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CONVERGENCE ANALYSIS OF A FULLY DISCRETE FINITE DIFFERENCE SCHEME FOR THE CAHN-HILLIARD-HELE-SHAW EQUATION

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Abstract. We present an error analysis for an unconditionally energy stable, fully discrete finite difference scheme for the Cahn-Hilliard-Hele-Shaw equation, a modified Cahn-Hilliard equation coupled with the Darcy flow law. The scheme, proposed by S. M. Wise, is based on the idea of convex splitting. In this paper, we rigorously prove first order convergence in time and second order convergence in space. Instead of the (discrete) $L_s^\infty(0,T;L_h^2)\cap L_s^2(0,T;H_h^2)$ error estimate, which would represent the typical approach, we provide a discrete $L_s^\infty(0,T;H_h^1)\cap L_s^2(0,T;H_h^3)$ error estimate for the phase variable, which allows us to treat the nonlinear convection term in a straightforward way. Our convergence is unconditional in the sense that the time step s is in no way constrained by the mesh spacing h. This is accomplished with the help of an $L_s^2(0,T;H_h^3)$ bound of the numerical approximation of the phase variable. To facilitate both the stability and convergence analyses, we establish a finite difference analog of a Gagliardo-Nirenberg type inequality.

1. Introduction

The Cahn-Hilliard-Hele-Shaw (CHHS) diffuse interface model describes the process of phase separation of a viscous, binary fluid into domains in which the fluid is very nearly pure in the respective components. We refer the reader to [28] for an overview of the model, its physical background, and some PDE analyses, such as existence, uniqueness and regularity. See also the related references [2, 3, 45–47].

The Cahn-Hilliard energy functional is given by [10]

$$E(\phi) := \int_\Omega \left[\frac{1}{4}\phi^4 - \frac{1}{2}\phi^2 + \frac{\varepsilon^2}{2}|\nabla\phi|^2\right] d\boldsymbol{x}, \tag{1.1}$$

and, with the appropriate boundary conditions, the Cahn-Hilliard equation takes the form

$$\phi_t = \Delta\mu, \quad \mu = \delta_\phi E = \phi^3 - \phi - \varepsilon^2\Delta\phi, \qquad \text{in } \Omega_T. \tag{1.2}$$

Here ϕ denotes the concentration of the binary fluid, $\Omega_T := \Omega\times(0,T]$, where $\Omega\subset\mathbb{R}^d$ is a bounded domain with, for example, a Lipschitz continuous boundary. Formally, the parameter ε gives the thickness of the transition region, *i.e.*, the diffuse interface thickness. It is well-known that the Cahn-Hilliard system is energy dissipative:

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$\frac{d}{dt}E = -\|\nabla\mu\|_{L^2}^2 \leq 0$. As shown in [28], the Cahn-Hilliard-Hele-Shaw equation also satisfies an energy dissipation law. Such an energy law plays a vital role in the PDE and numerical analyses.

The dynamical equations for the Cahn-Hilliard-Hele-Shaw model are given by

$$\partial_t \phi = \Delta\mu - \nabla\cdot(\phi \boldsymbol{u}), \qquad \text{in } \Omega_T, \tag{1.3}$$

$$\mu = \phi^3 - \phi - \varepsilon^2 \Delta\phi, \qquad \text{in } \Omega_T, \tag{1.4}$$

$$\boldsymbol{u} = -\nabla p - \gamma\phi\nabla\mu, \qquad \text{in } \Omega_T, \tag{1.5}$$

$$\nabla\cdot\boldsymbol{u} = 0, \qquad \text{in } \Omega_T, \tag{1.6}$$

where $\gamma \geq 0$ is related to surface tension, $\boldsymbol{u}$ is the advective velocity, and p is the pressure. The term $-\gamma\phi\nabla\mu$ is a diffuse interface approximation of the singular surface force. Also see the detailed derivations in [36, 37, 41, 47]. The initial and boundary conditions are assumed to be

$$\phi(\,\cdot\,, 0) = \phi_0(\,\cdot\,) \qquad \text{in } \Omega, \tag{1.7}$$

$$\frac{\partial\phi}{\partial\boldsymbol{n}} = \frac{\partial\mu}{\partial\boldsymbol{n}} = \frac{\partial p}{\partial\boldsymbol{n}} = 0 \qquad \text{on } \partial\Omega_T := \partial\Omega \times (0, T]\,, \tag{1.8}$$

where $\boldsymbol{n}$ is the unit outward normal vector. The system (1.3) – (1.6) is mass conservative, *i.e.*, $\int_\Omega \phi(x,t)d\boldsymbol{x} \equiv \int_\Omega \phi(x,0)d\boldsymbol{x}$, and energy dissipative [28, 47], *i.e.*,

$$d_t E(\phi) + \int_\Omega |\nabla\mu|^2 d\boldsymbol{x} + \frac{1}{\gamma}\int_\Omega |\boldsymbol{u}|^2 d\boldsymbol{x} = 0. \tag{1.9}$$

The construction and numerical analyses of schemes that preserve the energy stability of the CHHS system (and other gradient systems, in general) have become very important topics of research. Such schemes are especially valuable when large-time scale numerical simulations are required. In this direction, the idea of convex splitting of the energy into a purely convex part and a purely concave part, popularized by Eyre's earlier work [23], has attracted a great deal of attention in recent years. In a convex splitting scheme, one treats the terms of the variational derivative implicitly or explicitly according to whether the terms correspond to the convex or concave parts of the energy, respectively. The energy stability of the numerical scheme can be derived using simple convexity inequalities. In previous works, convex splitting schemes have been applied to various PDE systems, including the phase field crystal (PFC) equation [48], epitaxial thin film growth model [11, 43], and others. In addition, extensions to second order accurate (in time) schemes are available for these convex splitting approaches; see the related references [12, 34, 39].

For a gradient system coupled with fluid motion, such as the CHHS equation (1.3) – (1.6), the idea of convex splitting can still be applied. Indeed, the reference [47] describes a fully discrete convex splitting scheme for (1.3) – (1.6), with second order centered differences in space. An unconditional energy stability was proven for the proposed numerical scheme. Meanwhile, a combination of the proposed convex splitting and a finite element approximation in space was analyzed in the more recent article [28], and a weak convergence of the numerical approximation to a global-in-time weak solution was established in detail. Similar related works can also be found in [45, 46], in which approximate solutions constructed by the abstract Galerkin procedure were proven to converge to a weak solution.

