q+1}}^2 \\ & \quad + h^{2q} \left| \phi^{m+1} \right|_{H^{q+1}}^2 + h^{2q} \left| \phi^m \right|_{H^{q+1}}^2 + \gamma_m h^{2q} \left| \phi^{m-1} \right|_{H^{q+1}}^2 \\ & \quad + \tau^3 \int_{t_m}^{t_{m+1}} \left\| \partial_{sss} \phi(s) \right\|_{L^2}^2 ds + \tau^3 \int_{t_m}^{t_{m+1}} \left\| \partial_{ss} \phi^2(s) \right\|_{H^1}^2 ds \\ & \quad + \gamma_m \tau^3 \int_{t_{m-1}}^{t_m} \left\| \nabla \partial_{ss} \phi(s) \right\|_{L^2}^2 ds + \tau^3 \int_{t_m}^{t_{m+1}} \left\| \nabla \partial_{ss} \phi(s) \right\|_{L^2}^2 ds \\ & \quad + \gamma_m \tau^3 \int_{t_{m-1}}^{t_m} \left\| \nabla \Delta \partial_{ss} \phi(s) \right\|_{L^2}^2 ds + \tau^3 \int_{t_m}^{t_{m+1}} \left\| \nabla \Delta \partial_{ss} \phi(s) \right\|_{L^2}^2 ds. \end{aligned} \tag{4.84}$$

Proof. Define, for $0 \leq m \leq M - 1$, time-dependent spatial mass average

$$\overline{\mathcal{E}_h^{\mu, m+\frac{1}{2}}} := |\Omega|^{-1} \left(\mathcal{E}_h^{\mu, m+\frac{1}{2}}, 1 \right). \tag{4.85}$$

Using the Cauchy-Schwarz inequality, the Poincaré inequality, with the fact that

$$\left(\sigma_1^{m+\frac{1}{2}} + \sigma_2^{m+\frac{1}{2}}, 1 \right) = 0,$$

and the local truncation error estimates (4.65) and (4.66), we get the following estimate:

$$\begin{aligned}
\left| \left(\sigma_1^{m+\frac{1}{2}} + \sigma_2^{m+\frac{1}{2}}, \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right) \right| &= \left| \left(\sigma_1^{m+\frac{1}{2}} + \sigma_2^{m+\frac{1}{2}}, \mathcal{E}_h^{\mu, m+\frac{1}{2}} - \overline{\mathcal{E}_h^{\mu, m+\frac{1}{2}}} \right) \right| \\
&\leq \left\| \sigma_1^{m+\frac{1}{2}} + \sigma_2^{m+\frac{1}{2}} \right\|_{L^2} \left\| \mathcal{E}_h^{\mu, m+\frac{1}{2}} - \overline{\mathcal{E}_h^{\mu, m+\frac{1}{2}}} \right\|_{L^2} \\
&\leq C \left\| \sigma_1^{m+\frac{1}{2}} + \sigma_2^{m+\frac{1}{2}} \right\|_{L^2} \left\| \nabla \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right\|_{L^2} \\
&\leq C \left\| \sigma_1^{m+\frac{1}{2}} \right\|_{L^2}^2 + C \left\| \sigma_2^{m+\frac{1}{2}} \right\|_{L^2}^2 + \frac{\varepsilon}{2} \left\| \nabla \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right\|_{L^2}^2 \\
&\leq C \frac{h^{2q+2}}{\tau} \int_{t_m}^{t_{m+1}} \|\partial_s \phi(s)\|_{H^{q+1}}^2 ds \\
&\quad + C \frac{\tau^3}{640} \int_{t_m}^{t_{m+1}} \|\partial_{sss} \phi(s)\|_{L^2}^2 ds + \frac{\varepsilon}{2} \left\| \nabla \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right\|_{L^2}^2.
\end{aligned} \tag{4.86}$$

Standard finite element approximation theory shows that

$$\left\| \nabla \mathcal{E}_a^{\mu, m+\frac{1}{2}} \right\|_{L^2} = \left\| \nabla \left(R_h \mu^{m+\frac{1}{2}} - \mu^{m+\frac{1}{2}} \right) \right\|_{L^2} \leq Ch^q \left| \mu^{m+\frac{1}{2}} \right|_{H^{q+1}}.$$

Applying Lemma 2.2.22 and the last estimate, we have

$$\begin{aligned}
\left| \left(\mathcal{E}_a^{\mu, m+\frac{1}{2}}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) \right| &\leq C \left\| \nabla \mathcal{E}_a^{\mu, m+\frac{1}{2}} \right\|_{L^2} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h} \\
&\leq Ch^q \left| \mu^{m+\frac{1}{2}} \right|_{H^{q+1}} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h} \\
&\leq Ch^{2q} \left| \mu^{m+\frac{1}{2}} \right|_{H^{q+1}}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h}^2.
\end{aligned} \tag{4.87}$$

Using Lemma 2.2.22 and estimate (4.67), we find

$$\begin{aligned}
\varepsilon a \left(\sigma_3^{m+\frac{1}{2}}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) &= -\varepsilon \left(\Delta \sigma_3^{m+\frac{1}{2}}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) \\
&\leq C \left\| \nabla \Delta \sigma_3^{m+\frac{1}{2}} \right\|_{L^2} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h} \\
&\leq C \frac{\tau^3}{96} \int_{t_m}^{t_{m+1}} \left\| \nabla \Delta \partial_{ss} \phi(s) \right\|_{L^2}^2 ds + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h}^2.
\end{aligned} \tag{4.88}$$

Now, using Lemmas 4.4.2 and 2.2.22, we obtain

$$\begin{aligned}
\varepsilon^{-1} \left| \left(\sigma_4^{m+\frac{1}{2}}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) \right| &\leq C \left\| \nabla \sigma_4^{m+\frac{1}{2}} \right\|_{L^2} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h} \\
&\leq C \left\| \nabla \sigma_4^{m+\frac{1}{2}} \right\|_{L^2}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h}^2 \\
&\leq C \tau^3 \int_{t_m}^{t_{m+1}} \left\| \nabla \partial_{ss} \phi(s) \right\|_{L^2}^2 ds \\
&\quad + C \tau^3 \int_{t_m}^{t_{m+1}} \left\| \partial_{ss} \phi^2(s) \right\|_{H^1}^2 ds + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h}^2.
\end{aligned} \tag{4.89}$$

