AN EFFICIENT AND CONVERGENT FINITE ELEMENT SCHEME FOR CAHN–HILLIARD EQUATIONS WITH DYNAMIC BOUNDARY CONDITIONS

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Abstract. The Cahn–Hilliard equation is a widely used model that describes amongst others phase separation processes of binary mixtures or two-phase-flows. In the recent years, different types of boundary conditions for the Cahn–Hilliard equation were proposed and analyzed. In this publication, we are concerned with the numerical treatment of a recent model which introduces an additional Cahn–Hilliard type equation on the boundary as closure for the Cahn–Hilliard equation [C. Liu, H. Wu, Arch. Ration. Mech. An., 2019]. By identifying a mapping between the phase-field parameter and the chemical potential inside of the domain, we are able to postulate an efficient, unconditionally energy stable finite element scheme. Furthermore, we establish the convergence of discrete solutions towards suitable weak solutions of the original model, which serves also as an additional pathway to establish existence of weak solutions.

1. Introduction

Different approaches to model the hydrodynamics of fluid mixtures have been widely used in literature. In addition to the conventional sharp interface models which consist of separate hydrodynamic systems for each component of the mixture, there are diffuse interface models. In these models, the hyper-surface description of the fluid-fluid interface is replaced by a small transition region, where mixing of the macroscopically immiscible fluids is allowed, which leads to a smooth transition between the pure phases. In its easiest form, a diffuse interface model for two phases in a domain $\Omega$ with boundary $\Gamma = \partial \Omega$ reads

$$\begin{align*}
\partial_t \phi &= m \Delta \mu & \text{in } \Omega, \\
\mu &= -\delta \sigma \Delta \phi + \delta^{-1} \sigma F'(\phi) & \text{in } \Omega, \\
\nabla \mu \cdot n &= 0 & \text{on } \Gamma, \\
\nabla \phi \cdot n &= 0 & \text{on } \Gamma,
\end{align*}$$

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in combination with suitable initial conditions for the phase-field parameter $\phi$. Here, $n$ is the outer normal vector of the domain $\Omega$, $m > 0$ is a mobility constant, $\sigma > 0$ is a parameter related to surface tension, and the parameter $\delta > 0$ prescribes the width of the interfacial area. The chemical potential $\mu$ given as the first variation of the free energy

$$\mathcal{E}_\Omega(\phi) := \sigma \delta \int_{\Omega} \frac{1}{2} |\nabla \phi|^2 + \sigma \delta^{-1} \int_{\Omega} F(\phi),$$

where $F$ is a double-well potential with minima in $\phi = \pm 1$ representing the pure fluid phases. Typical choices for $F$ are $F(\phi) := \frac{\gamma}{2}(1 + \phi) \log (1 + \phi) + \frac{\gamma}{2}(1 - \phi) \log (1 - \phi) - \frac{\gamma}{2} \phi^2$ with $0 < \theta < \theta_c$ and $F(\phi) := \frac{1}{4}(\phi^2 - 1)^2$. The boundary condition (1.1c) states that there is no flux across $\Gamma$, i.e. $\int_{\Omega} \phi$ is conserved. The second boundary condition (1.1d) indicates that the fluid-fluid interface, i.e. the zero level set of $\phi$, intersects the boundary $\Gamma$ at a static contact angle of $\frac{\pi}{2}$. This can be interpreted as neglecting the interactions between the fluids and the walls of the surrounding container. Although (1.1) satisfies the energy balance equation

$$\mathcal{E}_\Omega(\phi)\big|_T + \int_0^T \int_{\Omega} m |\nabla \mu|^2 = \mathcal{E}_\Omega(\phi)\big|_0,$$

the boundary condition (1.1d) imposing a static contact angle is considered a major flaw and there are several attempts to improve this boundary condition. In [16], it was suggested to include the wetting energy $\int_{\Gamma} \gamma_{fs}(\phi)$ to the system’s energy and to replace (1.1d) by

$$\sigma \delta \nabla \phi \cdot n = -\alpha \partial_\phi \phi - \gamma_{fs}(\phi).$$

Here, $\gamma_{fs}$ interpolates between liquid-solid interfacial energies of the two fluid phases and prescribes the stationary contact angle via Young's formula. For $\alpha > 0$, (1.4) allows also for hysteresis effects in the evolution of the contact angles and changes the energy balance (1.3) to

$$\mathcal{E}_\Omega(\phi)\big|_T + \int_{\partial \Omega} \gamma_{fs}(\phi)\big|_T + \int_0^T \int_{\Omega} m |\nabla \mu|^2 + \alpha \int_{\partial \Omega} |\partial_\phi \phi|^2 = \mathcal{E}_\Omega(\phi)\big|_0 + \int_{\partial \Omega} \gamma_{fs}(\phi)\big|_0.$$

Other approaches for improving (1.1d) include — among others — using an Allen–Cahn-type equation to replace (1.1d). The resulting boundary condition reads

$$\delta_\Gamma \partial_\phi \phi = \kappa \delta_\Gamma \Delta_\Gamma \phi - \delta_\Gamma^{-1} G'(\phi) - \delta \sigma \nabla \phi \cdot n$$

on $\Gamma$ (1.6)

with $\Delta_\Gamma$ denoting the Laplace-Beltrami operator describing surface diffusion on $\Gamma$. This type of dynamic boundary condition was suggested in [11] and analyzed in [5]. Formally, it can be seen as an $L^2$-gradient flow of the surface free energy

$$\mathcal{E}_\Gamma(\phi) := \kappa \delta_\Gamma \int_{\Gamma} \frac{1}{2} |\nabla_\Gamma \phi|^2 + \delta_\Gamma^{-1} \int_{\Gamma} G(\phi),$$

where $\nabla_\Gamma$ denotes the tangential (surface) gradient operator defined on $\Gamma$ and $G$ is a surface potential function. In particular, the resulting model satisfies

$$\mathcal{E}_\Omega(\phi)\big|_T + \mathcal{E}_\Gamma(\phi)\big|_T + \int_0^T \int_{\Omega} m |\nabla \mu|^2 + \int_0^T \int_{\Gamma} |\partial_\phi \phi|^2 = \mathcal{E}_\Omega(\phi)\big|_0 + \mathcal{E}_\Gamma(\phi)\big|_0.$$
From a formal point of view, one may set $\delta = 1$, $\kappa = 0$, and $G \equiv \gamma_h$ in order to recover (1.4).

Recently, a new type of dynamic boundary condition was derived by C. Liu and H. Wu [13]. Using a variational approach with different flow maps for $\Omega$ and $\Gamma$, they derived a model closing the Cahn–Hilliard equation in $\Omega$ with an additional Cahn–Hilliard-type equation on $\Gamma$. The derived model assumes that $\phi$ is continuous on $\Omega$ and reads

$$\partial_t \phi = m \Delta \mu \quad \text{in } \Omega,$$  
(1.9a)

$$\mu = -\delta \sigma \Delta \phi + \delta^{-1} \sigma F'(\phi) \quad \text{in } \Omega,$$  
(1.9b)

$$\nabla \mu \cdot n = 0 \quad \text{on } \Gamma,$$  
(1.9c)

$$\partial_t \phi = m_\Gamma \Delta_\Gamma \mu_\Gamma \quad \text{on } \Gamma,$$  
(1.9d)

$$\mu_\Gamma = -\delta_\Gamma \kappa \Delta_\Gamma \phi + \delta_\Gamma^{-1} G'(\phi) + \delta \sigma \nabla \phi \cdot n \quad \text{on } \Gamma.$$  
(1.9e)

This model is derived from physical principles and satisfies conservation of mass on $\Omega$ and $\Gamma$, balance of forces, and dissipation of free energy. In particular, model (1.9) satisfies the energy equation

$$\mathcal{E}_\Omega(\phi)|_T + \mathcal{E}_\Gamma(\phi)|_T + \int_0^T \int_\Omega m |\nabla \mu|^2 + \int_0^T \int_\Gamma m_\Gamma |\nabla_\Gamma \mu_\Gamma|^2 = \mathcal{E}_\Omega(\phi)|_0 + \mathcal{E}_\Gamma(\phi)|_0. \quad (1.10)$$

Constructing solutions of a regularized system, where (1.9b) and (1.9c) are extended by $\alpha \partial_t \phi$, and taking the limit $\alpha \downarrow 0$ allowed them to prove existence and uniqueness of weak and strong solutions.

The authors of [7] interpreted model (1.9) as a gradient flow equation of the total free energy $\mathcal{E}_\Omega(\phi) + \mathcal{E}_\Gamma(\phi)$ and used this structure for their proof of existence and uniqueness of weak solutions.

The numerical treatment of the Cahn–Hilliard equation and its variants – often in combination with Navier–Stokes-equations – was intensely discussed through the last years. Consequently, there are various different discretization techniques at hand, which transfer the energy stability (1.3) to a discrete setting. These techniques include approaches based on convex-concave splittings of the energy (cf. [20, 17]) or the double-well potential (cf. [10, 8, 6, 9]), stabilized linearly implicit approaches (cf. [21, 18]), the method of invariant energy quadratization (cf. [4, 22]) and the recently developed scalar auxiliary variable approach (see [12]).

In this publication, we are interested in the numerical treatment of (1.9). A first finite element scheme was proposed in the Bachelor’s thesis [19] (see also [7] for numerical results). In this thesis, a straightforward discretization based on continuous, piecewise linear finite element functions was applied to model (1.9), and the arising nonlinear system was solved using Newton’s method. In this publication, we pursue a different approach and investigate the connection between $\phi$ and the chemical potentials.

The peculiarity of (1.9) is the coupling between the chemical potential defined inside of the domain and the one on the boundary. In the standard Cahn–Hilliard equation (1.1), the chemical potential is merely a definition in terms of $\phi$. This allows us to write (1.1) as a sole, nonlinear, fourth-order equation. In (1.9), however, the chemical potentials $\mu$ and $\mu_\Gamma$ are coupled via the normal derivative $\nabla \phi \cdot n$. Consequently, the chemical potentials
have to be determined by solving a system consisting of (1.9b), (1.9e), and the additional assumption that $\phi$ is continuous on $\Omega$. The latter one translates to the constraint that (1.9a) and (1.9d) yield compatible results. Deducing a suitable expression for $\mu$ will be key ingredient for the derivation of an efficient numerical scheme, but also for the numerical analysis, as the existence of a unique (discrete) $\mu$ for any given $\phi$ allows us to reuse techniques from the analysis of the standard Cahn–Hilliard equation.

The outline of the paper is as follows. In Section 2, we introduce the discrete function spaces and derive the discrete scheme. In Section 3, we will establish a first a priori estimate which is discrete counterpart of (1.10), and use this estimate to prove the existence of discrete solutions. The main convergence result, Theorem 4.4, can be found in Section 4, where we establish improved regularity results and show the convergence of discrete solutions towards weak solutions of (1.9). For the uniqueness results for these weak solutions, we refer the reader to Section 5 in [7]. We will conclude this manuscript by briefly discussing the case of Allen–Cahn-type boundary conditions (cf. Remark 4.5). By showing that the presented techniques are also applicable for Allen–Cahn-type boundary conditions, we also cover (1.4) as a special case of (1.6).