On the other hand, these convergence results only indicate a weak convergence without an associated order of convergence. In fact, a convergence analysis for any numerical scheme applied to the CHHS equation (1.3) – (1.6) is a challenging problem, one that we will begin to address herein. Compared to the standard analysis for the pure Cahn-Hilliard equation (1.2), the error estimate for the CHHS equation (1.3) – (1.6) is a much more delicate matter. The key reason is due to the appearance of a highly nonlinear convection term; the velocity error term turns out to be a Helmholtz projection (into the divergence-free vector space) of the nonlinear error associated with $-\gamma\phi\nabla\mu$. In turn, even the highest order diffusion term in the standard Cahn-Hilliard part is not able to control the numerical error term associated with the nonlinear convection. Moreover, the lack of regularity for the velocity field in the Darcy law (1.5) is an essential difficulty for establishing a convergence analysis with an optimal order. Some related issues can also be found in the works [16, 24, 25] for two-phase flow.

In this paper, we will provide a detailed convergence analysis for the fully discrete scheme formulated in [47], which is shown to be first order accurate in time and second order in space. In addition, the second order accuracy in space indicates a kind of super-convergence, as explained in Remark 3.15 below. A careful calculation shows that the standard $L_s^\infty(0,T;L_h^2) \cap L_s^2(0,T;H_h^2)$ error estimate does not work for the CHHS system (1.3) – (1.6) due to the lack of control for the highly nonlinear convection term. Instead, we perform an $L_s^\infty(0,T;H_h^1) \cap L_s^2(0,T;H_h^3)$ error estimate, and such an estimate in a higher order Sobolev norm is necessary to make the error term associated with the nonlinear convection term have a non-positive inner product with the appropriate error test function. This step is a crucial and novel feature of the convergence analysis.

To facilitate the stability and convergence analysis, we need to establish discrete Gagliardo-Nirenberg inequality for grid functions. This is accomplished via a discrete Fourier transformation over a uniform numerical grid, so that the discrete Parseval equality is valid and the equivalence between the discrete and continuous H^m (m an integer) norms for the numerical grid function and its continuous version, respectively, can be established. The discrete Gagliardo-Nirenberg inequality is crucial for obtaining the $L_s^\infty(0,T)$ bound of the discrete concentration, so that the convergence analysis can go through for the scheme.

We note that for the convex splitting scheme proposed in [47], the discrete $L_s^2(0,T;H_h^2)$ stability for the discrete concentration was also derived, in addition to the global-in-time $L_s^\infty(0,T;H_h^1)$ bound (which comes directly from the energy stability). Similar estimates are also valid for the same temporal discretization combined with finite element approximation in space, as reported in [28]. While these energy estimates are sufficient to pass to the limit and obtain a global-in-time weak solution to the PDE, they are not strong enough to derive an unconditional error estimate in 3-D, due to the high degree nonlinearity of the CHHS system. In this article, we will explore the numerical scheme in more detail and derive a discrete $L_s^2(0,T;H_h^3)$ stability for the fully discrete approximation of the concentration, $\phi_{h,s}$. Such an estimate is available since there is an $L_s^2(0,T;L_h^2)$ bound for $\nabla_h\mu_{h,s}$, where $\mu_{h,s}$ is the fully discrete approximation of chemical potential, combined with the global-in-time $L_s^\infty(0,T;H_h^1)$ bound on $\phi_{h,s}$ and a careful application of some discrete Sobolev inequalities to the nonlinear term in the definition of $\mu_{h,s}$. With the help of this $L_s^2(0,T;H_h^3)$ bound for $\phi_{h,s}$,[1] we are able to derive an unconditional convergence analysis in 3-D; *i.e.*, the convergence rate is valid without a scaling condition between the time step s and grid size h.

The rest of the paper is organized as follows. The fully discrete scheme is reviewed in Section 2. Therein we recall and derive some stability estimates for the fully discrete finite difference approximations. The refined stabilities, $L_s^2(0,T;H_h^3)\cap L_s^8(0,T;L_h^\infty)$ bounds of the discrete concentration, depend upon a discrete version of a Gagliardo-Nirenberg-type inequality, which is proved in Appendix B. In Section 3, we detail the convergence analysis for the scheme, which is undertaken in three steps. First, in Section 3.1 via consistency we establish an equation for the error function. In Section 3.2 we prove a stability estimate for the error function. Since we are not able to use the discrete Gronwall inequality directly with the error stability estimate in Section 3.3, we make an *a priori* assumption – which serves as the induction hypothesis in our convergence proof – about the error estimate at an arbitrary time step to make further progress. The main result and the final step of the convergence analysis follow by induction and are detailed in Section 3.4. In Appendix A, we define some notation and tools for the finite difference analysis in space.

2. The fully discrete scheme and a priori stabilities

For simplicity, we consider the cuboid $\Omega = (0,L_x)\times(0,L_y)\times(0,L_z)$ such that there are $N_x, N_y, N_z \in \mathbb{N} = \{1,2,3,\ldots\}$, with $h = L_x/N_x = L_y/N_y = L_z/N_z$, for some $h>0$. Let $s = \frac{T}{M} > 0$, for some $M\in\mathbb{N}$, be the time step size. The two-dimensional version of the fully discrete scheme for the CHHS system was given by [47]. The three-dimensional extension is as follows: for $0\le m\le M-1$, given $\phi^m\in\mathcal{C}_\Omega$, find the cell-centered grid functions $(\phi^{m+1},\mu^{m+1},p^{m+1})\in[\mathcal{C}_\Omega]^3$, each satisfying the discrete homogeneous Neumann boundary conditions (defined in Appendix A) such that

$$\phi^{m+1}-\phi^m = s\nabla_h\cdot\left(\mathcal{M}(A_h\phi^m)\nabla_h\mu^{m+1}\right)+s\nabla_h\cdot\left(A_h\phi^m\nabla_h p^{m+1}\right), \tag{2.1}$$

$$\mu^{m+1} = \left(\phi^{m+1}\right)^3-\phi^m-\varepsilon^2\Delta_h\phi^{m+1}, \tag{2.2}$$

$$-\Delta_h p^{m+1} = \gamma\nabla_h\cdot\left(A_h\phi^m\nabla_h\mu^{m+1}\right), \tag{2.3}$$

where $\mathcal{M}(r) := 1+r^2$, for any $r\in\mathbb{R}$. Here we are using a compact notation to make the structure of the scheme more transparent, but some further description may be necessary. First we point out that $\mathcal{M}(A_h\phi^m)\in\vec{\mathcal{E}}_\Omega$, the set of face-centered functions in the staggered grid, since $A_h\phi^m\in\vec{\mathcal{E}}_\Omega$, where A_h is the face-average operator defined in (A.15). For example, the x-component at a generic x-face grid point is given as $[\mathcal{M}(A_h\phi^m)]^x_{i\pm1/2,j,k} = \mathcal{M}(A_x\phi^m_{i\pm1/2,j,k})$. In our notation, $\mathcal{M}(A_h\phi^m)\nabla_h\mu^{m+1}\in\vec{\mathcal{E}}_\Omega$, as well. For instance, the y-component at a generic y-face grid point is given as

$$\left[\mathcal{M}(A_h\phi^m)\nabla_h\mu^{m+1}\right]^y_{i,j\pm1/2,k} = \mathcal{M}(A_y\phi^m_{i,j\pm1/2,k})D_y\mu^{m+1}_{i,j\pm1/2,k}.$$

Likewise, $A_h\phi^m\nabla_h p^{m+1}$, $A_h\phi^m\nabla_h\mu^{m+1}\in\vec{\mathcal{E}}_\Omega$. The definitions of the discrete operators used above can be found in Appendix A.2 and are similar to those found in [47].