Similarly, using Lemmas 4.4.3 and 2.2.21, the relation $\mathcal{E}^{\phi, m+1} = \mathcal{E}_a^{\phi, m+1} + \mathcal{E}_h^{\phi, m+1}$, and a standard finite element error estimate, we arrive at

$$\begin{aligned}
\varepsilon^{-1} \left| \left(\sigma_5^{m+\frac{1}{2}}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) \right| &\leq C \left\| \nabla \sigma_5^{m+\frac{1}{2}} \right\|_{L^2}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h}^2 \\
&\leq C \left\| \nabla \mathcal{E}^{\phi, m+1} \right\|_{L^2}^2 + C \left\| \nabla \mathcal{E}^{\phi, m} \right\|_{L^2}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h}^2 \\
&\leq C \left\| \nabla \mathcal{E}_a^{\phi, m+1} \right\|_{L^2}^2 + C \left\| \nabla \mathcal{E}_h^{\phi, m+1} \right\|_{L^2}^2 + C \left\| \nabla \mathcal{E}_a^{\phi, m} \right\|_{L^2}^2 \\
&\quad + C \left\| \nabla \mathcal{E}_h^{\phi, m} \right\|_{L^2}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h}^2 \\
&\leq C h^{2q} \left| \phi^{m+1} \right|_{H^{q+1}}^2 + C \left\| \nabla \mathcal{E}_h^{\phi, m+1} \right\|_{L^2}^2 + C h^{2q} \left| \phi^m \right|_{H^{q+1}}^2 \\
&\quad + C \left\| \nabla \mathcal{E}_h^{\phi, m} \right\|_{L^2}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h}^2.
\end{aligned} \tag{4.90}$$

Applying Lemmas 4.4.4 and 2.2.22, the relation $\mathcal{E}^{\phi, m+1} = \mathcal{E}_a^{\phi, m+1} + \mathcal{E}_h^{\phi, m+1}$, and a standard finite element error estimate,

$$\begin{aligned}
\varepsilon^{-1} \left| \left(\sigma_6^{m+\frac{1}{2}}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) \right| &\leq C \left\| \nabla \sigma_6^{m+\frac{1}{2}} \right\|_{L^2}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h}^2 \\
&\leq C \tau^3 \left(\gamma_m \int_{t_{m-1}}^{t_m} \left\| \nabla \partial_{ss} \phi(s) \right\|_{L^2}^2 ds + \int_{t_m}^{t_{m+1}} \left\| \nabla \partial_{ss} \phi(s) \right\|_{L^2}^2 ds \right) \\
&\quad + C \left\| \nabla \mathcal{E}_h^{\phi, m} \right\|_{L^2}^2 + C \gamma_m \left\| \nabla \mathcal{E}_h^{\phi, m-1} \right\|_{L^2}^2 \\
&\quad + C h^{2q} |\phi^m|_{H^{q+1}}^2 + C \gamma_m h^{2q} |\phi^{m-1}|_{H^{q+1}}^2 + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h}^2.
\end{aligned} \tag{4.91}$$

To finish up, using (4.69),

$$\frac{\gamma_m \varepsilon \tau^2}{4} a \left(\delta_\tau^2 \phi^m, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) \leq C \gamma_m \frac{\tau^3}{3} \int_{t_{m-1}}^{t_m} \left\| \nabla \Delta \partial_{ss} \phi(s) \right\|_{L^2}^2 ds + \frac{\alpha}{6} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h}^2. \tag{4.92}$$

Combining the estimates (4.86) – (4.92) with the error equation (4.64), the result follows. $\square$

Lemma 4.4.6. *Suppose that (ϕ, μ) is a weak solution to (4.55a) – (4.55b), with the additional regularities (4.53). Then, for any $h, \tau > 0$, there exists a constant $C > 0$, independent of h and τ , such that*

$$\left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1, h}^2 \leq 2 \varepsilon^2 \left\| \nabla \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right\|_{L^2}^2 + C \mathcal{R}^{m+\frac{1}{2}}, \tag{4.93}$$

where $\mathcal{R}^{m+\frac{1}{2}}$ is the consistency term given in (4.84).

Proof. Setting $\nu = \mathbb{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi, \frac{1}{2}} \right)$ in (4.60a) and $\nu = \mathbb{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right)$ in (4.61a) and combining, we have

$$\begin{aligned}
\left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1,h}^2 &= -\varepsilon a \left(\mathcal{E}_h^{\mu, m+\frac{1}{2}}, \mathbb{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) \right) + \left(\sigma_1^{m+\frac{1}{2}} + \sigma_2^{m+\frac{1}{2}}, \mathbb{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) \right) \\
&= -\varepsilon \left(\mathcal{E}_h^{\mu, m+\frac{1}{2}}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) + \left(\sigma_1^{m+\frac{1}{2}} + \sigma_2^{m+\frac{1}{2}}, \mathbb{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) \right) \\
&\leq \varepsilon \left\| \nabla \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right\|_{L^2} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1,h} \\
&\quad + \left\| \sigma_1^{m+\frac{1}{2}} + \sigma_2^{m+\frac{1}{2}} \right\|_{L^2} \left\| \mathbb{T}_h \left(\delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) \right\|_{L^2} \\
&\leq \varepsilon^2 \left\| \nabla \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right\|_{L^2}^2 + \frac{1}{4} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1,h}^2 \\
&\quad + C \left\| \sigma_2^{m+\frac{1}{2}} + \sigma_1^{m+\frac{1}{2}} \right\|_{L^2}^2 + \frac{1}{4} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1,h}^2 \\
&\leq \varepsilon^2 \left\| \nabla \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right\|_{L^2}^2 + \frac{1}{2} \left\| \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right\|_{-1,h}^2 + C \mathcal{R}^{m+\frac{1}{2}}, \tag{4.94}
\end{aligned}$$

for $0 \leq m \leq M-1$ and where we have used Lemma 4.4.1. The result now follows. $\square$