Notation. Given the spatial domain $\Omega$, we denote the space-time cylinder $\Gamma \times (0,T)$ by $\Omega_T$. By $W^{k,p}(\Omega)$ we denote the space of $k$-times weakly differentiable functions with weak derivatives in $L^p(\Omega)$. The symbol $W^{k,p}_0(\Omega)$ stands for the closure of $C^\infty(\Omega)$ in $W^{k,p}(\Omega)$. For $p = 2$, we will denote $W^{k,2}(\Omega)$ by $H^k(\Omega)$ and $W^{k,2}_0(\Omega)$ by $H^k_0(\Omega)$. The dual space of $H^1(\Omega)$ will be denoted by $(H^1(\Omega))^\prime$ and the corresponding dual pairing by $\langle \cdot , \cdot \rangle$. For a Banach space $X$ and a time interval $I$, the symbol $L^p(I; X)$ stands for the parabolic space of $L^p$-integrable functions on $I$ with values in $X$. Denoting the boundary of $\Omega$ by $\Gamma$ and the space-time cylinder $\Gamma \times (0,T)$ by $\Gamma_T$, we use a notation similar to the one introduced above for the function spaces defined on $\Gamma$ and denote the dual pairing between $(H^1(\Gamma))^\prime$ and $H^1(\Gamma)$ by $\langle \cdot , \cdot \rangle_\Gamma$. In addition, we define the space

$$X_\kappa := \begin{cases} \{ v \in H^1(\Omega) : \gamma(v) \in H^1(\Gamma) \} & \text{if } \kappa > 1, \\ H^1(\Omega) & \text{if } \kappa = 0, \end{cases} \quad (1.11)$$

where $\gamma$ defines the trace operator. The trace operator is uniquely defined and lies in $\mathcal{L}(W^{s,p}(\Omega), W^{s-1/p,p}(\Gamma))$ for $1 \leq p \leq \infty$ and $s > 1/p$, where $s-1/p$ is not an integer. For brevity, we will sometimes (in particular when the considered function is continuous) neglect the trace operator and write $v$ instead of $\gamma(v)$.

2. DERIVATION OF AN EFFICIENT NUMERICAL SCHEME

We start by introducing the general notation and the discretization techniques used in the considered scheme. Concerning the discretization with respect to time, we assume that

- $(T)$ the time interval $I := [0,T)$ is subdivided in intervals $I_n := [t_n, t_{n+1})$ with $t_{n+1} = t_n + \tau_n$ for time increments $\tau_n > 0$ and $n = 0, \ldots, N-1$ with $t_N = T$. For simplicity, we take $\tau_n \equiv \tau = \frac{T}{N}$ for $n = 0, \ldots, N-1$.

The spatial domain $\Omega \subset \mathbb{R}^d$ in spatial dimensions $d \in \{2,3\}$ is assumed to be bounded, convex, and polygonal (or polyhedral, respectively). We introduce partitions $\mathcal{T}_h$ of $\Omega$ and $\mathcal{T}_h^\Gamma$ of $\Gamma$ depending on a spatial discretization parameter $h > 0$ satisfying the following assumptions:
(S1) Let \( \{ \mathcal{T}_h \}_{h>0} \) a quasiuniform family (in the sense of [3]) of partitions of \( \Omega \) into disjoint, open, nonobtuse simplices \( K \), so that
\[
\overline{\Omega} \equiv \bigcup_{K \in \mathcal{T}_h} \overline{K} \quad \text{with} \quad \max_{K \in \mathcal{T}_h} \text{diam}(K) \leq h.
\]

(S2) Let \( \{ \mathcal{T}^\Gamma_h \}_{h>0} \) a quasiuniform family of partitions of \( \Gamma \) into disjoint, open, nonobtuse simplices \( K^\Gamma \), so that
\[
\forall K^\Gamma \in \mathcal{T}^\Gamma_h \; \exists ! K \in \mathcal{T}_h \text{ such that } \overline{K^\Gamma} = \overline{K} \cap \Gamma,
\]
and
\[
\Gamma \equiv \bigcup_{K^\Gamma \in \mathcal{T}^\Gamma_h} \overline{K^\Gamma} \quad \text{with} \quad \max_{K^\Gamma \in \mathcal{T}^\Gamma_h} \text{diam}(K^\Gamma) \leq h.
\]

(S2) implies that \( \mathcal{T}^\Gamma_h \) is compatible to \( \mathcal{T}_h \) in the sense that all elements in \( \mathcal{T}^\Gamma_h \) are edges of elements in \( \mathcal{T}_h \). For the approximation of the phase-field \( \phi \) and the chemical potential \( \mu \) we use continuous, piecewise linear finite element functions on \( \mathcal{T}_h \). This space will be denoted by \( U^\Omega_h \) and is given by functions \( \{ \chi_{h,k} \}_{k=1}^{\dim U^\Omega_h} \) forming a dual basis to the vertices \( \{ x_k \}_{k=1}^{\dim U^\Omega_h} \) of \( \mathcal{T}_h \), i.e. \( \chi_{h,k} (x_l) = \delta_{k,l} \) for \( k,l = 1, \ldots, \dim U^\Omega_h \). Analogously, we denote the space of continuous, piecewise linear finite element functions on \( \mathcal{T}^\Gamma_h \) by \( U^\Gamma_h \). This space is spanned by functions \( \{ \chi_{h,k}^\Gamma \}_{k=1}^{\dim U^\Gamma_h} \) forming a dual basis to the vertices \( \{ x_k^\Gamma \}_{k=1}^{\dim U^\Gamma_h} \) of \( \mathcal{T}^\Gamma_h \), i.e. \( \chi_{h,k}^\Gamma (x_l^\Gamma) = \delta_{k,l} \) for \( k,l = 1, \ldots, \dim U^\Gamma_h \).

Due to the compatibility condition for \( \mathcal{T}_h \) and \( \mathcal{T}^\Gamma_h \), we have
\[
U^\Gamma_h = \text{span} \{ \gamma (\theta_h) : \theta_h \in U^\Omega_h \}.
\]

Without loss of generality, we may assume that the first \( \dim U^\Gamma_h \) vertices of \( \mathcal{T}_h \) are located on \( \Gamma \), i.e. \( \{ x_k^\Gamma \}_{k=1}^{\dim U^\Gamma_h} = \{ x_k \}_{k=1}^{\dim U^\Omega_h} \). We define the nodal interpolation operators \( I_h : C^0(\Omega) \to U^\Omega_h \) and \( I^\Gamma_h : C^0(\Gamma) \to U^\Gamma_h \) by
\[
I_h \{ a \} := \sum_{k=1}^{\dim U^\Omega_h} a(x_k) \chi_{h,k}, \quad \text{and} \quad I^\Gamma_h \{ a \} := \sum_{k=1}^{\dim U^\Gamma_h} a(x_k) \chi_{h,k}^\Gamma.
\]

For future reference, we state the following estimate for the interpolation operators.

**Lemma 2.1.** Let \( \mathcal{T}_h \) and \( \mathcal{T}^\Gamma_h \) satisfy (S1) and (S2). Furthermore, let \( p \in [1, \infty) \), \( 1 \leq q \leq \infty \), and \( q^* = \frac{q}{q-1} \) for \( q < \infty \) or \( q^* = 1 \) for \( q = \infty \). Then
\[
\|(I - I_h) \{ f_h g_h \} \|_{L^p(\Omega)} \leq C h \| \nabla f_h \|_{L^{pq}(\Omega)} \| \nabla g_h \|_{L^{pq^*}(\Omega)},
\]
\[
\|(I - I^\Gamma_h) \{ f_h g_h \} \|_{L^p(\Gamma)} \leq C h \| \nabla \Gamma f_h \|_{L^{pq}(\Gamma)} \| \nabla \Gamma g_h \|_{L^{pq^*}(\Gamma)}.
\]

holds true for all \( f_h, g_h \in U^\Omega_h \)

**Proof.** Using the standard error estimates for the nodal interpolation operator (cf. [3]) and Hölder’s inequality, we compute on each \( K \in \mathcal{T}_h \):
\[
\int_K \|(I - I_h) \{ f_h g_h \} \|^p \leq C h^{2p} \int_K \| f_h g_h \|_{W^{2,\infty}(K)}^p \leq C h^{2p} \sum_{i,j=1}^d \int_K |\partial_i f_h|^p |\partial_j g_h|^p \leq C h^{2p} \| \nabla f_h \|_{L^{pq}(K)}^p \| \nabla g_h \|_{L^{pq^*}(K)}^p.
\]
Similar computations provide the result for $\mathcal{I}_h^n$. 

Concerning the potentials $F$ and $G$, we make the following assumptions:

(P1) $F, G \in C^1(\mathbb{R})$ are bounded from below, i.e. there exists a constant $C > 0$ such that $F(s) > -C$ and $G(s) > -C$ for all $s \in \mathbb{R}$. Furthermore, there exist convex, non-negative functions $F_+, G_+ \in C^1(\mathbb{R})$ and concave functions $F_-, G_- \in C^1(\mathbb{R})$ such that $F \equiv F_+ + F_-$ and $G \equiv G_+ + G_-$. 

(P2) The convex and concave parts of $F$ and $G$ can be further decomposed into a polynomial part of degree four and an additional part with a globally Lipschitz-continuous first derivative. Moreover, there exists $\beta \geq 0$ such that the concave parts satisfy

$$G_-(s_1 - s_2) \geq G_-(s_1) - G_-(s_2) + \beta |s_1 - s_2|^2$$

for all $s_1, s_2 \in \mathbb{R}$. In the case $\kappa = 0$, we assume that the above assumption holds true for $\beta > 0$.

Remark 2.2. The Assumptions (P1) and (P2) are in particular satisfied by the (penalized) polynomial double-well potential

$$W(\phi) := \frac{2}{3}(1 - \phi^2)^2 + C_{pen} \max \{(|\phi| - 1), 0\}^2 \quad \text{with } C_{pen} > 0,$$

as well as by the typical fluid-solid interfacial energy $\gamma_{fs}$ with

$$\gamma_{fs,+}(\phi) = \sin\left(\frac{\pi}{2} \min \{\max \{\phi, -1\}, 1\}\right) + \frac{1}{8} \pi^2 \phi^2 \quad \text{and} \quad \gamma_{fs,-}(\phi) = -\frac{1}{8} \pi^2 \phi^2.$$

Remark 2.3. In this publication, we consider only a convex-concave decomposition of the double-well potential. Other suitable, energy stable discretization techniques can be found in [9]. For a comparison of these techniques, we refer to [14].