[1] We will drop the subscripts h and s on the fully discrete finite difference approximations in the rest of the paper.

Note that the convex splitting treatment was applied to the chemical potential as given by (2.2). The unique solvability and unconditional stability have been established in [47]. The next theorem is a simple three-dimensional extension of the two-dimensional estimates in [47]:

Theorem 2.1. *Suppose that the initial profile $\phi_0 \in H^2(\Omega)$ satisfies homogeneous Neumann boundary conditions $\boldsymbol{n} \cdot \nabla \phi_0 = 0$ on $\partial\Omega$. The scheme* (2.1) – (2.3)*, with starting values $\phi^0_{i,j,k} = \phi_0(\xi_i, \xi_j, \xi_k)$, is unconditionally energy stable;* i.e., *for any $s > 0$ and $h > 0$, and any positive integer $1 \le \ell \le M$,*

$$s \sum_{m=1}^{\ell} \|\nabla_h \mu^m\|_2^2 + s \sum_{m=1}^{\ell} \|\boldsymbol{u}^m\|_2^2 + \|\nabla_h \phi^\ell\|_2^2 \le C_0, \tag{2.4}$$

where $C_0 >$ is a constant independent of s, h, and ℓ, and $\boldsymbol{u}^m \in \vec{\mathcal{E}}_\Omega$, given by

$$\boldsymbol{u}^m := -\nabla_h p^m - \gamma A_h \phi^{m-1} \nabla_h \mu^m. \tag{2.5}$$

In addition, a (discrete) $L^2_s(0,T;H^2_h)$ stability for the numerical solution was derived in the original article [47]; similar works can also be found in [28], in which the finite element approximations were taken. In this paper, we will derive a sharper estimate for (2.1) – (2.3): an $L^2_s(0,T;H^3_h)$ stability for the grid function ϕ. Such an estimate is crucial to derive an unconditional convergence analysis in 3-D. We need the following discrete Gagliardo-Nirenberg-type inequality. The proof is contained in Appendix B.

Lemma 2.2. *If the cell-centered grid function $\phi \in \mathcal{C}_\Omega$ satisfies the discrete homogeneous Neumann boundary conditions $\boldsymbol{n} \cdot \nabla_h \phi = 0$, as defined in Appendix* A, *then*

$$\left\|\phi - \bar{\phi}\right\|_\infty \le C_1 \left(\|\nabla_h \phi\|_2^{\frac{3}{4}} \|\nabla_h \Delta_h \phi\|_2^{\frac{1}{4}} + \|\nabla_h \phi\|_2 \right), \tag{2.6}$$

where $\bar{\phi} := \frac{1}{|\Omega|}(\phi, 1)$, and $C_1 > 0$ is a constant that is independent of h.

Theorem 2.3. *With the same hypotheses as in Theorem* 2.1*, we have the further stabilities for the scheme* (2.1) – (2.3)*: for any $s, h > 0$ and any $1 \le \ell \le M$, there exist constants $C_2, C_3, C_4 > 0$ such that*

$$s \sum_{m=1}^{\ell} \|\nabla_h \Delta_h \phi^m\|_2^2 \le C_2(t_\ell + 1) \le C_2(T+1), \tag{2.7}$$

$$s \sum_{m=1}^{\ell} \|\phi^m_{\mathbf{F}}\|_{H^3}^2 \le C_3(t_\ell + 1) \le C_3(T+1), \tag{2.8}$$

$$s \sum_{m=1}^{\ell} \|\phi^m\|_\infty^8 \le C_4(t_\ell + 1) \le C_4(T+1), \tag{2.9}$$

where $\phi^m_{\mathbf{F}}$ is the continuous cosine expansion of the numerical solution ϕ^m defined in Appendix B, *$t_\ell := s \cdot \ell$, and $T := s \cdot M$.*

Proof. Recall that the scheme is mass conservative. Therefore, $\overline{\phi^m} = \overline{\phi^0}$, for all $1 \le m \le M$. Thus

$$\|\phi^m\|_\infty \le \left\|\phi^m - \overline{\phi^m}\right\|_\infty + \left|\overline{\phi^0}\right| \le \left\|\phi^m - \overline{\phi^m}\right\|_\infty + C,$$

with $C > 0$ independent of h, by a standard consistency argument, leveraging the regularity of the initial data. By (2.2) and Young's inequality, we get

$$\begin{aligned}
\|\nabla_h \Delta_h \phi^{m+1}\|_2 =& \frac{1}{\varepsilon^2} \|\nabla_h \left(-\mu^{m+1} + (\phi^{m+1})^3 - \phi^m \right) \|_2 \\
\leq& C \left(\|\nabla_h \mu^{m+1}\|_2 + \|\nabla_h \phi^m\|_2 + \|\nabla_h (\phi^{m+1})^3\|_2 \right) \\
\leq& C \left(\|\nabla_h \mu^{m+1}\|_2 + \|\nabla_h \phi^m\|_2 + \|\phi^{m+1}\|_\infty^2 \cdot \|\nabla_h \phi^{m+1}\|_2 \right) \\
\leq& C \Big(\|\nabla_h \mu^{m+1}\|_2 + \|\nabla_h \phi^m\|_2 + \|\phi^{m+1} - \overline{\phi^{m+1}}\|_\infty^2 \cdot \|\nabla_h \phi^{m+1}\|_2 \\
&+ \|\nabla_h \phi^{m+1}\|_2 \Big) \\
\leq& C \Big(\|\nabla_h \mu^{m+1}\|_2 + \|\nabla_h \phi^m\|_2 + \|\nabla_h \phi^{m+1}\|_2^{\frac{5}{2}} \cdot \|\nabla_h \Delta_h \phi^{m+1}\|_2^{\frac{1}{2}} \\
&+ \|\nabla_h \phi^{m+1}\|_2^3 + \|\nabla_h \phi^{m+1}\|_2 \Big) \\
\leq& C \left(\|\nabla_h \mu^{m+1}\|_2 + C_0^{\frac{1}{2}} + C_0^{\frac{3}{2}} + C_0^{\frac{5}{2}} \right) + \frac{1}{2} \|\nabla_h \Delta_h \phi^{m+1}\|_2,
\end{aligned}$$

in which Lemma 2.2 was recalled in the fourth step, and the estimate (2.4) was used in the last step. The following discrete Hölder-type inequality was applied in the third step: for any $\phi \in \mathcal{C}_\Omega$,

$$\left\| \nabla_h \left(\phi^3 \right) \right\|_2 \leq C \left\| \phi \right\|_\infty^2 \cdot \left\| \nabla_h \phi \right\|_2 . \tag{2.10}$$