Lemma 4.4.7. *Suppose that (ϕ, μ) is a weak solution to (4.55a) – (4.55b), with the additional regularities (4.53). Then, for any $h, \tau > 0$, there exists a constant $C > 0$, independent of h and τ , but possibly dependent upon T , such that*

$$\begin{aligned}
&\frac{\varepsilon}{2} a \left(\mathcal{E}_h^{\phi, m+1} + \mathcal{E}_h^{\phi, m}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) + \frac{\gamma_m \tau^2 \varepsilon}{4} a \left(\delta_\tau^2 \mathcal{E}_h^{\phi, m}, \delta_\tau \mathcal{E}_h^{\phi, m+\frac{1}{2}} \right) + \frac{\varepsilon}{4} \left\| \nabla \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right\|_{L^2}^2 \\
&\leq C \left\| \nabla \mathcal{E}_h^{\phi, m+1} \right\|_{L^2}^2 + C \left\| \nabla \mathcal{E}_h^{\phi, m} \right\|_{L^2}^2 + \gamma_m C \left\| \nabla \mathcal{E}_h^{\phi, m-1} \right\|_{L^2}^2 + C \mathcal{R}^{m+1}. \tag{4.95}
\end{aligned}$$

Proof. This follows upon combining the last two lemmas and choosing α in (4.83) appropriately. $\square$

Using the last lemma, we are ready to show the main convergence result for our second-order splitting scheme.

Theorem 4.4.8. *Suppose (ϕ, μ) is a weak solution to (4.55a) – (4.55b), with the additional regularities (4.53). Then, provided $0 < \tau < \tau_0$, for some τ_0 sufficiently small,*

$$\max_{0 \leq m \leq M-1} \left\| \nabla \mathcal{E}_h^{\phi, m+1} \right\|_{L^2}^2 + \tau \sum_{m=0}^{M-1} \left\| \nabla \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right\|_{L^2}^2 \leq C(T)(\tau^4 + h^{2q}) \quad (4.96)$$

for some $C(T) > 0$ that is independent of τ and h .

Proof. Using Lemma 4.4.7, we have

$$\begin{aligned} & \frac{1}{2\tau} \left(\left\| \nabla \mathcal{E}_h^{\phi, m+1} \right\|_{L^2}^2 - \left\| \nabla \mathcal{E}_h^{\phi, m} \right\|_{L^2}^2 \right) + \frac{1}{4} \left\| \nabla \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right\|_{L^2}^2 \\ & + \frac{\gamma_m}{8\tau} \left(\left\| \nabla \mathcal{E}_h^{\phi, m+1} - \nabla \mathcal{E}_h^{\phi, m} \right\|_{L^2}^2 - \left\| \nabla \mathcal{E}_h^{\phi, m} - \nabla \mathcal{E}_h^{\phi, m-1} \right\|_{L^2}^2 \right) \\ & \leq C \left\| \nabla \mathcal{E}_h^{\phi, m+1} \right\|_{L^2}^2 + C \left\| \nabla \mathcal{E}_h^{\phi, m} \right\|_{L^2}^2 + \gamma_m C \left\| \nabla \mathcal{E}_h^{\phi, m-1} \right\|_{L^2}^2 + C\mathcal{R}^{m+\frac{1}{2}}. \end{aligned} \quad (4.97)$$

Letting $m = 0$ in the previous equation and noting that $\mathcal{E}_h^{\phi, 0} \equiv 0$ and $\gamma_0 = 0$, then

$$\frac{1}{2\tau} \left\| \nabla \mathcal{E}_h^{\phi, 1} \right\|_{L^2}^2 + \frac{1}{4} \left\| \nabla \mathcal{E}_h^{\mu, \frac{1}{2}} \right\|_{L^2}^2 \leq C_1 \left\| \nabla \mathcal{E}_h^{\phi, 1} \right\|_{L^2}^2 + C\mathcal{R}^{\frac{1}{2}}. \quad (4.98)$$

If $0 < \tau \leq \tau_0 := \frac{1}{2C_1} < \frac{1}{C_1}$, it follows from the last estimate that

$$\left\| \nabla \mathcal{E}_h^{\phi, 1} \right\|_{L^2}^2 + \frac{\tau}{2} \left\| \nabla \mathcal{E}_h^{\mu, \frac{1}{2}} \right\|_{L^2}^2 \leq \tau C\mathcal{R}^{\frac{1}{2}} \leq C(\tau^4 + h^{2q}), \quad (4.99)$$

where we have used the regularity assumptions to conclude $\tau C\mathcal{R}^{\frac{1}{2}} \leq C(\tau^4 + h^{2q})$.

Now, applying $\tau \sum_{m=0}^{\ell}$ to (4.97),

$$\begin{aligned} \left\| \nabla \mathcal{E}_h^{\phi, \ell+1} \right\|_{L^2}^2 + \frac{\tau}{2} \sum_{m=0}^{\ell} \left\| \nabla \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right\|_{L^2}^2 & \leq C\tau \sum_{m=0}^{\ell} \mathcal{R}^{m+\frac{1}{2}} + C_2\tau \sum_{m=0}^{\ell} \left\| \nabla \mathcal{E}_h^{\phi, m+1} \right\|_{L^2}^2 \\ & + \frac{1}{4} \left\| \nabla \mathcal{E}_h^{\phi, 1} \right\|_{L^2}^2. \end{aligned} \quad (4.100)$$

If $0 < \tau \leq \tau_0 := \frac{1}{2C_2} < \frac{1}{C_2}$, it follows from the last estimate that

$$\begin{aligned} \left\| \nabla \mathcal{E}_h^{\phi, \ell+1} \right\|_{L^2}^2 &\leq C\tau \sum_{m=0}^{\ell} \mathcal{R}^{m+\frac{1}{2}} + \frac{C_2\tau}{1-C_2\tau} \sum_{m=0}^{\ell} \left\| \nabla \mathcal{E}_h^{\phi, m} \right\|_{L^2}^2 + \frac{1}{4} \left\| \nabla \mathcal{E}_h^{\phi, 1} \right\|_{L^2}^2 \\ &\leq C(\tau^4 + h^{2q}) + C\tau \sum_{m=0}^{\ell} \left\| \nabla \mathcal{E}_h^{\phi, m} \right\|_{L^2}^2, \end{aligned} \quad (4.101)$$

where we have used (4.99) and the regularity assumptions to conclude $\tau \sum_{m=0}^{M-1} \mathcal{R}^{m+\frac{1}{2}} \leq C(\tau^4 + h^{2q})$. Appealing to the discrete Gronwall inequality 2.2.26, it follows that, for any $0 < \ell \leq M-1$,

$$\left\| \nabla \mathcal{E}_h^{\phi, \ell+1} \right\|_{L^2}^2 \leq C(T)(\tau^4 + h^{2q}). \quad (4.102)$$