Defining the backward difference quotient $\partial^-a^\tau := \tau^{-1}(a^n - a^{n-1})$, we have all tools at hand to propose a fully discrete finite element scheme. Due to the compatibility condition (2.1), we may write the scheme as

$$\int_{\Omega} \mathcal{I}_h \{\phi^n_h \theta_h\} + \tau m \int_{\Omega} \nabla \mu^n_h \cdot \nabla \theta_h = \int_{\Omega} \mathcal{I}_h \{\phi^{n-1}_h \theta_h\}, \quad (2.6a)$$

$$\int_{\Gamma} \mathcal{I}^T_h \{\phi^n_h \theta_h\} + \tau m_{\Gamma} \int_{\Gamma} \nabla \mu^n_{\Gamma,h} \cdot \nabla \theta_h = \int_{\Gamma} \mathcal{I}^T_h \{\phi^{n-1}_h \theta_h\}, \quad (2.6b)$$

$$\int_{\Omega} \mathcal{I}_h \{\mu^n_h \theta_h\} + \int_{\Gamma} \mathcal{I}^T_h \{\mu^n_{\Gamma,h} \theta_h\} = \delta \sigma \int_{\Omega} \nabla \phi^n_h \cdot \nabla \theta_h + \delta^{-1} \sigma \int_{\Omega} \mathcal{I}_h \{(F'_+(\phi^n_h) + F'_-(\phi^{n-1}_h)) \theta_h\}$$

$$+ \kappa \delta \int_{\Gamma} \nabla \phi^n_h \cdot \nabla \theta_h + \delta^{-1} \int_{\Gamma} \mathcal{I}^T_h \{(G'_+(\phi^n_h) + G'_-(\phi^{n-1}_h)) \theta_h\} \quad (2.6c)$$

for all $\theta_h \in U^n_\Omega$. At this point, the main difference between (2.8) and the established schemes developed for the Cahn–Hilliard models without dynamic boundary conditions becomes evident. While schemes for the standard Cahn–Hilliard equation (see e.g. [10, 9, 6]) allow us to compute $\mu^n_h$ for given $\phi^n_h$ and $\phi^{n-1}_h$ in an easy way, model (1.9) with the dynamic boundary conditions provides only the expression (2.6c) for $\mu^n_h$ and $\mu^n_{\Gamma,h}$ and the constraint that (2.6a) and (2.6b) have to yield the same results for $\gamma(\phi^n_h)$. Consequently,
the goal for this section will be to derive an equivalent formulation for (2.6) which allows to compute the chemical potentials in an efficient way.

We define the lumped mass matrices \( M_\Omega \) and \( M_\Gamma \) via

\[
(M_\Omega)_{ij} := \int_\Omega \{ \chi_{hj} \chi_{hi} \} \quad \forall i, j = 1, \ldots, \dim U_h^\Omega, \tag{2.7a}
\]

\[
(M_\Gamma)_{ij} := \int_\Gamma \{ \chi_{hj} \chi_{hi} \} \quad \forall i, j = 1, \ldots, \dim U_h^\Gamma, \tag{2.7b}
\]

and the stiffness matrices \( L_\Omega \) and \( L_\Gamma \) via

\[
(L_\Omega)_{ij} := \int_\Omega \nabla \chi_{hj} \cdot \nabla \chi_{hi} \quad \forall i, j = 1, \ldots, \dim U_h^\Omega, \tag{2.7c}
\]

\[
(L_\Gamma)_{ij} := \int_\Gamma \nabla_\Gamma \chi_{hj} \cdot \nabla_\Gamma \chi_{hi} \quad \forall i, j = 1, \ldots, \dim U_h^\Gamma. \tag{2.7d}
\]

Furthermore, we collect the nodal values of \( \phi^n_h, \phi^{n-1}_h, \mu^n_h, \) and \( \mu_{\Gamma,h}^n \) in the vectors \( \Phi^n, \Phi^{n-1} \), \( P^n \), and \( P_\Gamma^n \). In a slight misuse of notation, we will write \( F(\Phi^n) \), when we apply a function \( F \) to all components of \( \Phi^n \). With this notation, we are able to rewrite (2.6) as

\[
M_\Omega \Phi^n + \tau m L_\Omega P^n = M_\Omega \Phi^{n-1}, \tag{2.8a}
\]

\[
M_\Gamma (\Phi^n|_\Gamma) + \tau m_\Gamma L_\Gamma P_\Gamma^n = M_\Gamma (\Phi^{n-1}|_\Gamma), \tag{2.8b}
\]

\[
M_\Omega P^n + (M_\Gamma P_\Gamma^n)|^\Omega = \delta \sigma L_\Omega \Phi^n + \delta^{-1} \sigma M_\Omega F'_+ (\Phi^n) + \delta^{-1} \sigma M_\Omega F'_- (\Phi^{n-1}) \\
+ (\delta_\Gamma \kappa L_\Gamma (\Phi^n|_\Gamma) + \delta^{-1}_\Gamma M_\Gamma G'_+ (\Phi^n|_\Gamma) + \delta^{-1}_\Gamma M_\Gamma G'_- (\Phi^{n-1}|_\Gamma))|^\Omega. \tag{2.8c}
\]

Here, we used the extension operator \( |^\Omega : \mathbb{R}^{\dim U_h^\Omega} \to \mathbb{R}^{\dim U_h^\Omega} \) defined via

\[
\mathbb{R}^{\dim U_h^\Omega} \ni A \mapsto \left( \begin{array}{c} \hat{A} \\ \end{array} \right) \in \mathbb{R}^{\dim U_h^\Omega} \tag{2.9}
\]

and the restriction operator \( |_\Gamma : \mathbb{R}^{\dim U_h^\Omega} \to \mathbb{R}^{\dim U_h^\Gamma} \), which restricts a vector its first \( \dim U_h^\Gamma \) entries.

In order to derive a scheme allowing to solve (2.8) efficiently, we define restriction operators for matrices. In particular, we will split a matrix \( A \in \mathbb{R}^{\dim U_h^\Omega \times \dim U_h^\Omega} \) into submatrices

\[
A|_{\Gamma \times \Gamma} \in \mathbb{R}^{\dim U_h^\Gamma \times \dim U_h^\Gamma}, \quad A|_{\Gamma \times \hat{\Omega}} \in \mathbb{R}^{\dim U_h^\Gamma \times \dim U_h^\hat{\Omega}}, \quad A|_{\hat{\Omega} \times \Gamma} \in \mathbb{R}^{\dim U_h^\hat{\Omega} \times \dim U_h^\Gamma}, \quad A|_{\hat{\Omega} \times \hat{\Omega}} \in \mathbb{R}^{\dim U_h^\hat{\Omega} \times \dim U_h^\hat{\Omega}}, \tag{2.10}
\]

such that

\[
A = \begin{pmatrix} A|_{\Gamma \times \Gamma} & A|_{\Gamma \times \hat{\Omega}} \\ A|_{\hat{\Omega} \times \Gamma} & A|_{\hat{\Omega} \times \hat{\Omega}} \end{pmatrix} = \begin{pmatrix} A|_{\Gamma \times \hat{\Omega}} & A|_{\hat{\Omega} \times \Gamma} \\ A|_{\Gamma \times \hat{\Omega}} & A|_{\hat{\Omega} \times \hat{\Omega}} \end{pmatrix} = \begin{pmatrix} A|_{\Gamma \times \Gamma} & A|_{\Gamma \times \hat{\Omega}} \\ A|_{\hat{\Omega} \times \Gamma} & A|_{\hat{\Omega} \times \hat{\Omega}} \end{pmatrix}. \tag{2.11}
\]
Hence, the chemical potentials are given as solutions of the \((\dim U_h^\Omega + \dim U_h^\Gamma) \times (\dim U_h^\Omega + \dim U_h^\Gamma)\)-system

\[
\begin{pmatrix}
M_\Omega|_{\Gamma \times \Gamma} & 0 & M_\Gamma & \left( P^n \right)_{\Gamma} \\
0 & m M_\Omega^{-1} |_{\Gamma \times \Omega} L_\Omega |_{\Omega \times \Gamma} & m M_\Omega^{-1} |_{\Gamma \times \Omega} L_\Omega |_{\Omega \times \Omega} & -m_\Gamma M_\Gamma^{-1} L_\Gamma \\
\end{pmatrix}
\begin{pmatrix}
0 \\
0 \\
\end{pmatrix}
= \begin{pmatrix}
R_\Gamma (\Phi^n) \\
R_\Omega (\Phi^n) \\
\end{pmatrix}
\]

(2.12)

with \( R_\Gamma (\Phi^n) := \delta \sigma L_\Omega |_{\Gamma \times \Omega} \Phi^n + \delta^{-1} \sigma M_\Omega |_{\Gamma \times \Omega} F'_+ (\Phi^n) + \delta^{-1} \sigma M_\Omega |_{\Gamma \times \Omega} F'_- (\Phi^{n-1}) + \kappa \delta_T L_\Gamma \Phi^n |_{\Gamma} + \delta^{-1} \Gamma \sigma G''_+ (\Phi^n |_{\Gamma}) + \delta^{-1} \Gamma \sigma G''_- (\Phi^{n-1} |_{\Gamma}) \)

and \( R_\Omega (\Phi^n) := \delta \sigma L_\Omega |_{\Omega \times \Omega} \Phi^n + \delta^{-1} \sigma M_\Omega |_{\Omega \times \Omega} F'_+ (\Phi^n) + \delta^{-1} \sigma M_\Omega |_{\Omega \times \Omega} F'_- (\Phi^{n-1}) \). Here, the first two lines are a consequence of (2.8c) and the last line guarantees that (2.8a) and (2.8b) provide the same result for \( \Phi^n |_{\Gamma} \).

As the (2.8) is nonlinear in \( \Phi^n \), computing a possible solution requires the application of an iterative scheme (e.g. Newton’s method) and therefore solving (2.12) multiple times per time step. Hence, solving a \((\dim U_h^\Omega + \dim U_h^\Gamma) \times (\dim U_h^\Omega + \dim U_h^\Gamma)\)-system each time is not desirable and we have to continue reducing the complexity of the system.