We now arrive at the following estimate:

$$\|\nabla_h \Delta_h \phi^{m+1}\|_2 \leq C \|\nabla_h \mu^{m+1}\|_2 + C. \tag{2.11}$$

By summation, we are able to derive the following bound using estimate (2.4) again:

$$s \sum_{m=1}^{\ell} \|\nabla_h \Delta_h \phi^m\|_2^2 \leq C s \sum_{m=1}^{\ell} \|\nabla_h \mu^m\|_2^2 + C\, t_\ell \leq C_0 + CT. \tag{2.12}$$

Estimate (2.7) follows.

Meanwhile, using the fact that $\overline{\phi_{\mathbf{F}}^m} = \overline{\phi^m} = \overline{\phi^0}$, a consistency argument to bound the norm of $\overline{\phi^0}$ independent of h, and an application of an elliptic regularity result, we have

(2.13)

$$\|\phi_{\mathbf{F}}^m\|_{H^3}^2 \leq 2 \left\| \phi_{\mathbf{F}}^m - \overline{\phi_{\mathbf{F}}^m} \right\|_{H^3}^2 + 2 \left\| \overline{\phi^0} \right\|_{L^2}^2 \leq C \left\| \nabla \Delta \phi_{\mathbf{F}}^m \right\|_{L^2}^2 + C \leq C \left\| \nabla_h \Delta_h \phi^m \right\|_2^2 + C,$$

with the equivalence estimate (B.15) (between the discrete and continuous norms) applied in the last step. With a summation of (2.13) and an application of (2.7), we have the desired estimate (2.8).

To derive the $L_s^8(0,T;L_h^\infty)$ bound for ϕ, we apply (2.6):

$$\|\phi^m\|_\infty^8 \leq C \left\| \phi^m - \overline{\phi^m} \right\|_\infty^8 + C \leq C \left\| \nabla_h \phi^m \right\|_2^6 \left\| \nabla_h \Delta_h \phi^m \right\|_2^2 + C \left\| \nabla_h \phi^m \right\|_2^8 . \tag{2.14}$$

With a summation of the above bound and applying (2.4), as well as (2.7), we have estimate (2.9), and the proof of Theorem 2.3 is complete. □

Remark 2.4. The constant C_0 appearing in Theorem 2.1 and the constants C_2, C_3, C_4 appearing in Theorem 2.3 are all time independent, but they do depend on integer powers of ε^{-1}. For instance, a careful derivation shows that $C_0 = O(\varepsilon^{-2})$. Similarly, $C_2 = O(\varepsilon^{-5})$, $C_3 = O(\varepsilon^{-5})$, and $C_3 = O(\varepsilon^{-11})$.

3. Convergence analysis

In this section we provide error estimates in three steps. First, in Section 3.1, we establish an equation for the error function using a standard consistency argument. In Section 3.2 we prove a stability estimate for the error function. Since we are not able to use the discrete Gronwall inequality directly with the error stability to derive an error estimate, in Section 3.3 we make an *a priori* assumption about the error estimate, which serves as an induction hypothesis, to make further progress. The final step of the convergence analysis follows by induction and an application of the discrete Gronwall inequality, which can then be rigorously justified. The main theorem is proved in Section 3.4.

3.1. **Error equations.** We need the following definition.

Definition 3.1. The subspaces $\mathcal{F}, \mathcal{G} \subset \vec{\mathcal{E}}_\Omega$ are defined as

$$\mathcal{G} := \left\{ \boldsymbol{f} \in \vec{\mathcal{E}}_\Omega \;\middle|\; \boldsymbol{n} \cdot \boldsymbol{f} = 0 \text{ on } \partial\Omega \right\}, \quad \mathcal{F} := \left\{ \boldsymbol{f} \in \vec{\mathcal{E}}_\Omega \;\middle|\; \nabla_h \cdot \boldsymbol{f} = 0 \text{ in } \Omega \right\} \cap \mathcal{G}. \tag{3.1}$$

(The discrete boundary conditions $\boldsymbol{n} \cdot \boldsymbol{f} = 0$ are defined in Appendix A.) We define the projection $\mathcal{P}_h : \mathcal{G} \to \mathcal{F}$ as follows: for every $\boldsymbol{f} \in \mathcal{G}$,

$$\mathcal{P}_h(\boldsymbol{f}) = \nabla_h p + \boldsymbol{f}, \tag{3.2}$$

where $p \in \mathring{\mathcal{C}}_\Omega := \{u \in \mathcal{C}_\Omega \mid (u,1) = 0\}$ is the unique solution to

$$-\Delta_h p - \nabla_h \cdot \boldsymbol{f} = 0 \text{ in } \Omega \quad \text{and} \quad \boldsymbol{n} \cdot \nabla_h p = 0 \text{ on } \partial\Omega. \tag{3.3}$$

The projection operator is linear and has the following properties:

$$(\boldsymbol{q}, \mathcal{P}_h(\boldsymbol{f}) - \boldsymbol{f}) = 0, \ \forall \boldsymbol{q} \in \mathcal{F}, \quad \text{and} \quad \|\mathcal{P}_h(\boldsymbol{f})\|_2 \le \|\boldsymbol{f}\|_2 . \tag{3.4}$$

Using this projection operator we may write the scheme compactly as

$$\phi^{m+1} - \phi^m = s\Delta_h \mu^{m+1} - s\nabla_h \cdot \left(A_h \phi^m \boldsymbol{u}^{m+1}\right), \tag{3.5}$$

$$\mu^{m+1} = \left(\phi^{m+1}\right)^3 - \phi^m - \varepsilon^2 \Delta_h \phi^{m+1}, \tag{3.6}$$

$$\boldsymbol{u}^{m+1} = -\mathcal{P}_h\left(\gamma A_h \phi^m \nabla_h \mu^{m+1}\right). \tag{3.7}$$

We denote $(\phi_e, \mu_e, \boldsymbol{u}_e)$ as the exact solution to the original CHHS equation and take $\Phi^\ell_{i,j,k} = \phi_e(\xi_i, \xi_j, \xi_k, t_\ell)$. We assume that the exact solution has regularity of class $\mathcal{R}$, *i.e.*,

$$\phi_e \in \mathcal{R} := H^2(0,T;C^0) \cap H^1(0,T;C^2) \cap L^\infty(0,T;C^6). \tag{3.8}$$