Considering estimates (4.99), (4.100), and (4.102) we get the desired result. $\square$

Remark 4.4.9. *From here it is straightforward to establish an optimal error estimate of the form*

$$\max_{0 \leq m \leq M-1} \left\| \nabla \mathcal{E}_h^{\phi, \ell+1} \right\|_{L^2}^2 + \tau \sum_{m=0}^{M-1} \left\| \nabla \mathcal{E}_h^{\mu, m+\frac{1}{2}} \right\|_{L^2}^2 \leq C(T)(\tau^4 + h^{2q}) \quad (4.103)$$

using $\mathcal{E}^\phi = \mathcal{E}_a^\phi + \mathcal{E}_h^\phi$, et cetera, the triangle inequality, and the standard spatial approximations. We omit the details for the sake of brevity.

4.5 Numerical Experiments

In this section, we provide some numerical experiments to gauge the accuracy and reliability of the fully discrete finite element method developed in the previous sections. We use a square domain $\Omega = (0, 1)^2 \subset \mathbb{R}^2$ and take $\mathcal{T}_h$ to be a regular triangulation of Ω consisting of right isosceles triangles. To refine the mesh, we assume that $\mathcal{T}_\ell$, $\ell = 0, 1, \dots, L$, is an hierarchy of nested triangulations of Ω where $\mathcal{T}_\ell$ is obtained by subdividing the triangles of $\mathcal{T}_{\ell-1}$ into four congruent sub-triangles. Note that $h_{\ell-1} = 2h_\ell$, $\ell = 1, \dots, L$ and that $\{\mathcal{T}_\ell\}$ is a quasi-uniform family. (We use

a family of meshes $\mathcal{T}_h$ such that no triangle in the mesh has more than one edge on the boundary.) We use the $\mathcal{P}_2$ finite element space for the phase field and chemical potential. In short, we take $q = 2$.

We solve the scheme (4.7a) – (4.10b) with $\epsilon = 6.25 \times 10^{-2}$. The initial data for the phase field is taken to be

$$\phi_h^0 = \mathcal{I}_h \left\{ \frac{1}{2} \left(1.0 - \cos(4.0\pi x) \right) \cdot \left(1.0 - \cos(2.0\pi y) \right) - 1.0 \right\}, \quad (4.104)$$

where $\mathcal{I}_h : H^2(\Omega) \rightarrow S_h$ is the standard nodal interpolation operator. Recall that our analysis does not specifically cover the use of the operator $\mathcal{I}_h$ in the initialization step. But, since the error introduced by its use is optimal, a slight modification of the analysis shows that this will lead to optimal rates of convergence overall. (See Remark 4.3.4.) To solve the system of equations above numerically, we are using the finite element libraries from the FEniCS Project [47].

Note that source terms are not naturally present in the system of equations (1.2a) – (1.2c). Therefore, it is somewhat artificial to add them to the equations in attempt to manufacture exact solutions. To get around the fact that we do not have possession of exact solutions, we measure error by a different means. Specifically, we compute the rate at which the Cauchy difference, $\delta_\zeta := \zeta_{h_f}^{M_f} - \zeta_{h_c}^{M_c}$, converges to zero, where $h_f = 2h_c$, $\tau_f = 2\tau_c$, and $\tau_f M_f = \tau_c M_c = T$. Then, using a linear refinement path, *i.e.*, $\tau = Ch$, and assuming $q = 2$, we have

$$\|\delta_\zeta\|_{H^1} = \left\| \zeta_{h_f}^{M_f} - \zeta_{h_c}^{M_c} \right\|_{H^1} \leq \left\| \zeta_{h_f}^{M_f} - \zeta(T) \right\|_{H^1} + \left\| \zeta_{h_c}^{M_c} - \zeta(T) \right\|_{H^1} = \mathcal{O}(h_f^q + \tau_f^2) = \mathcal{O}(h_f^2). \quad (4.105)$$

The results of the H^1 Cauchy error analysis are found in Table 4.1 and confirm second-order convergence in this case. Additionally, we have proved that (at the theoretical level) the modified energy is non-increasing at each time step. This is observed in our computations and shown below in Figures 4.1 and 4.2.

Table 4.1: H^1 Cauchy convergence test. The final time is $T = 4.0 \times 10^{-1}$, and the refinement path is taken to be $\tau = .001\sqrt{2}h$ with $\varepsilon = 6.25 \times 10^{-2}$. The Cauchy difference is defined via $\delta_\phi := \phi_{h_f} - \phi_{h_c}$, where the approximations are evaluated at time $t = T$, and analogously for δ_μ . Since $q = 2$, *i.e.*, we use $\mathcal{P}_2$ elements for these variables, the norm of the Cauchy difference at T is expected to be $\mathcal{O}(\tau_f^2) + \mathcal{O}(h_f^2) = \mathcal{O}(h_f^2)$.

h_c	h_f	$\ \delta_\phi\ _{H^1}$	rate	$\ \delta_\mu\ _{H^1}$	rate
$\sqrt{2}/16$	$\sqrt{2}/32$	1.148×10^{-1}	—	1.307×10^{-1}	—
$\sqrt{2}/32$	$\sqrt{2}/64$	2.939×10^{-2}	1.95	3.299×10^{-2}	1.98
$\sqrt{2}/64$	$\sqrt{2}/128$	7.468×10^{-3}	1.97	8.295×10^{-3}	1.99
$\sqrt{2}/128$	$\sqrt{2}/256$	1.913×10^{-3}	1.95	2.087×10^{-3}	1.99