From the second line in (2.12), we immediately get

\[
P^n |_{\Omega} = M_\Omega |_{\Omega \times \Omega} R_\Omega (\Phi^n),
\]

(2.13)

while the first line provides

\[
P^n |_{\Gamma} = -M_\Gamma^{-1} M_\Omega |_{\Gamma \times \Gamma} P^n |_{\Gamma} + M_\Gamma^{-1} R_\Gamma (\Phi^n).
\]

(2.14)

Plugging this into the last line, we obtain

\[
m M_\Omega^{-1} |_{\Gamma \times \Omega} L_\Omega |_{\Omega \times \Gamma} P^n |_{\Gamma} = -m M_\Omega^{-1} |_{\Gamma \times \Omega} L_\Omega |_{\Omega \times \Omega} P^n |_{\Omega} + m_\Gamma M_\Gamma^{-1} L_\Gamma P^n |_{\Gamma} = -m M_\Omega^{-1} |_{\Gamma \times \Omega} L_\Omega |_{\Omega \times \Omega} M_\Omega^{-1} |_{\Omega \times \Omega} R_\Omega (\Phi^n) + m_\Gamma M_\Gamma^{-1} L_\Gamma M_\Gamma^{-1} R_\Gamma (\Phi^n) \]  (2.15)

and therefore

\[
\left( m M_\Omega^{-1} |_{\Gamma \times \Omega} L_\Omega |_{\Omega \times \Gamma} + m_\Gamma M_\Gamma^{-1} L_\Gamma M_\Gamma^{-1} M_\Omega |_{\Gamma \times \Gamma} \right) P^n |_{\Gamma} = -m M_\Omega^{-1} |_{\Gamma \times \Omega} L_\Omega |_{\Omega \times \Omega} M_\Omega^{-1} |_{\Omega \times \Omega} R_\Omega (\Phi^n) + m_\Gamma M_\Gamma^{-1} L_\Gamma M_\Gamma^{-1} R_\Gamma (\Phi^n). \]  (2.16)

As \( M_\Omega^{-1} \) is a diagonal matrix, \( M_\Omega^{-1} |_{\Gamma \times \Omega} L_\Omega |_{\Omega \times \Gamma} = M_\Omega^{-1} |_{\Gamma \times \Gamma} L_\Omega |_{\Gamma \times \Gamma} \) holds true. This allows us to multiply (2.16) by \( M_\Omega |_{\Gamma \times \Gamma} \) to obtain

\[
\left( m L_\Omega |_{\Gamma \times \Gamma} + m_\Gamma M_\Gamma^{-1} L_\Gamma M_\Gamma^{-1} M_\Omega |_{\Gamma \times \Gamma} \right) P^n |_{\Gamma} = -m L_\Omega |_{\Gamma \times \Omega} M_\Omega^{-1} |_{\Omega \times \Omega} R_\Omega (\Phi^n) + m_\Gamma M_\Gamma^{-1} L_\Gamma M_\Gamma^{-1} R_\Gamma (\Phi^n). \]  (2.17)

In order to show that (2.17) is well defined, we need to prove that the matrix on the left-hand side is indeed invertible.
Lemma 2.4. The matrix \( \left( m L_\Gamma |_{\Gamma \times \Gamma} + m_\Gamma M_\Gamma |_{\Gamma \times \Gamma} M_\Gamma^{-1} L_\Gamma M_\Gamma^{-1} M_\Omega |_{\Gamma \times \Gamma} \right) \), that is defined via (2.7) and (2.10), is symmetric, positive definite.

Proof. It is obvious that \( m L_\Omega |_{\Gamma \times \Gamma} \) and \( m_\Gamma M_\Omega |_{\Gamma \times \Gamma} M_\Gamma^{-1} L_\Gamma M_\Gamma^{-1} M_\Omega |_{\Gamma \times \Gamma} \) are symmetric, positive semi-definite matrices. Therefore, it will be sufficient to show that \( A^T L_\Omega |_{\Gamma \times \Gamma} A > 0 \) for all \( 0 \neq A \in \mathbb{R}^{\dim U_h^T \times U_h^T} \) to complete the proof. This is equivalent to showing

\[
\tilde{A}^T L_\Omega \tilde{A} > 0 \quad \text{with} \quad \tilde{A} = A |^{\Omega} = (A \ 0) \quad \text{for all} \quad 0 \neq A \in \mathbb{R}^{\dim U_h^T \times U_h^T} .
\]  

(2.18)

From (2.7), we have that \( L_\Omega \) is symmetric, positive semi-definite with only constant vectors corresponding to the zero eigenvalue. As the restrictions in (2.18) do not allow for constant vectors, the proof is complete. \( \square \)

Combining (2.17) with (2.13), we obtain an expression for the chemical potential which requires to solve only a \( \dim U_h^T \) by \( \dim U_h^T \) linear system with a sparse, symmetric, positive definite matrix. Having an expression for the chemical potential, we propose the following nonlinear equation for \( \Phi^n \).

\[
\Phi^n + \tau m M_\Omega^{-1} L_\Omega \left( \begin{array}{cc}
(m L_\Omega |_{\Gamma \times \Gamma} + m_\Gamma M_\Omega |_{\Gamma \times \Gamma} M_\Gamma^{-1} L_\Gamma M_\Gamma^{-1} M_\Omega |_{\Gamma \times \Gamma})^{-1} & 0 \\
0 & I
\end{array} \right) .
\]

(2.19)

This nonlinear equation can be tackled using e.g. Newton’s method. Thereby, a linear system with the matrix \( \left( m L_\Omega |_{\Gamma \times \Omega} + m_\Gamma M_\Omega |_{\Gamma \times \Omega} M_\Gamma^{-1} L_\Gamma M_\Gamma^{-1} M_\Omega |_{\Gamma \times \Gamma} \right) \) has to be solved repeatedly. As this matrix is symmetric, positive definite, it is predestined for the application of a conjugate gradient method or a Cholesky decomposition.

3. Stability and existence of discrete solutions

In this section, we analyze the discrete scheme (2.19) proposed in the previous section. Although (2.19) is entirely written in terms of the unknown quantity \( \Phi^n \), we will continue using \( P^n \) and \( P^n_\Gamma \), which are defined in (2.17), (2.13), and (2.14), to simplify the notation. For the ease of representation, we will set \( \sigma = \delta = \delta_\Gamma = 1 \) for the remainder of this publication. As a first step, we shall verify that (2.19) indeed satisfies the compatibility constraint \( m M_\Omega^{-1} |_{\Gamma \times \Omega} L_\Omega |_{\Gamma \times \Omega} P^n = m_\Gamma M_\Gamma^{-1} L_\Gamma P^n_\Gamma \). This auxiliary result allows us derive an a priori stability result for (2.19) which serves as the corner stone for proving the existence of discrete solutions.

Lemma 3.1. Let \( P^n \) and \( P^n_\Gamma \) be defined via (2.17), (2.13), and (2.14). Then the identity

\[
m_\Gamma M_\Gamma^{-1} L_\Gamma P^n_\Gamma - m M_\Omega^{-1} L_\Omega |_{\Gamma \times \Omega} P^n = 0
\]

holds true.
Corollary 3.2. Recalling (2.17) and (2.14), we obtain

Lemma 3.3. We test (2.19) by \(1 \in \mathbb{R}^{\dim U^\Omega}\) and by \(1^T M^\Omega \Gamma\) proves the following corollary.

Corollary 3.2. Let \(\Phi^n\) be a discrete solution of (2.19). Then

\[
1^T M^\Omega \Phi^n = 1^T M^\Omega \Phi^{n-1} - 1^T M^\Gamma \Phi^n\big|_\Gamma = 1^T M^\Gamma \Phi^{n-1}\big|_\Gamma
\]

with \(1 := (1, ..., 1)^T \in \mathbb{R}^{\dim U^\Omega}\) and \(1^\Gamma := 1\big|_\Gamma\).

Using the above auxiliary results, we are now able to state a first stability result which is a discrete version of the energy equality (1.10).

Lemma 3.3. Let the assumptions \((T), (S1), (S2), (P1),\) and \((P2)\) hold true and let \(\Phi^{n-1} \in \mathbb{R}^{\dim U^\Omega}\) be given. Then a solution \(\Phi^n \in \mathbb{R}^{\dim U^\Omega}\) to (2.19), if it exists, satisfies

\[
\frac{1}{2} \Phi^n L^\Omega \Phi^n + \frac{1}{2} (\Phi^n - \Phi^{n-1})^T L^\Omega (\Phi^n - \Phi^{n-1}) + 1^T M^\Omega F(\Phi^n) + \frac{1}{2} \Phi^n L^\Gamma M^\Gamma L^\Gamma T \Phi^n
\]

\[
+ \frac{1}{2} \kappa (\Phi^n - \Phi^{n-1}) L^\Gamma (\Phi^n - \Phi^{n-1})\big|_\Gamma + 1^T M^\Gamma G(\Phi^n)\big|_\Gamma
\]

\[
+ \beta (\Phi^n - \Phi^{n-1}) M^\Gamma (\Phi^n - \Phi^{n-1})\big|_\Gamma + \tau m P^n T L^\Omega P^n + \tau m T P^n T L^\Gamma P^n\]

\[
\leq \frac{1}{2} \Phi^{n-1} T L^\Omega \Phi^{n-1} + 1^T M^\Omega F(\Phi^{n-1}) + \frac{1}{2} \kappa \Phi^{n-1} L^\Gamma \Phi^{n-1}\big|_\Gamma + 1^T M^\Gamma G(\Phi^{n-1})\big|_\Gamma,
\]

with \(1 := (1, ..., 1)^T \in \mathbb{R}^{\dim U^\Omega}\), \(1^\Gamma := 1\big|_\Gamma\), and \(P^n\) and \(P^n\) defined in (2.13), (2.17), and (2.14).

Proof. We test (2.19) by \((M^\Omega P^n + \left(M^\Gamma P^n\right))\) and use Lemma 3.1 to obtain

\[
0 = (\Phi^n - \Phi^{n-1})^T M^\Omega P^n + (\Phi^n - \Phi^{n-1})^T M^\Gamma P^n
\]

\[
+ \tau m (P^n)^T L^\Omega P^n + \tau m T P^n T L^\Gamma P^n
\]

\[
=: I + II + III + IV.
\]

As \(III\) and \(IV\) provide the dissipative parts of the desired estimate, we have show to that \(I\) and \(II\) yield the time difference of the energy. Recalling (2.14), we compute

\[
II = - (\Phi^n - \Phi^{n-1})^T L^\Omega \big|_{\Gamma \times \Gamma} P^n \big|_\Gamma + (\Phi^n - \Phi^{n-1})^T R^\Gamma (\Phi^n).
\]
Consequently, we obtain from (2.17)
\[
I + II = (\Phi^n - \Phi^{n-1})^T \Omega \Omega_{\Gamma} (\Phi^n) + (\Phi^n - \Phi^{n-1})^T \Omega \Omega_{\Gamma} (\Phi^n)
\]
\[
= (\Phi^n - \Phi^{n-1})^T \Omega \Omega_{\Gamma} (\Phi^n) + (\Phi^n - \Phi^{n-1})^T M_{\Omega} (F'_+ (\Phi^n)) + \kappa (\Phi^n - \Phi^{n-1})^T L_{\Gamma} \Phi^n + (\Phi^n - \Phi^{n-1})^T M_{\Gamma} (G'_+ (\Phi^n) + G'_{-} (\Phi^{n-1}))
\]
For (3.5).

As $M_{\Omega}$ and $M_{\Gamma}$ are diagonal matrices, we may combine $(F'_+ (\Phi^n) + F'_{-} (\Phi^{n-1}))$ and $(\Phi^n - \Phi^{n-1})$, and $(G'_+ (\Phi^n) + G'_{-} (\Phi^{n-1}))$ and $(\Phi^n - \Phi^{n-1})$ componentwise. In combination with $s_1(s_1 - s_2) = \frac{1}{2}s_1^2 + \frac{1}{2}(s_1 - s_2)^2 - \frac{1}{2}s_2^2$, this provides the result.