To facilitate our error analysis, we need to construct an approximate solution to the chemical potential via the exact solution ϕ_e. In addition, we note that the exact velocity $\boldsymbol{u}_e$ is not divergence-free at the discrete level ($\nabla_h \cdot \boldsymbol{u}_e \neq 0$). To overcome this difficulty, we must also construct an approximate solution to the velocity vector (again through the exact solution) which satisfies the divergence-free conditions at the discrete level. Therefore, we define the cell-centered grid functions

$$\Gamma^{m+1} := (\Phi^{m+1})^3 - \Phi^m - \varepsilon^2 \Delta_h \Phi^{m+1}, \quad \mathbf{U}^{m+1} := -\mathcal{P}_h\left(\gamma A_h \Phi^m \nabla_h \Gamma^{m+1}\right), \tag{3.9}$$

for $1 \le m \le M$, where $\mathcal{P}_h$ is given by Definition 3.1. We need to enforce the discrete homogeneous Neumann boundary conditions for the chemical potential: $\boldsymbol{n} \cdot \nabla_h \Gamma^m = 0$, for all $1 \le m \le M$, so that, in particular, $\mathcal{P}_h\left(A_h \Phi^m \nabla_h \Gamma^{m+1}\right)$ is well defined.

Remark 3.2. In order to assure the divergence-free property of the velocity vector at the discrete level, we choose a staggered grid for the velocity field, in which the individual components of a given velocity, say, $\boldsymbol{v} = (v^x, v^y, v^z)$, are evaluated at the ($x$, y, and z face) mesh points $(ih, (j+1/2)h, (k+1/2)h)$, $((i+1/2)h, jh, (k+1/2)h)$, $((i+1/2)h, (j+1/2)h, kh)$, respectively. This staggered grid is also known as the marker and cell (MAC) grid and was first proposed in [31] to deal with the incompressible Navier-Stokes equations. Also see [38] for related applications to the 3-D primitive equations.

One key advantage of this staggered grid can be inferred from the following fact: the discrete divergence of $\boldsymbol{U}$ (defined in (3.9)), specifically, $\nabla_h \cdot \boldsymbol{U} = d_x U^x + d_y U^y + d_z U^z$, is identically zero at every (cell-center) mesh point $((i+1/2)h, (j+1/2)h, (k+1/2)h)$. Such a divergence-free property at the discrete level comes from the special structure of the MAC grid and assures that the velocity field is orthogonal to a corresponding discrete pressure gradient at the discrete level; see also reference [18].

Moreover, we observe that the velocity component U^x has zero boundary values at mesh points $(0, (j+1/2)h, (k+1/2)h)$ and $(N_x h, (j+1/2)h, (k+1/2)h)$, corresponding to the boundaries at $x = 0$ and $x = L_x$. Similarly, the velocity component U^y has zero boundary values at mesh points $((i+1/2)h, 0, (k+1/2)h)$ and $((i+1/2)h, N_y h, (k+1/2)h)$, and the velocity component U^z has zero boundary values at mesh points $((i+1/2)h, (j+1/2)h, 0)$ and $((i+1/2)h, (j+1/2)h, N_z h)$, so that the boundary condition of $\boldsymbol{n} \cdot \boldsymbol{U} = 0$ is satisfied at the point-wise (global) level at all six boundary faces.

With the assumed regularities, the constructed approximations Γ^m and $\mathbf{U}^m$ obey the following estimates:

$$\|\nabla_h \Gamma^m\|_\infty \le C_5, \quad \|\mathbf{U}^m\|_\infty \le C_6, \tag{3.10}$$

for $1 \le m \le M$, where the constants $C_5, C_6 > 0$ are independent of $h > 0$ and $s > 0$.

It follows that $(\Phi, \Gamma, \mathbf{U})$ satisfies the numerical scheme with an $O(s + h^2)$ truncation error:

$$\frac{\Phi^{m+1} - \Phi^m}{s} = \Delta_h \Gamma^{m+1} - \nabla_h \cdot \left(A_h \Phi^m \mathbf{U}^{m+1}\right) + \tau^{m+1}, \tag{3.11}$$

$$\Gamma^{m+1} = (\Phi^{m+1})^3 - \Phi^m - \varepsilon^2 \Delta_h \Phi^{m+1}, \tag{3.12}$$

$$\mathbf{U}^{m+1} = -\mathcal{P}_h \left(\gamma A_h \Phi^m \nabla_h \Gamma^{m+1}\right), \tag{3.13}$$

where the local truncation error satisfies

$$\|\tau^m\|_2 \le (s + h^2)\beta_m, \quad s \sum_{m=1}^{M} \beta_m^2 \le C_7, \tag{3.14}$$

and where $s \cdot M = T$, and C_7 is independent of h and s.

Remark 3.3. The regularity estimates (3.8) and the local truncation error analysis (3.11) are based on a detailed Taylor expansion of the exact solution ϕ_e in both time and space, combined with the standard analysis for the discrete Helmholtz projection.

The global-in-time weak solution of the PDE has a regularity of $L^\infty(0, T; H^1)$; see [28] for the derivation. Moreover, a global-in-time existence of strong and smooth solutions for the 2-D CHHS flow and a local in time existence for the 3-D model have been established in recent works [45, 46]. As a result, we are always able to make the regularity assumption (3.8) for the exact solution of the 3-D CHHS equation (1.3) – (1.6) over a finite time interval, with the interval length dependent on the the initial data and the physical parameter ε. In turn, the convergence analysis presented in this article is over this finite time interval.

We note that the regularity requirement (3.8) is much higher than the uniform in time $L^\infty(0,T;H^1)$ regularity for the weak solution derived in [28]. Such a higher regularity requirement comes from the $O(s+h^2)$ convergence analysis that is conducted in the high order discrete norms associated to the space $L_s^\infty(0,T;H_h^1)\cap L_h^2(0,T;H_h^3)$. If, instead, a convergence analysis was conducted in the discrete norms associated to the "classical" space $L_s^\infty(0,T;L_h^2)\cap L_h^2(0,T;H_h^2)$, the regularity requirement could be reduced.

On the other hand, we remark that the regularity assumption (3.8) does not represent the optimal regularity requirement for the exact solution. In fact, a reduced regularity assumption

$$\phi_e \in H^2(0,T;C^0)\cap H^1(0,T;H^2)\cap L^\infty(0,T;H^6) \tag{3.15}$$

is sufficient for the $L_s^2(0,T;L_h^2)$ bound of the local truncation error τ, following a subtle consistency analysis as in the style reported in [9, 44]. The details are suppressed for brevity of presentation.