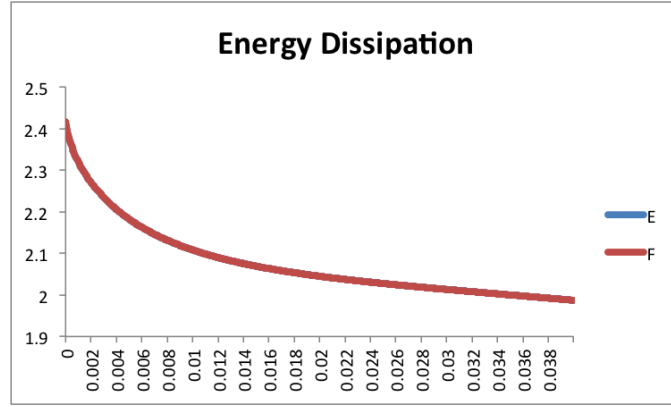


Figure 4.1: Energy dissipation for the second order numerical scheme for the Cahn-Hilliard problem. All parameters are as listed in Table 4.1 and we have taken $h = \frac{\sqrt{2}}{32}$.

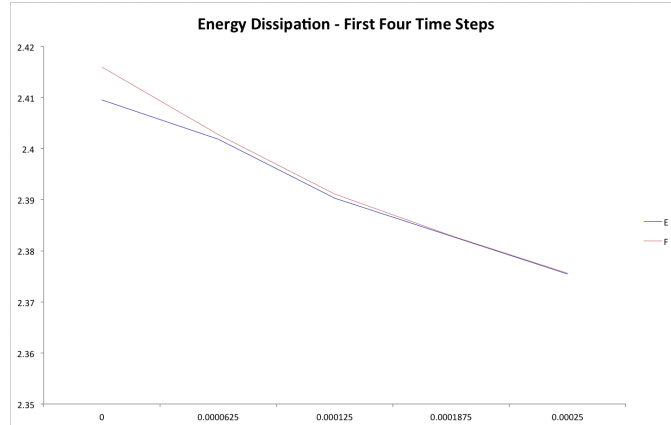


Figure 4.2: Energy dissipation for the second order numerical scheme for the Cahn-Hilliard problem. If we zoom in on the first four time steps, we are able to see the difference between the modified energy $F(\phi)$ and the Cahn-Hilliard energy $E(\phi)$. All parameters are as listed in Table 4.1 and we have taken $h = \frac{\sqrt{2}}{32}$.

Chapter 5

Future Directions

Chapter 5 is devoted to outlining a few possible avenues for the continuation of research presented in this dissertation.

5.1 Global-in-Time Estimates

Note that while all the stability and error estimates presented throughout this dissertation are unconditional with respect to the time and space step sizes, τ and h , they are not global-in-time, since the bounds depend on the final time T . Recently, Guo *et al.* [32] have developed analysis tools to show that solutions to their finite difference version of the scheme (4.7b)–(4.7b) are bounded globally-in-time for the phase field variable in the $L^\infty(0, T; L^\infty(\Omega))$ norm, but at the price of a mild time step restriction. With their success in mind, we would like to revisit the analysis of the finite element version of the second-order convex splitting scheme for the Cahn-Hilliard problem (1.2a)–(1.2c) with the goal of obtaining global-in-time stability results. Furthermore, we would like to develop and analyze a second order convex-splitting scheme for a *CHS* system of equations, similar to (3.7a)–(3.7e) described in Chapter 3. In particular, investigation of whether it is possible to prove stability estimates that are unconditional with respect to the time and space step sizes *and*

global-in-time should be completed. A rigorous proof of optimal-order error estimates for the second-order convex splitting schemes could then be examined.

5.2 The Cahn-Hilliard-Navier-Stokes Equations

Chapter 3 of this dissertation presented a numerical scheme for a mathematical model which could be used to describe the flow of a very viscous block copolymer fluid. The model paired the Darcy-Stokes equations (used to describe the fluid motion) with the Cahn-Hilliard equations creating a diffuse interface setting. However, the Darcy-Stokes equations can be somewhat limiting in describing the behavior of fluids. To capture more complicated dynamics of two-phase fluid flows, one should consider the Navier-Stokes equations. These equations have become the leading equations in modeling incompressible, viscous Newtonian fluids and, due to the wide range of applications, continue to be of tremendous mathematical interest. In particular, much research has been done on the so called Model H [36] which pairs the Navier-Stokes equations with the Cahn-Hilliard equations and which has become the accepted model for flows involving incompressible components with matched densities [21, 22, 24, 38, 40, 29, 57, 56] and references therein. Most recently, Jie Shen and Xiaofeng Yang [58] proposed two new numerical schemes for the Cahn-Hilliard-Navier-Stokes equation, one based on stabilization and the other based on convex splitting. Their new schemes have the advantage of being totally decoupled, linear, and unconditionally energy stable. However, no formal error analysis has been performed. Using the theory set forth in this dissertation, we would like to complete the formal error analysis for the convex splitting scheme presented in [58] if possible.

Additionally, there still remains a question of how to treat the case where the fluid densities do not match. Jie Shen and Xiaofeng Yang [56] likewise address this issue in [58]. The *CHNS* model they present is thermodynamically consistent and satisfies an energy dissipation law. They go on to introduce two numerical methods similar to those presented for the matched density case above. Abels *et. al.* [1] introduce

a thermodynamically consistent generalization to the Cahn-Hilliard-Navier-Stokes model for the case of non-matched densities based on a solenoidal velocity field. The authors demonstrate that their model satisfies a free energy inequality and conserves mass. As a follow-up, Garcke *et. al.* [27] present a new time discretization scheme for the numerical simulation for this model. They show that their scheme satisfies a discrete in time energy law and go on to develop a fully discrete model which preserves that energy law. They are furthermore able to show existence of solutions to both the time discrete and fully discrete schemes. Again, however, no formal error analysis is constructed for either of these schemes.