Using the a priori estimate from Lemma 3.3, we are able to prove the existence of discrete solutions.

**Lemma 3.4.** Let the assumptions $(T)$, $(S1)$, $(S2)$, and $(P1)$ hold true and let $\Phi^{n-1} \in \mathbb{R}^{\dim U_0}$ be given. Then, there exists at least one vector $\Phi^n \in \mathbb{R}^{\dim U_0}$ solving (2.19).

**Proof.** We will prove the existence of discrete solutions by contradiction. Let $\| \cdot \|$ denote the discrete $L^2$-norm which is derived from the inner product $(A, B) := A^T M_{\Omega} B$. According to Corollary 3.2, the mean-value of the phase-field is conserved in $\Omega$. This allows us to assume w.l.o.g. that $1^T M_{\Omega} \Phi^n = 1^T M_{\Omega} \Phi^{n-1} = 0$. Therefore, $\sqrt{\Phi^n} M_{\Omega} \Phi^n$ is also a norm of $\Phi^n$. Under the assumption that (2.19) has no solution in
\[
B_R := \{ A \in \mathbb{R}^{\dim U_0} : 1^T M_{\Omega} A = 0 \text{ and } \| A \| \leq R \}
\]
for any $R > 0$, the function $\mathcal{H}$ defined via
\[
\Phi - \Phi^{n-1} + \tau m M_{\Omega}^{-1} L_{\Omega} \left( \begin{array}{cc}
(m L_{\Omega})_{\Gamma \times \Gamma} + m_{\Gamma} M_{\Omega}|_{\Gamma \times \Gamma} M_{\Gamma}^{-1} L_{\Gamma} M_{\Gamma}^{-1} M_{\Omega}|_{\Gamma \times \Gamma} & 0 \\
0 & 1
\end{array} \right)^{-1} 0
\]
\[
= \begin{pmatrix}
-\tau m L_{\Omega}|_{\Gamma \times \Omega} M_{\Omega}^{-1} R_{\Omega} (\Phi) + m_{\Gamma} M_{\Omega}|_{\Gamma \times \Omega} M_{\Gamma}^{-1} L_{\Gamma} M_{\Gamma}^{-1} R_{\Gamma} (\Phi) \\
M_{\Omega}|^{-1}_{\Omega \times \Omega} R_{\Omega} (\Phi)
\end{pmatrix}
\]
has no root and is continuous on $B_R$. This allows us to define a function $A : B_R \rightarrow \partial B_R \subset B_R$ as
\[
A(\Phi) := -R \frac{\mathcal{H}(\Phi)}{\| \mathcal{H}(\Phi) \|}.
\]
As $A$ is continuous and maps a closed set onto itself, Brouwer’s fixed point theorem provides the existence of at least one fixed point $\Phi^*$. In the following, we will show
\[
0 < (\Phi^*, \Psi) < 0
\]
for a suitable $\Psi \in B_R$ and $R$ large enough. This contradiction shows that the initial assumption of (2.19) not having solutions in $B_R$ is wrong. To prove the contradiction
(3.9), we choose $\Psi = \tilde{\Psi}_1 + \tilde{\Psi}_2 - 1^T M_\Omega (\tilde{\Psi}_1 + \tilde{\Psi}_2) (1^T M_\Omega 1)^{-1} 1$ with
\[
\tilde{\Psi}_1 := \left( m L_\Omega |_{\Gamma \times \Gamma} + m_\Gamma M_\Omega |_{\Gamma \times \Gamma} M_\Gamma^{-1} L_\Gamma M_\Gamma^{-1} M_\Omega |_{\Gamma \times \Gamma} \right)^{-1} 0 \quad 0
\]
\[
\cdot \left( -m L_\Omega |_{\Omega \times \Omega} M_\Omega |_{\Omega \times \Omega} R_\Omega (\Phi^* ) + m_\Gamma M_\Omega |_{\Gamma \times \Gamma} M_\Gamma^{-1} L_\Gamma M_\Gamma^{-1} R_\Gamma (\Phi^* ) \right)
\]
and
\[
\tilde{\Psi}_2 := \left( M_\Omega^{-1} |_{\Gamma \times \Gamma} M_\Gamma \left( -M_\Gamma^{-1} M_\Omega |_{\Gamma \times \Gamma} \tilde{\Psi}_1 |_{\Gamma} + M_\Gamma^{-1} R_\Gamma (\Phi^* ) \right) \right) \quad (3.10)
\]
i.e. the test function is the sum of the chemical potentials deprived of their mean values. The computations from the proof of Lemma 3.3 provide
\[
(\mathcal{H}(\Phi^*), \Psi) \geq \frac{1}{2} \Phi^*^T L_\Omega \Phi^* - C,
\]
where the constant $C$ depends on $\Phi^{n-1}$ and the lower bound from (P1), but not on the fixed point $\Phi^*$ or $R$. Since all norms on finite dimensional spaces are equivalent, there exists $c > 0$ such that $\frac{1}{2} \Phi^*^T L_\Omega \Phi^* \geq c \Phi^*^T M_\Omega \Phi^*$ and we obtain
\[
(\mathcal{H}(\Phi^*), \Psi) \geq c \| \Phi^* \|^2 - C = c R^2 - C > 0 \quad (3.13)
\]
for $R$ large enough. This provides the second inequality in (3.9). In order to establish the first inequality we again use the computations from the proof of Lemma 3.3 to show
\[
(\Phi^*, \Psi) = \Phi^*^T L_\Omega \Phi^* + \Phi^*^T M_\Omega (F_+^0 (\Phi^*) + F_-^0 (0))
+ \Phi^*^T M_\Omega (F_+ (\Phi^{n-1}) - F_-^0 (0)) + \kappa \Phi^*^T |_{\Gamma} L_\Gamma \Phi^* |_{\Gamma}
+ \Phi^*^T |_{\Gamma} M_\Gamma (G^+ (\Phi^{n-1} |_{\Gamma}) + G_- (0)) + \Phi^*^T |_{\Gamma} M_\Gamma (G_-^0 (\Phi^{n-1} |_{\Gamma}) - G_+^0 (0))
\geq c \| \Phi^* \|^2 + 1^T M_\Omega (F(\Phi^*) - F_-^0 (0)) - \varepsilon \| \Phi^* \|^2 - C_{\varepsilon} \| F_-^0 (\Phi^{n-1}) - F_-^0 (0) \|^2
+ \kappa \Phi^*^T |_{\Gamma} L_\Gamma \Phi^* |_{\Gamma} + 1^T M_\Gamma (G(\Phi^* |_{\Gamma}) - G(0)) - \varepsilon \Phi^*^T |_{\Gamma} M_\Gamma \Phi^* |_{\Gamma}
- C_{\varepsilon} (G^+_0 (\Phi^{n-1} |_{\Gamma}) - G_-^0 (0))^T M_\Gamma (G^-_0 (\Phi^{n-1} |_{\Gamma}) - G_-^0 (0))
\]
with $0 < \varepsilon, \tilde{\varepsilon} \ll 1$. For every fixed $h$, there is a constant $C_h > 0$ such that $\Phi^*^T |_{\Gamma} M_\Gamma \Phi^* |_{\Gamma} \leq C_h \Phi^*^T M_\Omega \Phi^*$. Hence, we have
\[
(\Phi^*, \Psi) \geq (c - \varepsilon - C_h \tilde{\varepsilon}) \| \Phi^* \|^2 - C_{\varepsilon, \tilde{\varepsilon}} = (c - \varepsilon - C_h \tilde{\varepsilon}) R^2 - C_{\varepsilon, \tilde{\varepsilon}}
\]
with $C_{\varepsilon, \tilde{\varepsilon}} > 0$ independent of $\Phi^*$ and $R$. Choosing $\varepsilon$ and $\tilde{\varepsilon}$ small enough provides $(c - \varepsilon - C_h \tilde{\varepsilon}) > 0$. Hence, we obtain the first inequality in (3.9) for $R$ large enough, which completes the proof. \qed

**Remark 3.5.** The existence result in Lemma 3.3 implies no constraints on the time increment $\tau$. Therefore, we have the existence of discrete solutions for arbitrary time increments.
4. CONVERGENCE OF THE DISCRETE SCHEME

In this section, we show that the discrete solutions established in the last section converge towards suitable weak solutions of (1.9). This requires some assumptions on the initial data. In particular, we will assume that

(I) the initial data \( \phi_0 \in X_\kappa \) and its projection \( \phi_0^0 \) onto \( U_h^\Omega \) satisfies

\[
\int_\Omega |\nabla \phi_0^0|^2 + \int_\Omega \mathcal{I}_h \{F(\phi_0^0)\} + \kappa \int_\Gamma |\nabla \phi_0^0|^2 + \int_\Gamma \mathcal{I}_h \{G(\phi_0^0)\} \leq C
\]

with some \( C > 0 \) independent of \( h \) and \( \tau \).

Furthermore, the regularity results provided in this section require additional assumptions on \( h \) and \( \tau \). In particular, we will need

(C) that \( \frac{k^2}{\tau} \searrow 0 \) for \( (h, \tau) \searrow 0 \) when \( \kappa > 0 \) and that \( \frac{k^2}{\tau} \searrow 0 \) for \( (h, \tau) \searrow 0 \) when \( \kappa = 0 \).

Assumption (I) allows us to state our first regularity result.

**Corollary 4.1.** Let the assumptions (T), (S1), (S2), (P1), (P2), and (I) hold true and let \( h > 0 \) be small enough. Then a solution \( (\phi^0_n, \mu^0_n, \mu^I_n, h)_{n=1,...,N} \) to (2.6) satisfies

\[
\max_{n=0,...,N} \|\phi^0_n\|_{H^1(\Omega)}^2 + \max_{n=0,...,N} \int_\Omega \mathcal{I}_h \{F(\phi^0_n)\} + \kappa \max_{n=0,...,N} \|\phi^0_n\|_{H^1(\Gamma)}^2 \\
+ \max_{n=0,...,N} \int_\Omega \mathcal{I}_h \{G(\phi^0_n)\} + \sum_{n=1}^N \int_\Omega |\nabla \phi^0_n - \nabla \phi^{n-1}_h|^2 + \kappa \sum_{n=1}^N \int_\Gamma |\nabla \phi^0_n - \nabla \phi^{n-1}_h|^2 \\
+ \beta \sum_{n=1}^N \int_\Gamma |\phi^0_n - \phi^{n-1}_h|^2 + \tau \mu^0_n \sum_{n=1}^N \|\mu^0_n\|_{H^1(\Omega)}^2 + \tau \mu^I_n \sum_{n=1}^N \|\mu^I_n\|_{H^1(\Gamma)}^2 \leq C,
\]

with a constant \( C > 0 \) independent of \( h \) and \( \tau \).