The numerical error functions are denoted as

$$\tilde{\phi}^m := \Phi^m - \phi^m, \quad \tilde{\mu}^m := \Gamma^m - \mu^m, \quad \tilde{\boldsymbol{u}}^m := \mathbf{U}^m - \boldsymbol{u}^m. \tag{3.16}$$

Subtracting (3.11) – (3.13) from (3.5) – (3.7) yields

$$\frac{\tilde{\phi}^{m+1}-\tilde{\phi}^m}{s} = \Delta_h\tilde{\mu}^{m+1} - \nabla_h\cdot\left(A_h\tilde{\phi}^m\mathbf{U}^{m+1} + A_h\phi^m\tilde{\boldsymbol{u}}^{m+1}\right) + \tau^{m+1}, \tag{3.17}$$

$$\tilde{\mu}^{m+1} = \mathcal{N}^{m+1}\tilde{\phi}^{m+1} - \tilde{\phi}^m - \varepsilon^2\Delta_h\tilde{\phi}^{m+1}, \tag{3.18}$$

$$\tilde{\boldsymbol{u}}^{m+1} = -\gamma\mathcal{P}_h\left(A_h\tilde{\phi}^m\nabla_h\Gamma^{m+1} + A_h\phi^m\nabla_h\tilde{\mu}^{m+1}\right), \tag{3.19}$$

$$\mathcal{N}^{m+1} := \left(\left(\Phi^{m+1}\right)^2 + \Phi^{m+1}\phi^{m+1} + \left(\phi^{m+1}\right)^2\right), \tag{3.20}$$

for $0\le m\le M-1$. Observe that $\tilde{\phi}^0\equiv 0$.

3.2. **Stability of the error functions.** In this subsection, we prove a stability estimate for the error function.

Lemma 3.4. *Assume the exact solution is of regularity class $\mathcal{R}$. Then, for any $1\le m\le M$,*

$$\|\tilde{\phi}^m\|_2 \le C_8\left(\|\nabla_h\tilde{\phi}^m\|_2 + h^2\right), \tag{3.21}$$

$$\|\tilde{\phi}^m\|_\infty \le C_9\left(\|\nabla_h\tilde{\phi}^m\|_2^{\frac{3}{4}}\|\nabla_h\Delta_h\tilde{\phi}^m\|_2^{\frac{1}{4}} + \|\nabla_h\tilde{\phi}^m\|_2 + h^2\right) \tag{3.22}$$

for some constants $C_8, C_9 > 0$ that are independent of s, h, and m.

Proof. The estimates follow from a discrete version of the Poincaré inequality (see, for example, [44]) and the discrete Gagliardo-Nirenberg inequality (2.6) in

Lemma 2.2 and the fact that

$$\begin{aligned}\left|\overline{\tilde{\phi}^m}\right| &= \left|\overline{\Phi^m} - \overline{\phi^m}\right| = \left|\overline{\Phi^m} - \overline{\phi^0}\right| \\ &= \left|\overline{\Phi^m} - |\Omega|^{-1}\int_\Omega \phi_e(\boldsymbol{x}, t_m)\, d\boldsymbol{x} - \left(\overline{\phi^0} - |\Omega|^{-1}\int_\Omega \phi_e(\boldsymbol{x}, t_0)\, d\boldsymbol{x}\right)\right| \\ &\leq \left|\overline{\Phi^m} - |\Omega|^{-1}\int_\Omega \phi_e(\boldsymbol{x}, t_m)\, d\boldsymbol{x}\right| + \left|\overline{\phi^0} - |\Omega|^{-1}\int_\Omega \phi_0(\boldsymbol{x})\, d\boldsymbol{x}\right| \\ &\leq Ch^2, \end{aligned} \tag{3.23}$$

owing to consistency. Here the overline refers only to the discrete average. □

The following theorem states the stability of the numerical error functions satisfying the error equations by (3.17) – (3.19).

Theorem 3.5. *Assume the exact solution is of regularity class $\mathcal{R}$. Then the error function $\tilde{\phi}^m$ obeys the following discrete energy stability law: for any $m = 0, \ldots, M-1$,*

$$\begin{aligned}\|\nabla_h\tilde{\phi}^{m+1}\|_2^2 - \|\nabla_h\tilde{\phi}^m\|_2^2 + \varepsilon^2 s\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2 &\leq sC_{10}D_1^{m+1}\|\nabla_h\tilde{\phi}^{m+1}\|_2^2 \\ &+ sC_{11}D_2^m\|\nabla_h\tilde{\phi}^m\|_2^2 + C_{12}D_3^{m+1}sh^4 + s(s^2+h^4)\beta_{m+1}^2,\end{aligned} \tag{3.24}$$

where

$$\begin{aligned} D_1^{m+1} &:= \left(\alpha_m^4+1\right)\alpha_{m+1}^4 + \alpha_m^{\frac{16}{3}}\left(\alpha_{m+1}^{\frac{8}{3}}+1\right)+1, \\ D_2^m &:= \alpha_m^4+\alpha_m^2+1, \\ D_3^{m+1} &:= \alpha_m^4\left(\alpha_{m+1}^2+1\right)+\alpha_m^2+\alpha_{m+1}^2+1, \end{aligned} \tag{3.25}$$

with $\alpha_m := \|\phi^m\|_\infty$, and $C_{10}, C_{11}, C_{12} > 0$ are constants that are independent of s and h.

Proof. Taking a discrete inner product of (3.17) with $-s\Delta_h\tilde{\phi}^{m+1}$ gives

$$\begin{aligned}&\frac{1}{2}\|\nabla_h\tilde{\phi}^{m+1}\|_2^2 - \frac{1}{2}\|\nabla_h\tilde{\phi}^m\|_2^2 + \frac{1}{2}\|\nabla_h(\tilde{\phi}^{m+1}-\tilde{\phi}^m)\|_2^2 \\ &\quad - s(\nabla_h\Delta_h\tilde{\phi}^{m+1}, \nabla_h\tilde{\mu}^{m+1}) \\ &= -s(\nabla_h\Delta_h\tilde{\phi}^{m+1}, A_h\tilde{\phi}^m\mathbf{U}^{m+1} + A_h\phi^m\tilde{\boldsymbol{u}}^{m+1}) - s(\tau^{m+1}, \Delta_h\tilde{\phi}^{m+1}),\end{aligned} \tag{3.26}$$

with repeated applications of the summation by parts formulas (A.26) and (A.27). The term associated with the local truncation error can be bounded as

$$\begin{aligned}-(\tau^{m+1}, \Delta_h\tilde{\phi}^{m+1}) &\leq C(s+h^2)^2\beta_{m+1}^2 + \left\|\Delta_h\tilde{\phi}^{m+1}\right\|_2^2 \\ &\leq C(s^2+h^4)\beta_{m+1}^2 + C\|\nabla_h\tilde{\phi}^{m+1}\|_2^2 + \frac{\varepsilon^2}{8}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2.\end{aligned} \tag{3.27}$$