A third model/scheme for consideration for the Cahn-Hilliard-Navier-Stokes equations is presented in [33] by Daozhi Han and Xiaoming Wang. The scheme is presented as a second order in time, uniquely solvable, unconditionally stable numerical scheme for the *CHNS* equations with match density. The scheme is based on second order convex splitting for the Cahn-Hilliard equation and pressure-projection for the Navier-Stokes equation. The authors show that the scheme satisfies a modified energy law which mimics the continuous version of the energy law and prove unique solvability. However, no formal error analysis is presented and stability estimates are restricted to those gleaned from the energy law. No advanced stability estimates are obtained. The overall scheme is based on the Crank Nicholson time discretization and a second order Adams Bashforth extrapolation. Recall that the second order scheme we present in this dissertation for the Cahn-Hilliard equations is also based on the Crank Nicholson time discretization and a second order Adams Bashforth extrapolation but includes an additional second order advection term. In order to achieve advanced stability estimates and provide a formal convergence analysis, we suggest adding this additional term into the authors' proposed scheme. As a preliminary step to the course of action described below, we will make the necessary alteration to the scheme presented in [33] and complete the stability and convergence analyses following the work presented in this dissertation.

We now describe a course of action for pursuing numerical analyses for *CHNS* models with density and viscosity disparity. As a first step, we would like to build on the models described in the papers above and develop and analyze both first and second-order convex splitting schemes for the density-matched *CHNS* system with the goal of achieving unconditional stability and optimal order error estimates in line with the analyses presented in this dissertation. Again, it may be possible to obtain some or all of the anterior stability estimates unconditionally with respect to τ and h , and investigation of whether it is possible to obtain some of the stability bounds globally-in-time would follow. If the stability $\phi_h \in L^\infty(0, T; L^\infty(\Omega))$ is available, as preliminary evidence suggests, then it should be possible to derive optimal-order error estimates. The completion of the analyses in the first two steps would then open the door for investigation of first and second-order convex splitting schemes for the general *CHNS* system for density and viscosity mismatch. Because the structure of the diffusion equation is unchanged in all of the model variations, there is significant reason to be optimistic that some or all of the stabilities described herein will be achievable and will lead to optimally convergent and efficient numerical schemes for the *CHNS* systems.

5.3 Variable Parameters and Mobilities

From Chapter 3, we note that we have only considered parameters and mobilities of constant values. However, this simplifying assumption may prove to be physically unrealistic. Therefore, as a future direction, it would be natural to consider mobilities and parameters which take on physical meaning such as viscosity, permeability, density etc. as variable rather than static in line with their physical meanings.

5.4 Fast Solvers

The numerical schemes (3.7a) - (3.7e) and (4.7a) - (4.10b) require solving very large non-linear systems. Therefore, taking fine discretizations in practice require long computational run times. However, there are a few options to improving the amount of required computational work and, thus, reducing run times. One promising option is the finite element multigrid method. In their book, Brenner and Scott [5] describe a multigrid method which provides an optimal order algorithm for solving a two dimensional piecewise linear elliptic boundary value problem. The two main features of the multigrid method are smoothing on the current grid and error correction on a coarser grid. The advantage is that the amount of computational work is then only proportional to the number of unknowns in the discretized equations. We believe a multigrid method for the schemes presented in Chapters 3 and 4 are possible and well worth exploring.

Bibliography

- [1] H Abels, H Garcke, and G Grün. Thermodynamically Consistent, Frame Indifferent Diffuse Interface Models for Incompressible Two-Phase Flows with Different Densities. *Mathematical Models and Methods in Applied Sciences*, 22(03):1150013, 2012. 4, 28, 111
- [2] R A Adams. *Sobolev Spaces*. Academic Press, New York, 1975. 20
- [3] A Aristotelous, O Karakashian, and S M Wise. A Mixed Discontinuous Galerkin, Convex Splitting Scheme for a Modified Cahn-Hilliard Equation and an Efficient Nonlinear Multigrid Solver. *Discrete Contin. Dyn. Syst. Ser. B*, 18(9), 2013. 6, 8, 29
- [4] A Aristotelous, O A Karakashian, and S M Wise. Adaptive, Second-Order in Time, Primitive-Variable Discontinuous Galerkin Schemes for a Cahn-Hilliard Equation with a Mass Source. *IMA Journal of Numerical Analysis*, 2014. 8, 68
- [5] S C Brenner and L R Scott. *The Mathematical Theory of Finite Element Methods*. Springer-Verlag, Berlin, third edition, 2008. 16, 17, 18, 22, 31, 63, 114
- [6] J W Cahn. On Spinodal Decomposition. *Acta Metall.*, 9:795, 1961. 1, 2
- [7] J W Cahn and J E Hilliard. Free Energy of a Nonuniform System. I. Interfacial Free Energy. *J. Chem. Phys.*, 28:258, 1958. 1, 2
- [8] L Q Chen and J Shen. Applications of Semi-Implicit Fourier-Spectral Method to Phase Field Equations. *Computer Physics Communications*, 108(2):147–158, 1998. 8, 68
- [9] W Chen, Y Liu, C Wang, and S Wise. Global-in-Time Smooth Solutions to a Three Dimension Cahn-Hilliard-Stokes Model. *ZAMP*, (In Review). 21, 27

- [10] R Choksi, M Maras, and J F Williams. 2D Phase Diagram for Minimizers of a Cahn-Hilliard Functional with Long-range Interactions. *SIAM J. Appl. Dyn. Sys.*, 10(4):1344–1362, 2011. 4, 6, 29
- [11] R Choksi and X Ren. On a Derivation of a Density Functional Theory for Microphase Separation of Diblock Copolymers. *J. Stat. Phys.*, 113, 2003. 4, 6, 29
- [12] C Collins, J Shen, and S M Wise. Unconditionally Stable Finite Difference Multigrid Schemes for the Cahn-Hilliard-Brinkman Equation. *Commun. Comput. Phys.*, 13:929–957, 2013. 29
- [13] A Diegel, X Feng, and S M Wise. Analysis of a Mixed Finite Element Method for a Cahn-Hilliard-Darcy-Stokes System. *SIAM Journal on Numerical Analysis*, 53(1):127–152, January 2015. xi, 6
- [14] Q Du and R Nicolaides. Numerical Analysis of a Continuum Model of a Phase Transition. *SIAM J. Num. Anal.*, 28:1310–1322, 1991. 8, 68
- [15] C M Elliott. The Cahn-Hilliard Model for the Kinetics of Phase Separation. In J F Rodrigues, editor, *Mathematical Models for Phase Change Problems: Proceedings of the European Workshop held at Óbidos, Portugal, October 1-3, 1988*, International Series of Numerical Mathematics, pages 35–73, Berlin, 1989. Birkhäuser Verlag. 8, 68
- [16] C M Elliott and S Larsson. Error Estimates with Smooth and Nonsmooth Data for a Finite Element Method for the Cahn-Hilliard Equation. *Math. Comp.*, 58:603–630, 1992. 8
- [17] C M Elliott and A M Stuart. The Global Dynamics of Discrete Semilinear Parabolic Equations. *SIAM J. Numer. Anal.*, 30:1622–1663, 1993. 8
- [18] C M Elliott and A M Stuart. Viscous Cahn-Hilliard Equation. II. Analysis. *J. Diff. Eq.*, 128:387–414, 1996. 8