**Proof.** After summing the result of Lemma 3.3 over all time steps and recalling Corollary 3.2 and (I), it remains to show that we have indeed control over the complete \( H^1 \) norm of \( \mu^0_n \) and \( \mu^I_n, h \). To establish this result, we will follow the lines of [7]. Testing (2.6c) by \( \mathcal{I}_h \{\eta\} \) with \( \eta \in C_0^\infty(\Omega; [0, 1]) \), which is not identically zero, we obtain

\[
\int_\Omega \mathcal{I}_h \{\mu^0_n \eta\} = \int_\Omega \nabla \phi^0_n \cdot \nabla \mathcal{I}_h \{\eta\} + \int_\Omega \mathcal{I}_h \{(F^+_h(\phi^0_n) + F^-(\phi^{n-1}_h)) \eta\}.
\]

From (P2) and (I), we obtain

\[
\left| \int_\Omega \mathcal{I}_h \{(F^+_h(\phi^0_n) + F^-(\phi^{n-1}_h)) \eta\} \right| \\
\leq C \|\phi^0_n\|_{L^3(\Omega)}^3 + C \|\phi^0_n\|_{L^3(\Omega)} + C \|\phi^{n-1}_h\|_{L^3(\Omega)}^3 + C \|\phi^{n-1}_h\|_{L^3(\Omega)} + C \leq C \quad (4.2)
\]

Hence, there exists a constant \( \tilde{C}(\eta) \) independent of \( h \) and \( \tau \) such that \( \int_\Omega \mathcal{I}_h \{\mu^0_n \eta\} \leq \tilde{C}(\eta) \).

We now define

\[
\mathcal{M}_\eta := \left\{ v \in H^1(\Omega) : \int_\Omega \mathcal{I}_h \{v \eta\} \leq \tilde{C}(\eta) \right\}.
\]

(4.3)
From standard error estimates for the interpolation operator \( I_h \) (cf. [3]), we derive the existence of \( c(\eta) > 0 \) such that \( \int_{\Omega} I_h \{ \eta \} \geq c(\eta) \) for \( h \) small enough. Therefore, we may use the generalized Poincaré inequality (cf. [1]), which we cite in the appendix as Lemma A.1, with \( u_0 \equiv 0 \) and \( C_0 := \tilde{C}(\eta)/c(\eta) \) to obtain
\[
\| \mu^n_h \|_{L^2(\Omega)} \leq C(1 + \| \nabla \mu^n_h \|_{L^2(\Omega)}) \quad \text{for all } n \in \{1, \ldots, N\}.
\] (4.4)
To obtain the \( L^2 \)-bound for \( \mu^n_{\Gamma,h} \), we test (2.6c) by \( \theta_h \equiv 1 \) and obtain
\[
\left| \int_{\Gamma} \mu^n_{\Gamma,h} \right| \leq \int_{\Omega} \mu^n_h + \int_{\Omega} I_h \{ F'_+ (\phi^n_h) + F'_-(\phi^n_{h-1}) \} + \int_{\Gamma} I^n_h \{ G'_+ (\phi^n_h) + G'_-(\phi^n_{h-1}) \}.
\]
Considerations similar to (4.2) show that the last term on the right-hand side is also bounded by a constant independent of \( h \) and \( \tau \). Therefore, we may use Poincaré’s inequality to complete the proof. \( \square \)

In a second step, we derive uniform bounds for the time difference quotient of the phase-field parameter on \( \Omega \) and \( \Gamma \).

**Lemma 4.2.** Let the assumptions \((T), (S_1), (S_2), (P_1), (P_2), (I), \) and \((C)\) hold true. Furthermore, let \( h > 0 \) be small enough such that Corollary 4.1 holds true. Then a solution \((\phi^n_h)_{n=1,\ldots,N}\) to (2.6) satisfies
\[
\tau \sum_{n=1}^{N} \| \partial^-_\tau \phi^n_h \|_{(H^1(\Omega))'}^2 \leq C, \quad \text{and} \quad \tau \sum_{n=1}^{N} \| \partial^-_\tau \phi^n_h \|_{(H^1(\Gamma))'}^2 \leq C,
\] (4.5)
with \( C > 0 \) independent of \( h \) and \( \tau \).

**Proof.** We take \( \theta \in H^1(\Omega) \) and test (2.6a) by \( \theta_h := \mathcal{P}_{U^\Omega} \theta \), where \( \mathcal{P}_{U^\Omega} \) is the orthogonal \( L^2 \)-projection onto \( U^\Omega_h \). We decompose the first term in (2.6a) into
\[
\int_{\Omega} I_h \{ \partial^-_\tau \phi^n_h \theta_h \} = \int_{\Omega} \partial^-_\tau \phi^n_h \theta - \int_{\Omega} (I - I_h) \{ \partial^-_\tau \phi^n_h \theta \}.
\] (4.6)
The first term will be used to obtain a norm on the dual space of \( H^1(\Omega) \). The second term can be controlled via Lemma 2.1 and the \( H^1 \)-stability of \( \mathcal{P}_{U^\Omega} \) (cf. [2]). Using these considerations and Hölder’s inequality, we obtain
\[
\left| \int_{\Omega} \partial^-_\tau \phi^n_h \theta \right| \leq C h^2 \left\| \nabla \phi^n_h - \nabla \phi^{n-1}_h \right\|_{L^2(\Omega)} \left\| \theta \right\|_{H^1(\Omega)} + \left\| \nabla \mu^n_h \right\|_{L^2(\Omega)} \left\| \theta \right\|_{H^1(\Omega)}.
\] (4.7)
Dividing by \( \| \theta \|_{H^1(\Omega)} \), taking the second power on both sides, multiplying by \( \tau \), and summing over all time steps provides
\[
\tau \sum_{n=1}^{N} \| \partial^-_\tau \phi^n_h \|_{(H^1(\Omega))'}^2 \leq C h^4 \sum_{n=1}^{N} \left\| \nabla \phi^n_h - \nabla \phi^{n-1}_h \right\|_{L^2(\Omega)}^2 + C \tau \sum_{n=1}^{N} \left\| \nabla \mu^n_h \right\|_{L^2(\Omega)}^2.
\] (4.8)
Applying the already established regularity results and \((C)\) completes the proof of the left inequality in (4.5). For the case \( \kappa > 0 \), the right inequality in (4.5) can be established using similar computations. In the case \( \kappa = 0 \), we combine Lemma 2.1 with an inverse estimate and obtain
\[
\tau \sum_{n=1}^{N} \| \partial^-_\tau \phi^n_h \|_{(H^1(\Gamma))'}^2 \leq C h^2 \tau \sum_{n=1}^{N} \left\| \phi^n_h - \phi^{n-1}_h \right\|_{L^2(\Gamma)}^2 + C \tau \sum_{n=1}^{N} \left\| \nabla \mu^n_{\Gamma,h} \right\|_{L^2(\Gamma)}^2.
\] (4.9)
Again, the already established regularity results and (C) complete the proof.

In order to pass to the limit \((h, \tau) \searrow 0\), we define time-interpolants of time-discrete functions \(a^n, n = 0, \ldots, N\), and introduce some time-index-free notation as follows.

\[
a^\tau(\cdot, t) := \frac{t-n^{-1}}{\tau}a^n(\cdot) + \frac{n^{-1}}{\tau}a^{n-1}(\cdot) \quad t \in [t^{n-1}, t^n], n \geq 1, \quad (4.10a)
\]
\[
a^{\tau+}(\cdot, t) := a^n(\cdot), \quad a^{\tau-}(\cdot, t) := a^{n-1}(\cdot) \quad t \in (t^{n-1}, t^n], n \geq 1. \quad (4.10b)
\]

We want to point out that the time derivative of \(a^\tau\) coincides with the difference quotient, i.e.

\[
\partial_\tau a^\tau = \partial_\tau \left( \frac{t-n^{-1}}{\tau}a^n + \frac{n^{-1}}{\tau}a^{n-1} \right) = \frac{1}{\tau}a^n - \frac{1}{\tau}a^{n-1} = \partial_\tau a^n. \quad (4.11)
\]

If a statement is valid for \(a^\tau, a^{\tau+}, \) and \(a^{\tau-}\), we use the abbreviation \(a^{\tau,(\pm)}\). With this notation, system (2.6) reads as follows.

\[
\begin{align*}
\int_{\Omega_T} I_h \{ \partial_\tau \phi_h^+ \theta_h \} + m \int_{\Omega_T} \nabla \mu_h^{\tau+} \cdot \nabla \theta_h &= 0, \quad (4.12a) \\
\int_{\Gamma_T} I_h^T \{ \partial_\tau \phi_h^+ \theta_h \} + m_T \int_{\Gamma_T} \nabla \mu_h^{\tau+} \cdot \nabla \theta_h &= 0, \quad (4.12b)
\end{align*}
\]

\[
\int_{\Omega_T} I_h \{ \mu_h^{\tau+} \theta_h \} + \int_{\Gamma_T} I_h^T \{ \mu_{\Gamma,h}^{\tau+} \theta_h \} = \int_{\Omega_T} \nabla \phi_h^{\tau+} \cdot \nabla \theta_h \\
+ \int_{\Omega_T} I_h \{ (F_+^{\prime}(\phi_h^{\tau+}) + F_-^{\prime}(\phi_h^{\tau-})) \theta_h \} \\
+ \kappa \int_{\Gamma_T} \nabla \phi_h^{\tau+} \cdot \nabla \theta_h + \int_{\Gamma_T} I_h^T \{ (G_+^{\prime}(\phi_h^{\tau+}) + G_-^{\prime}(\phi_h^{\tau-})) \theta_h \} \quad (4.12c)
\]

for all \(\theta_h \in L^2(0,T;U_h^{\Omega})\). Similarly, we can rewrite the regularity results obtained in Corollary 4.1 and Lemma 4.2 as

\[
\left\| \phi_h^{\tau,(-)} \right\|_{L^\infty(0,T;H^1(\Omega))}^2 + \kappa \left\| \phi_h^{\tau,(\pm)} \right\|_{L^\infty(0,T;H^1(\Omega))}^2 \\
+ \tau^{-1} \left\| \nabla \phi_h^{\tau+} - \nabla \phi_h^{\tau-} \right\|_{L^2(0,T;L^2(\Omega))}^2 + \kappa \tau^{-1} \left\| \nabla \phi_h^{\tau+} - \nabla \phi_h^{\tau-} \right\|_{L^2(0,T;L^2(\Gamma))}^2 \\
+ \beta \tau^{-1} \left\| \phi_h^{\tau+} - \phi_h^{-} \right\|_{L^2(0,T;L^2(\Gamma))}^2 + \left\| \mu_h \right\|_{L^2(0,T;H^1(\Omega))}^2 + \left\| \mu_{\Gamma,h} \right\|_{L^2(0,T;H^1(\Gamma))}^2 \leq C, \quad (4.13a)
\]

as well as

\[
\left\| \partial_\tau \phi_h^+ \right\|_{L^2(0,T;H^1(\Gamma)')} \leq C \quad \text{and} \quad \left\| \partial_\tau \phi_h^- \right\|_{L^2(0,T;H^1(\Gamma)')} \leq C. \quad (4.13b)
\]