In the second step we have used the estimate

$$\left\|\Delta\tilde{\phi}^{m+1}\right\|_2^2 = -\left(\nabla_h\tilde{\phi}^{m+1}, \nabla_h\Delta_h\tilde{\phi}^{m+1}\right) \leq \frac{C}{\varepsilon^2}\|\nabla_h\tilde{\phi}^{m+1}\|_2^2 + \frac{\varepsilon^2}{8}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2. \tag{3.28}$$

The regular diffusion term has the following decomposition:

$$\begin{aligned}(\nabla_h\Delta_h\tilde{\phi}^{m+1}, \nabla_h\tilde{\mu}^{m+1}) &= (\nabla_h\Delta_h\tilde{\phi}^{m+1}, \nabla_h(\mathcal{N}^{m+1}\tilde{\phi}^{m+1})) - (\nabla_h\Delta_h\tilde{\phi}^{m+1}, \nabla_h\tilde{\phi}^m) \\ &\quad - \varepsilon^2\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2.\end{aligned} \tag{3.29}$$

The concave term can be controlled by

$$-(\nabla_h\Delta_h\tilde{\phi}^{m+1},\nabla_h\tilde{\phi}^m)\leq C\|\nabla_h\tilde{\phi}^m\|_2^2+\frac{\varepsilon^2}{8}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2. \tag{3.30}$$

For the nonlinear error term, we have

$$\begin{aligned}\|\nabla_h(\mathcal{N}^{m+1}\tilde{\phi}^{m+1})\|_2 \leq& 3\left(\|A_h\phi^{m+1}\|_\infty+\|A_h\Phi^{m+1}\|_\infty\right)\\ &\cdot\left(\|\nabla_h\phi^{m+1}\|_2+\|\nabla_h\Phi^{m+1}\|_2\right)\|A_h\tilde{\phi}^{m+1}\|_\infty\\ &+\frac{3}{2}\left(\|A_h\Phi^{m+1}\|_\infty^2+\|A_h\phi^{m+1}\|_\infty^2\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2\\ \leq& C\left(\alpha_{m+1}+1\right)\|\tilde{\phi}^{m+1}\|_\infty+C\left(\alpha_{m+1}^2+1\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2.\end{aligned} \tag{3.31}$$

As a result, we have, using estimate (3.22) and Young's inequality,

$$\begin{aligned}(\nabla_h\Delta_h\tilde{\phi}^{m+1},&\nabla_h(\mathcal{N}^{m+1}\tilde{\phi}^{m+1}))\\ \leq& C\left(\alpha_{m+1}+1\right)\|\tilde{\phi}^{m+1}\|_\infty\cdot\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2\\ &+C\left(\alpha_{m+1}^2+1\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2\cdot\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2\\ \leq& C\left(\alpha_{m+1}^2+1\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2\cdot\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2\\ &+C\left(\alpha_{m+1}+1\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2^{\frac{3}{4}}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^{\frac{5}{4}}\\ &+C\left(\alpha_{m+1}+1\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2\\ &+C\left(\alpha_{m+1}+1\right)h^2\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2\\ \leq& C\left(\alpha_{m+1}^4+1\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2^2+\frac{\varepsilon^2}{32}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2\\ &+C\left((\alpha_{m+1})^{\frac{8}{3}}+1\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2^2+\frac{\varepsilon^2}{32}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2\\ &+C\left((\alpha_{m+1})^2+1\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2^2+\frac{\varepsilon^2}{32}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2\\ &+C\left((\alpha_{m+1})^2+1\right)h^4+\frac{\varepsilon^2}{32}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2\\ \leq& C\left(\alpha_{m+1}^4+1\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2^2+\frac{\varepsilon^2}{8}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2+C\left(\alpha_{m+1}^2+1\right)h^4.\end{aligned} \tag{3.32}$$

These above estimates imply that

$$\begin{aligned}(\nabla_h\Delta_h\tilde{\phi}^{m+1},\nabla_h\tilde{\mu}^{m+1})\leq& C\left(\alpha_{m+1}^4+1\right)\left\|\nabla_h\tilde{\phi}^{m+1}\right\|_2^2+C\left\|\nabla_h\tilde{\phi}^m\right\|_2^2\\ &-\frac{3\varepsilon^2}{4}\left\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\right\|_2^2+C\left(\alpha_{m+1}^2+1\right)h^4.\end{aligned} \tag{3.33}$$

Next we focus our attention on the terms associated with the nonlinear convection part. Since $\|\mathbf{U}^m\|_\infty\leq C_6$, for all $1\leq m\leq M$, the first part can be bounded by

$$\begin{aligned}-(\nabla_h\Delta_h\tilde{\phi}^{m+1},A_h\tilde{\phi}^m\mathbf{U}^{m+1})\leq& C\left\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\right\|_2\cdot\left(\left\|\nabla_h\tilde{\phi}^m\right\|_2+h^2\right)\\ \leq&\frac{\varepsilon^2}{16}\left\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\right\|_2^2+C\left\|\nabla_h\tilde{\phi}^m\right\|_2^2+Ch^4.\end{aligned} \tag{3.34}$$

For the second part, the expansion for the velocity numerical error indicates that

$$
\begin{aligned}
-(\nabla_h \Delta_h \tilde{\phi}^{m+1}, A_h \phi^m \tilde{\boldsymbol{u}}^{m+1}) =& \gamma(A_h \phi^m \nabla_h \Delta_h \tilde{\phi}^{m+1}, \mathcal{P}_h(A_h \tilde{\phi}^m \nabla_h \Gamma^{m+1})) \\
&+ \gamma(A_h \phi^m \nabla_h \Delta_h \tilde{\phi}^{m+1}, \mathcal{P}_h(A_h \phi^m \nabla_h \tilde{\mu}^{m+1})).
\end{aligned} \tag{3.35}
$$