- [19] C M Elliott and S Zheng. On the Cahn-Hilliard Equation. *Arch. Rational Mech. Anal.*, 96:339–357, 1986. 68
- [20] D Eyre. Unconditionally Gradient Stable Time Marching the Cahn-Hilliard Equation. In J W Bullard, R Kalia, M Stoneham, and L Q Chen, editors, *Computational and Mathematical Models of Microstructural Evolution*, volume 53, pages 1686–1712, Warrendale, PA, USA, 1998. Materials Research Society. 7
- [21] X Feng. Fully Discrete Finite Element Approximations of the Navier–Stokes–Cahn-Hilliard Diffuse Interface Model for Two-Phase Fluid Flows. *SIAM J. Numer. Anal.*, 44(3):1049–1072, 2006. 4, 8, 28, 111
- [22] X Feng, Y He, and C Liu. Analysis of Finite Element Approximations of a Phase Field Model for Two-Phase Fluids. *Math. Comp.*, 76(258):539–571, 2007. 28, 29, 30, 111
- [23] X Feng and A Prohl. Error Analysis of a Mixed Finite Element Method for the Cahn-Hilliard Equation. *Numer. Math.*, 99:47–84, 2004. 8
- [24] X Feng and S M Wise. Analysis of a Darcy–Cahn–Hilliard Diffuse Interface Model for the Hele-Shaw Flow and Its Fully Discrete Finite Element Approximation. *SIAM J. Numer. Anal.*, 50(3):1320–1343, 2012. 27, 28, 111
- [25] P Fratzl, O Penrose, and J L Lebowitz. Modelling of Phase Separation in Alloys with Coherent Elastic Misfit. *J. Stat. Physics*, 95:1429–1503, 1999. 4
- [26] D Furihata. A Stable and Conservative Finite Difference Scheme for the Cahn-Hilliard Equation. *Numer. Math.*, 87:675–699, 2001. 8, 68
- [27] H Garcke, M Hinze, and C Kahle. A Stable and Linear Time Discretization for a Thermodynamically Consistent Model for Two-Phase Incompressible Flow. February 2014. 112

- [28] H Garcke and U Weikard. Numerical Approximation of the Cahn-Larché Equation. *Numer. Math.*, 100:639–662, 2005. 4
- [29] G Grün. On Convergent Schemes for Diffuse Interface Models for Two-Phase Flow of Incompressible Fluids with General Mass Densities. *SIAM J. Numer. Anal.*, 51(6):3036–3061, 2013. 4, 28, 48, 111
- [30] G Grün and F Klingbeil. Two-Phase Flow with Mass Density Contrast: Stable Schemes for a Thermodynamic Consistent and Frame Indifferent Diffuse-Interface Model. *J. Comput. Phys.*, 257:708–725, 2014. 4, 28
- [31] Z Guan, C Wang, and S M Wise. A Convergent Convex Splitting Scheme for the Periodic Nonlocal Cahn-Hilliard Equation. *Numerische Mathematik*, pages 1–30, 2013. 8
- [32] J Guo, C Wang, S Wise, and X Yue. An H^2 Convergence of a Second-Order Convex-Splitting, Finite Difference Scheme for the Three-Dimensional Cahn-Hilliard Equation. *Commun Math Sci*, 2014. 69, 110
- [33] D Han and X Wang. A Second Order in Time, Uniquely Solvable, Unconditionally Stable Numerical Scheme for Cahn-Hilliard-Navier-Stokes Equation . *Journal of Computational Physics*, 290(0):139 – 156, 2015. 112
- [34] Y He, Y Liu, and T Tang. On Large Time-Stepping Methods for the Cahn-Hilliard Equation. *Appl. Numer. Math.*, 57(4):616–628, 2006. 8
- [35] J G Heywood and R Rannacher. Finite Element Approximation of the Nonstationary Navier-Stokes Problem. IV. Error Analysis for the Second-Order Time Discretization. *SIAM J. Numer. Anal.*, 27:353–384, 1990. 24
- [36] P C Hohenberg and B I Halperin. Theory of Dynamic Critical Phenomena. *Rev. Mod. Phys.*, 49(3):435, 1977. 111

- [37] Z Hu, S M Wise, C Wang, and J S Lowengrub. Stable and Efficient Finite-Difference Nonlinear-Multigrid Schemes for the Phase-Field Crystal Equation. *J. Comput. Phys.*, 228:5323–5339, 2009. 7, 71
- [38] D Kay, V Styles, and R Welford. Finite Element Approximation of a Cahn-Hilliard-Navier-Stokes System. *Interfaces Free Bound.*, 10(1):15–43, 2008. 28, 111
- [39] D Kay and R Welford. A Multigrid Finite Element Solver for the Cahn-Hilliard Equation. *J. Comput. Phys.*, 212:288–304, 2006. 8
- [40] D Kay and R Welford. Efficient Numerical Solution of Cahn-Hilliard-Navier-Stokes Fluids in 2D. *SIAM J. Sci. Comput.*, 29(6):2241–2257, 2007. 4, 8, 28, 111
- [41] J S Kim, K Kang, and J S Lowengrub. Conservative Multigrid Methods for Cahn-Hilliard Fluids. *J. Comput. Phys.*, 193:511–543, 2003. 4, 8
- [42] F C Larché and J W Cahn. The Effect of Self-Stress on Diffusion in Solids. *Acta Metall.*, 30:1835–1845, 1982. 4
- [43] W Layton. *Introduction to the Numerical Analysis of Incompressible Viscous Flows*. SIAM, Philadelphia, PA, USA, 2008. 24
- [44] H G Lee, J S Lowengrub, and J Goodman. Modeling Pinchoff and Reconnection in a Hele-Shaw cell. I. The Models and Their Calibration. *Physics of Fluids*, 14:492–513, 2002. 4
- [45] H G Lee, J S Lowengrub, and J Goodman. Modeling Pinchoff and Reconnection in a Hele-Shaw cell. II. Analysis and Simulation in the Nonlinear Regime. *Physics of Fluids*, 14:514–545, 2002. 4