These regularity results can be used to identify converging subsequences.
Lemma 4.3. Let the assumptions (T), (S1), (S2), (P1), (P2), (I), and (C) hold true. Furthermore, let \((\phi_h^{\tau, (\pm)}, \mu_h^{\tau, +}, \mu_{T, h}^{\tau, +})\) be a solution to (4.12). Then there exists a subsequence (again denoted by \((\phi_h^{\tau, (\pm)}, \mu_h^{\tau, +}, \mu_{T, h}^{\tau, +})\)) and functions

\[
\phi \in L^\infty(0, T; H^1(\Omega)) \cap H^1(0, T; (H^1(\Omega))^d),
\]
\[
\psi \in \begin{cases} L^\infty(0, T; H^1(\Gamma)) \cap H^1(0, T; (H^1(\Gamma))^d) & \text{if } \kappa > 0, \\ L^\infty(0, T; H^{1/2}(\Gamma)) \cap H^1(0, T; (H^1(\Gamma))^d) & \text{if } \kappa = 0, \end{cases}
\]
\[
\mu \in L^2(0, T; H^1(\Omega)),
\]
\[
\mu_T \in L^2(0, T; H^1(\Gamma)),
\]

such that \(\gamma(\phi) = \psi\) almost everywhere on \(\Gamma_T\) and for \((h, \tau) \searrow 0\)

\[
\phi_h^{\tau, (\pm)} \rightharpoonup \phi \quad \text{in } L^\infty(0, T; H^1(\Omega)),
\]
\[
\partial_t \phi_h^{\tau, (\pm)} \rightharpoonup \partial_t \phi \quad \text{in } L^2(0, T; (H^1(\Omega))^d),
\]
\[
\phi_h^{\tau, (\pm)} \rightharpoonup \phi \quad \text{in } L^p(0, T, L^s(\Omega)),
\]
\[
\gamma(\phi_h^{\tau, (\pm)}) \rightharpoonup \psi \quad \text{in } \begin{cases} L^\infty(0, T; H^1(\Gamma)) & \text{if } \kappa > 0, \\ L^\infty(0, T; H^{1/2}(\Gamma)) & \text{if } \kappa = 0, \end{cases}
\]
\[
\partial_t \gamma(\phi_h^{\tau, (\pm)}) \rightharpoonup \partial_t \psi \quad \text{in } L^2(0, T; (H^1(\Gamma))^d),
\]
\[
\gamma(\phi_h^{\tau, (\pm)}) \rightharpoonup \psi \quad \text{in } \begin{cases} L^p(0, T; L^\infty(\Gamma)) & \text{if } \kappa > 0, \\ L^p(0, T; L^s(\Gamma)) & \text{if } \kappa = 0, \end{cases}
\]
\[
\mu_h^{\tau, +} \rightharpoonup \mu \quad \text{in } L^2(0, T; H^1(\Omega)),
\]
\[
\mu_{T, h}^{\tau, +} \rightharpoonup \mu_T \quad \text{in } L^2(0, T; H^1(\Gamma))
\]

for all \(p < \infty, s \in [1, \frac{2d}{d-2})\), and \(s \in [1, \frac{2(d-1)}{d-2})\).

Proof. The weak and weak* convergence expressed in (4.15a), (4.15b), (4.15g), and (4.15h) follows directly from the bounds in (4.13a) and (4.13b). The strong convergence in (4.15c) then follows from the bounds for \(\phi_h^{\tau, (\pm)}\) in \(L^\infty(0, T; H^1(\Omega))\), the bounds on \(\partial_t \phi_h^{\tau, (\pm)}\) in \(L^2(0, T; (H^1(\Omega))^d)\), the Aubin–Lions theorem, and the fact that \(\phi_h^{\tau, +}, \phi_h^{\tau, -},\) and \(\phi_h^{\tau, (\pm)}\) converge towards the same limit function due to the bound on \(\tau^{-1} \| \nabla \phi_h^{\tau, +} - \nabla \phi_h^{\tau, -}\|_{L^2(0, T; L^2(\Omega))}^2\).

Similar arguments provide (4.15d)-(4.15f) in the case \(\kappa > 0\). In the case \(\kappa = 0\), we use the uniform bound on \(\|\phi_h^\tau\|_{H^1(\Omega)}\) to deduce a uniform bound for \(\|\gamma(\phi_h^\tau)\|_{H^{1/2}(\Gamma)}\). As \(H^{1/2}(\Gamma)\) is compactly embedded in \(L^\infty(\Gamma)\) for \(s \in [1, \frac{2(d-1)}{d-2})\) (cf. [15]), we verify (4.15d)-(4.15f) for \(\kappa = 0\). It remains to show that \(\psi\) can be identified with \(\gamma(\phi)\). We choose \(\theta \in L^2(0, T; (C^\infty(\Omega))^d)\) and compute

\[
\int_{\Omega_T} \phi \div \theta \leftarrow \int_{\Omega_T} \phi_h^{\tau, (\pm)} \div \theta = -\int_{\Omega_T} \nabla \phi_h^{\tau, (\pm)} \cdot \theta + \int_{\Gamma_T} \gamma(\phi_h^{\tau, (\pm)}) \theta \cdot n
\]
\[
\quad \rightarrow -\int_{\Omega_T} \nabla \phi \cdot \theta + \int_{\Gamma_T} \psi \theta \cdot n = \int_{\Omega_T} \phi \div \theta - \int_{\Gamma_T} \gamma(\phi) \theta \cdot n + \int_{\Gamma_T} \psi \theta \cdot n.
\]
Theorem 4.4. Let $d \in \{2, 3\}$ and let the assumptions $(T)$, $(S1)$, $(S2)$, $(P1)$, $(P2)$, $(I)$, and $(C)$ hold true. Then a tuple $(\phi, \mu, \mu_T)$ can be obtained from discrete solutions to (2.6) by passing to the limit $(h, \tau) \rightarrow 0$ that solves (1.9) in the following weak sense:

\[
\int_0^T \langle \partial_t \phi, \theta \rangle + m \int_{\Omega_T} \nabla \mu \cdot \nabla \theta = 0 \quad \forall \theta \in L^2(0, T; H^1(\Omega)),
\]

(4.17a)

\[
\int_0^T \langle \partial_t \gamma(\phi), \theta \rangle_T + m_T \int_{\Gamma_T} \nabla \mu_T \cdot \nabla_T \theta = 0 \quad \forall \theta \in L^2(0, T; H^1(\Gamma)),
\]

(4.17b)

\[
\int_{\Omega_T} \mu \theta + \int_{\Gamma_T} \mu_T \theta = \int_{\Omega_T} \nabla \phi \cdot \nabla \theta + \int_{\Omega_T} F'(\phi) \theta
\]

\[
+ \kappa \int_{\Gamma_T} \nabla \gamma(\phi) \cdot \nabla_T \theta + \int_{\Gamma_T} G'(\gamma(\phi)) \theta \quad \forall \theta \in L^2(0, T; X_\kappa).
\]

(4.17c)

Proof. We start by passing to the limit in (4.12a). Choosing $\theta_h := \mathcal{I}_h\{\theta\}$ for $\theta \in L^2(0, T; C^\infty(\overline{\Omega}))$, we have $\theta_h \rightarrow \theta$ in $L^2(0, T; H^1(\Omega))$ (cf. [3]). We decompose the first term as

\[
\int_{\Omega_T} \mathcal{I}_h\{ \partial_t \phi^*_h \theta_h \} = \int_{\Omega_T} \partial_t \phi^*_h \theta_h - \int_{\Omega_T} (I - \mathcal{I}_h)\{ \partial_t \phi^*_h \theta \}.
\]

(4.18)

This allows us to combine the results from (4.6) and (4.7) with (4.15b) and (4.15g) to derive (4.17a) for $\theta \in L^2(0, T; C^\infty(\overline{\Omega}))$. Noting that $L^2(0, T; C^\infty(\overline{\Omega}))$ is dense in $L^2(0, T; H^1(\Omega))$ yields the result. Similar arguments allow us to pass to the limit in (4.12b) to obtain (4.17b).

In order to pass to the limit in (4.12c), we choose $\theta_h := \mathcal{I}_h\{\theta\}$ with $\theta \in L^2(0, T; C^\infty(\overline{\Omega}))$ and assume that $\gamma(\phi^*_h) \in L^\infty(0, T; H^{1/2}(\Gamma))$, which is the case for $\kappa > 0$ and $\kappa = 0$. While the convergence of the left-hand side of (4.12c) and the gradient terms is straightforward, the convergence of the terms including the derivative of the potential functions $F$ and $G$ require more finesse. We will showcase the convergence of $\int_T \mathcal{I}_h\{ G'_h(\phi^*_h) \theta_h \}$.

Then, the convergence of the remaining parts can be obtained in an analogous manner. According to (P2), $G'_h$ can be written as the sum of a polynomial of degree three and a globally Lipschitz-continuous component $G'_\infty$. We start with the decomposition

\[
\int_{\Gamma_T} \mathcal{I}_h(\phi^+_h)^3 \theta_h = \int_{\Gamma_T} (\phi^+_h)^3 \theta_h - \int_{\Gamma_T} (I - \mathcal{I}_h)\{ \phi^+_h \}^2 \phi^+_h \theta_h
\]

\[
- \int_{\Gamma_T} (I - \mathcal{I}_h)\{ \phi^+_h \}^2 \phi^+_h \theta_h - \int_{\Gamma_T} (I - \mathcal{I}_h)\{ \phi^+_h \} (\phi^+_h)^3 \theta_h.
\]

(4.19)

The convergence of the first term on the right-hand side follows directly from (4.15f) and the strong convergence of $\theta_h \rightarrow \theta$. Therefore, it remains to show that the remaining terms vanish when passing to the limit. Recalling that $H^{1/2}(\Gamma)$ is continuously embedded in $L^4(\Gamma)$ (cf. [15]), the estimates in Lemma 2.1 and the standard inverse estimates (cf. [3])
provide
\[
\left| \int_{\Gamma} (I - \mathcal{T}_h) \left\{ \mathcal{T}_h^T \left\{ (\phi_h^{+,T})^3 \right\} \theta_h \right\} \right| \leq C h \| \mathcal{T}_h^T \left\{ (\phi_h^{+,T})^3 \right\} \|_{L^2(\Gamma)} \| \nabla \Gamma \theta_h \|_{H^1(\Gamma)} \\
\leq C h \| \phi_h^{+,T} \|^3_{L^6(\Gamma)} \| \nabla \Gamma \theta_h \|_{H^1(\Gamma)} \leq C h^{1/2} \| \phi_h^{+,T} \|^3_{L^4(\Gamma)} \| \nabla \Gamma \theta_h \|_{H^1(\Gamma)} .
\]

Therefore, the last term in (4.19) vanishes. Furthermore, we derive the estimates
\[
\left| \int_{\Gamma} (I - \mathcal{T}_h) \left\{ \mathcal{T}_h^T \left\{ (\phi_h^{+,T})^2 \right\} \phi_h^{+,T} \right\} \theta_h \right| \\
\leq \left\| (I - \mathcal{T}_h) \left\{ \mathcal{T}_h^T \left\{ (\phi_h^{+,T})^2 \right\} \phi_h^{+,T} \right\} \right\|_{L^{5/4}(\Gamma)} \| \theta_h \|_{H^1(\Gamma)} \\
\leq C h^2 \| \nabla \phi_h^{+,T} \|_{L^{10/3}(\Gamma)} \left\| \nabla \mathcal{T}_h \left\{ (\phi_h^{+,T})^2 \right\} \right\|_{L^2(\Gamma)} \| \theta_h \|_{H^1(\Gamma)} \\
\leq C h^{2/5} \| \phi_h^{+,T} \|^3_{L^4(\Gamma)} \| \theta_h \|_{H^1(\Gamma)}
\]

and
\[
\left| \int_{\Gamma} (I - \mathcal{T}_h) \left\{ (\phi_h^{+,T})^2 \right\} \phi_h^{+,T} \theta_h \right| \\
\leq \left\| (I - \mathcal{T}_h) \left\{ (\phi_h^{+,T})^2 \right\} \right\|_{L^{3/2}(\Gamma)} \left\| \phi_h^{+,T} \right\|_{L^4(\Gamma)} \| \theta_h \|_{H^1(\Gamma)} \\
\leq C h^2 \| \nabla \phi_h^{+,T} \|^2_{L^3(\Gamma)} \| \phi_h^{+,T} \|_{L^4(\Gamma)} \| \theta_h \|_{H^1(\Gamma)} \leq C h^{1/6} \| \phi_h^{+,T} \|^3_{L^4(\Gamma)} \| \theta_h \|_{H^1(\Gamma)} .
\]

As \( \phi_h^{+,T} \in L^p(0, T; L^4(\Gamma)) \), we obtain the convergence of the polynomial part of \( G'_+ \). To deal with the Lipschitz-continuous part \( G''_+ \), we start with the decomposition
\[
\int_{\Gamma_T} \mathcal{T}_h \left\{ G''_+(\phi_h^{+,T}) \theta_h \right\} = \int_{\Gamma_T} \mathcal{T}_h \left\{ G''_+(\phi_h^{+,T}) \theta_h \right\} - \int_{\Gamma_T} (I - \mathcal{T}_h) \left\{ G''_+(\phi_h^{+,T}) \right\} \theta_h - \int_{\Gamma_T} (I - \mathcal{T}_h) \left\{ \mathcal{T}_h \left\{ G''_+(\phi_h^{+,T}) \right\} \theta_h \right\} := I + II + III .
\]

Combining Lemma 2.1 with a standard inverse estimate, we compute
\[
|III| \leq \int_0^T C h^2 \left\| \nabla \Gamma \mathcal{T}_h^T \left\{ G''_+(\phi_h^{+,T}) \right\} \right\|_{L^2(\Gamma)} \| \nabla \Gamma \theta_h \|_{L^2(\Gamma)} \\
\leq \int_0^T C h^{3/2} \left\| \mathcal{T}_h^T \left\{ G''_+(\phi_h^{+,T}) \right\} \right\|_{L^4(\Gamma)} \| \nabla \Gamma \theta_h \|_{L^2(\Gamma)} .
\]

Using the Lipschitz-continuity of \( G''_+ \), we deduce
\[
\left\| G''_+(\phi_h^{+,T}) \right\|_{L^\infty(0, T; L^4(\Gamma))} + \left\| \mathcal{T}_h \left\{ G''_+(\phi_h^{+,T}) \right\} \right\|_{L^\infty(0, T; L^4(\Gamma))} \leq C \| \phi_h^{+,T} \|_{L^\infty(0, T; L^4(\Gamma))} + C ,
\]

(4.25)
with a constant $C$ depending on the Lipschitz-constant of $G^L_+$. Furthermore, the Lipschitz-continuity provides on every $K^\Gamma \in \mathcal{T}_h^\Gamma$

$$
\int_{K^\Gamma} \left| \mathcal{T}_h^\Gamma \left\{ G^L_+ (\phi_h^{\tau,+}) \right\} - G^L_+ (\phi_h^{\tau,+}) \right|^2 \leq C \int_{K^\Gamma} \max_{K^\Gamma} \{ \phi_h^{\tau,+} \} - \min_{K^\Gamma} \{ \phi_h^{\tau,+} \}^2
\leq C h^2 \int_{K^\Gamma} |\nabla \phi_h^{\tau,+}|^2 . \quad (4.26)
$$

Consequently, an inverse estimate yields

$$
\left\| (I - \mathcal{T}_h^\Gamma) \left\{ G^L_+ (\phi_h^{\tau,+}) \right\} \right\|_{L^2(\Gamma)} \leq C h \left\| \nabla \phi_h^{\tau,+} \right\|_{L^2(\Gamma)} \leq C h^{1/2} \left\| \phi_h^{\tau,+} \right\|_{L^4(\Gamma)} , \quad (4.27)
$$

which proves that $II$ will also vanish when passing to the limit. From the strong convergence (4.15f), we deduce $G^L_+ (\phi_h^{\tau,+}) \rightarrow G^L_+ (\gamma(\phi))$ almost everywhere. Recalling $G^L_+ (\phi_h^{\tau,+}) \in L^\infty(0,T; L^8(\Gamma))$, we may use Vitali’s convergence theorem (see e.g. [1]) to show $G^L_+ (\phi_h^{\tau,+}) \rightarrow G^L_+ (\gamma(\phi))$ in $L^\infty(0,T; L^8(\Gamma))$ for $\delta < 4$. The convergence of derivatives of the concave parts of $G$ follows from the same arguments. The uniform bounds of $\phi_h^{\tau,+}$ in $L^\infty(0,T; H^1(\Omega))$ provide enough regularity, to adapt the previously presented arguments to three spatial dimensions, which proves the convergence of the remaining terms. Then, a denseness argument concludes the proof. \hfill \Box

**Remark 4.5.** The results presented in the preceding sections carry over to the case of Allen–Cahn-type dynamic boundary conditions (cf. (1.6)), where we use

$$
\int_{\Gamma} \mathcal{T}_h^\Gamma \{ \partial_\tau \phi_h^{n+} \theta_h \} = -m_\Gamma \int_{\Gamma} \mathcal{T}_h^\Gamma \{ \mu_{n+}^\Gamma \theta_h \} \quad \text{for all } \theta_h \in U_h^\Omega , \quad (4.28)
$$

instead of (2.6b). The resulting scheme reads

$$
\Phi^n + \tau m_\Omega M_\Omega^{-1} L_\Omega \left( \left( m L_\Omega |_{\Gamma \times \Gamma} + m_\Gamma M_\Omega |_{\Gamma \times \Gamma} M_\Omega^{-1} M_\Omega |_{\Gamma \times \Gamma} \right)^{-1} \Phi^n \right) - \tau m_\Omega M_\Omega |_{\Gamma \times \Omega} R_\Omega (\Phi^n) = m_\Gamma M_\Omega |_{\Gamma \times \Omega} M_\Omega^{-1} L_\Omega M_\Omega^{-1} R_\Omega (\Phi^n) \quad \text{for all } \theta_h \in U_h^\Omega , \quad (4.29)
$$

and is well defined, as $\left( m L_\Omega |_{\Gamma \times \Gamma} + m_\Gamma M_\Omega |_{\Gamma \times \Gamma} M_\Omega^{-1} M_\Omega |_{\Gamma \times \Gamma} \right)$ is obviously a symmetric, positive definite matrix.

Although, $\int_{\Gamma} \phi_h^{\tau,+}$ is not conserved when using Allen–Cahn-type boundary conditions, testing (4.28) by $1$ shows that $\left| \int_{\Gamma} \phi_h^{\tau,+} \right|$ is bounded. Consequently, the energy estimate still provides control over $\| \phi_h^{\tau,+} \|_{H(\Gamma)}$.

Testing (4.28) by $\partial_\tau \phi_h^{n+}$ shows $\tau \sum_{n=1}^N \| \partial_\tau \phi_h^{n+} \|_{L^2(\Gamma)}^2 \leq C$, i.e. we obtain a slightly better regularity result for the discrete time derivative than we obtained for Cahn–Hilliard-type boundary conditions. Using the time-index-free notation introduced in (4.10), the bounds
read
\[
\left\| \phi_h^{T(\pm)} \right\|^2_{L^2(0,T;H^1(\Omega))} + \kappa \left\| \phi_h^{T(\pm)} \right\|^2_{L^\infty(0,T;H^1(\Omega))} + \tau^{-1} \left\| \nabla \phi_h^{T,\pm} - \nabla \phi_h^{T,-} \right\|^2_{L^2(0,T;L^2(\Gamma))} + \kappa \tau^{-1} \left\| \nabla \phi_h^{T,\pm} - \nabla \phi_h^{T,-} \right\|^2_{L^2(0,T;L^2(\Gamma))} + \beta \tau^{-1} \left\| \phi_h^{T,\pm} - \phi_h^{T,-} \right\|^2_{L^2(0,T;L^2(\Gamma))} + \left\| \mu_h^{T,\pm} \right\|^2_{L^2(0,T;H^1(\Omega))} + \left\| \mu_h^{T,\pm} \right\|^2_{L^2(0,T;L^2(\Gamma))} + \left\| \partial_t \phi_h^{T,\pm} \right\|^2_{L^2(0,T;L^2(\Gamma)^\prime)} + \left\| \partial_t \phi_h^{T,-} \right\|^2_{L^2(0,T;L^2(\Gamma)^\prime)} \leq C \quad (4.30a)
\]
with \( C > 0 \) independent of \( h \) and \( \tau \). Based on these uniform bounds, we are able to identify converging subsequences and pass to the limit.

**Appendix A. Appendix**

For the reader’s convenience, we provide the generalized Poincaré inequality which can be found in [1].

**Lemma A.1.** Let \( \Omega \subset \mathbb{R}^d \) be open, bounded and connected with Lipschitz boundary \( \partial \Omega \). Moreover, let \( 1 < p < \infty \) and let \( \mathcal{M} \subset W^{1,p}(\Omega) \) be nonempty, closed and convex. Then the following items are equivalent for every \( u_0 \in \mathcal{M} \):

1. There exists a constant \( C_0 < \infty \) such that for all \( \xi \in \mathbb{R} \)
   \[
   u_0 + \xi \in \mathcal{M} \quad \Rightarrow \quad |\xi| \leq C_0.
   \]
2. There exists a constant \( C < \infty \) with
   \[
   \|u\|_{L^p(\Omega)} \leq C(1 + \|\nabla u\|_{L^p(\Omega)})
   \]
   for all \( u \in \mathcal{M} \).

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