- [46] C Liu and J Shen. A Phase Field Model for the Mixture of Two Incompressible Fluids and its Approximation by a Fourier-Spectral Method. *Physica D*, 179:211–228, 2003. 4
- [47] A Logg, K A Mardal, and G N Wells. *Automated Solution of Differential Equations by the Finite Element Method: The FEniCS Book*. Springer Verlag, Berlin, 2012. 63, 108
- [48] J S Lowengrub and L Truskinovsky. Quasi-Incompressible Cahn–Hilliard Fluids and Topological Transitions. *Proc. R. Soc. Lond. A*, 454:2617–2654, 1998. 4
- [49] A D McNaught. *Compendium of Chemical Terminology*, volume 1669. Blackwell Science Oxford, 1997. 1
- [50] Louis Nirenberg. *On Elliptic Partial Differential Equations*. Springer, 2011. 21
- [51] T Ohta and K Kawasaki. Equilibrium Morphology of Block Copolymer Melts. *Macromolecules*, 19, 1986. 4, 6
- [52] A Onuki. Phase Transitions of Fluids in Shear Flow. *Journal of Physics: Condensed Matter*, 9(29):6119, 1997. 4
- [53] Lord Rayleigh. XX. On the theory of surface forces. II. Compressible fluids. *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science*, 33(201):209–220, 1892. 3
- [54] J S Rowlinson and B Widom. *Molecular Theory of Capillarity*. Courier Dover Publications, 2013. 3
- [55] J Shen, C Wang, X Wang, and S M Wise. Second-Order Convex Splitting Schemes for Gradient Flows with Ehrlich–Schwoebel Type Energy: Application to Thin Film Epitaxy. *SIAM Journal on Numerical Analysis*, 50(1):105–125, 2012. 8, 68

- [56] J Shen and X Yang. A Phase-Field Model and its Numerical Approximation for Two-Phase Incompressible Flows with Different Densities and Viscosities. *SIAM J. Sci. Comput.*, 32:1159–1179, 2010. 4, 28, 111
- [57] J Shen and X Yang. Numerical Approximations of Allen-Cahn and Cahn-Hilliard Equations. *Discrete Contin. Dyn. Syst.*, 28:1669–1691, 2010. 8, 28, 68, 111
- [58] J Shen and X Yang. Decoupled, energy stable schemes for phase-field models of two-phase incompressible flows. *SIAM Journal on Numerical Analysis*, 53(1):279–296, 2015. 111
- [59] V Thomée. *Galerkin Finite Element Methods for Parabolic Problems*, volume 25 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, second edition, 2006. 7, 16, 17, 68
- [60] J D van der Waals. Verhandel. Konink. Akad. Weten. Amsterdam (Sect. 1); see Rowlinson, JS 1979 Translation of JD van der Waals\' The Thermodynamic Theory of Capillarity Under the Hypothesis of a Continuous Variation of Density.”. *J. Stat. Phys*, 20:197–244, 1893. 3
- [61] S M Wise. *Diffuse Interface Model for Microstructural Evolution of Stressed, Binary Thin Films on Patterned Substrates*. PhD thesis, University of Virginia, 2003. x, 2
- [62] S M Wise. Unconditionally Stable Finite Difference, Nonlinear Multigrid Simulation of the Cahn-Hilliard-Hele-Shaw System of Equations. *J. Sci. Comput.*, 44:38–68, 2010. 4, 8
- [63] S M Wise. Notes on some Discrete Sobolev Inequalities. A Reference for the Discrete Gagliardo-Nirenberg Inequality, 2015. 21
- [64] S M Wise, J S Lowengrub, J S Kim, K Thornton, P W Voorhees, and W C Johnson. Quantum Dot Formation on a Strain-Patterned Epitaxial Thin Film. *Appl. Phys. Lett.*, 87:133102, 2005. 4

- [65] X Wu, G J van Zwieten, and K G van der Zee. Stabilized Second-order Convex Splitting Schemes for Cahn-Hilliard Models with Application to Diffuse-Interface Tumor-Growth Models. *International Journal for Numerical Methods in Biomedical Engineering*, 30:180–203, 2014. 8, 68, 69
- [66] A V Zvelindovsky, G J A Sevink, B A C van Vlimmeren, N M Maurits, and J.G.E.M Fraaije. Three-Dimensional Mesoscale Dynamics of Block Copolymers Under Shear: The Dynamic Density-Functional Approach. *Phys. Rev. E*, 57:4879, 1998. xi, 4, 6
- [67] A V Zvelindovsky, B A C van Vlimmeren, G J A Sevink, N M Maurits, and J.G.E.M Fraaije. Three-Dimensional Simulation of Hexagonal Phase of a Specific Polymer System Under Shear: The Dynamic Density Functional Approach. *J. Chem. Phys.*, 109(20):8751, 1998. xi, 4, 6

Vita

Amanda Emily Diegel was born in Knoxville, TN, to the parents of Charles Kevin (Kevin) and Anne O'Dell (Dell) Diegel. She has one younger brother by the name of Charles Alexander (Alex). She attended Blue Grass Elementary School before moving on to the Farragut Middle and High School System. She decided to stay in Knoxville to attend the University of Tennessee where she graduated Summa Cum Laude with a Bachelor of Science degree in Mathematics and Statistics. After working as an actuarial analyst of the first six years following her undergraduate career, she returned to the University of Tennessee to pursue Master of Science and Doctorate of Philosophy degrees in Mathematics. Upon her return, she was introduced to the numerical analysis of nonlinear partial differential equations which captured her interest and is the subject of concentration of her dissertation. She plans to continue these interests as a postdoctoral researcher at Louisiana State University.