The first term can be estimated in a straightforward way. Using the L_h^2 stability of the projection and the regularity estimate $\|\nabla_h \Gamma^m\|_\infty \le C_6$, we have

$$
\begin{aligned}
&\gamma(A_h \phi^m \nabla_h \Delta_h \tilde{\phi}^{m+1}, \mathcal{P}_h(A_h \tilde{\phi}^m \nabla_h \Gamma^{m+1})) \\
&\quad \le \gamma \|\phi^m\|_\infty \cdot \|\nabla_h \Delta_h \tilde{\phi}^{m+1}\|_2 \cdot \|\mathcal{P}_h(A_h \tilde{\phi}^m \nabla_h \Gamma^{m+1})\|_2 \\
&\quad \le C \alpha_m \|\nabla_h \Delta_h \tilde{\phi}^{m+1}\|_2 \cdot \|\tilde{\phi}^m\|_2 \\
&\quad \le C \alpha_m \|\nabla_h \Delta_h \tilde{\phi}^{m+1}\|_2 \cdot \left(\|\nabla_h \tilde{\phi}^m\|_2 + h^2\right) \\
&\quad \le C \alpha_m^2 \left(\|\nabla_h \tilde{\phi}^m\|_2^2 + h^4\right) + \frac{\varepsilon^2}{32} \|\nabla_h \Delta_h \tilde{\phi}^{m+1}\|_2^2,
\end{aligned} \tag{3.36}
$$

with the discrete Poincaré inequality (3.21) applied in the third step. The second term can be expanded as

$$
\begin{aligned}
&\gamma(A_h \phi^m \nabla_h \Delta_h \tilde{\phi}^{m+1}, \mathcal{P}_h(A_h \phi^m \nabla_h \tilde{\mu}^{m+1})) \\
&\quad = \gamma(A_h \phi^m \nabla_h \Delta_h \tilde{\phi}^{m+1}, \mathcal{P}_h(A_h \phi^m \nabla_h (\mathcal{N}^{m+1} \tilde{\phi}^{m+1}))) \\
&\quad\quad - \gamma(A_h \phi^m \nabla_h \Delta_h \tilde{\phi}^{m+1}, \mathcal{P}_h(A_h \phi^m \nabla_h \tilde{\phi}^m)) \\
&\quad\quad - \gamma \varepsilon^2 (A_h \phi^m \nabla_h \Delta_h \tilde{\phi}^{m+1}, \mathcal{P}_h(A_h \phi^m \nabla_h \Delta_h \tilde{\phi}^{m+1})).
\end{aligned} \tag{3.37}
$$

It is observed that the third term of the right-hand side of (3.37) is always non-positive. Indeed, using a property of the projection,

$$
-(A_h \phi^m \nabla_h \Delta_h \tilde{\phi}^{m+1}, \mathcal{P}_h(A_h \phi^m \nabla_h \Delta_h \tilde{\phi}^{m+1})) = -\|\mathcal{P}_h(A_h \phi^m \nabla_h \Delta_h \tilde{\phi}^{m+1})\|_2^2 \le 0. \tag{3.38}
$$

The analysis for the second term of the right-hand side of (3.37) is standard:

$$
\begin{aligned}
-\gamma(A_h \phi^m \nabla_h \Delta_h \tilde{\phi}^{m+1}, \mathcal{P}_h(A_h \phi^m \nabla_h \tilde{\phi}^m)) &\le \gamma \|A_h \phi^m \nabla_h \Delta_h \tilde{\phi}^{m+1}\|_2 \cdot \|A_h \phi^m \nabla_h \tilde{\phi}^m\|_2 \\
&\le C \alpha_m^2 \|\nabla_h \Delta_h \tilde{\phi}^{m+1}\|_2 \cdot \|\nabla_h \tilde{\phi}^m\|_2 \\
&\le \frac{\varepsilon^2}{64} \|\nabla_h \Delta_h \tilde{\phi}^{m+1}\|_2^2 + C \alpha_m^4 \|\nabla_h \tilde{\phi}^m\|_2^2.
\end{aligned} \tag{3.39}
$$

For the first term of the right-hand side of (3.37), the estimates are as follows:

(3.40)
$$\begin{aligned}
&\gamma(A_h\phi^m\nabla_h\Delta_h\tilde{\phi}^{m+1},\mathcal{P}_h(A_h\phi^m\nabla_h(\mathcal{N}^{m+1}\tilde{\phi}^{m+1})))\\
&\quad\le C\alpha_m^2\left(\alpha_{m+1}^2+1\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2\cdot\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2\\
&\qquad+C\alpha_m^2\left(\alpha_{m+1}+1\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2^{\frac{3}{4}}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^{\frac{5}{4}}\\
&\qquad+C\alpha_m^2\left(\alpha_{m+1}+1\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2\\
&\qquad+C\alpha_m^2\left(\alpha_{m+1}+1\right)h^2\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2\\
&\quad\le C\alpha_m^4\left(\alpha_{m+1}^4+1\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2^2+\frac{\varepsilon^2}{256}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2\\
&\qquad+C\alpha_m^{\frac{16}{3}}\left(\alpha_{m+1}^{\frac{8}{3}}+1\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2^2+\frac{\varepsilon^2}{256}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2\\
&\qquad+C\alpha_m^4\left(\alpha_{m+1}^2+1\right)\|\nabla_h\tilde{\phi}^{m+1}\|_2^2+\frac{\varepsilon^2}{256}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2\\
&\qquad+C\alpha_m^4\left(\alpha_{m+1}^2+1\right)h^4+\frac{\varepsilon^2}{256}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2\\
&\quad\le C\left\{\alpha_m^4\alpha_{m+1}^4+\alpha_m^{\frac{16}{3}}\left(\alpha_{m+1}^{\frac{8}{3}}+1\right)+1\right\}\|\nabla_h\tilde{\phi}^{m+1}\|_2^2\\
&\qquad+\frac{\varepsilon^2}{64}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2+C\alpha_m^4\left(\alpha_{m+1}^2+1\right)h^4.
\end{aligned}$$

A combination of estimates (3.36), (3.38), (3.39), and (3.40) yields

$$\begin{aligned}
&-(\nabla_h\Delta_h\tilde{\phi}^{m+1},A_h\tilde{\phi}^m\tilde{\boldsymbol{u}}^{m+1})\\
&\quad\le C\left\{\alpha_m^4\alpha_{m+1}^4+\alpha_m^{\frac{16}{3}}\left(\alpha_{m+1}^{\frac{8}{3}}+1\right)+1\right\}\|\nabla_h\tilde{\phi}^{m+1}\|_2^2\\
&\qquad+C\alpha_m^2\left(1+\alpha_m^2\right)\|\nabla_h\tilde{\phi}^m\|_2^2+\frac{\varepsilon^2}{16}\|\nabla_h\Delta_h\tilde{\phi}^{m+1}\|_2^2\\
&\qquad+C\left(\alpha_m^2+\alpha_m^4\left(\alpha_{m+1}^2+1\right)\right)h^4.
\end{aligned}\tag{3.41}$$

Finally, from (3.26), (3.27), (3.33), (3.34), and (3.41), we obtain estimate (3.24). □

Remark 3.6. Note that we have suppressed the dependence of the constants on the parameters ε and γ. Typically, one would expect the constants to depend on ε^{-p} for small positive integers p. We also point out that C_{10}, C_{11}, C_{12} can depend upon T, but only indirectly. This is because C_{10}, C_{11}, C_{12} depend upon the regularity bounds for the exact PDE solution – for example, C_5, C_6 – which could possibly depend upon time.

Remark 3.7. In the classical numerical analyses for the pure Cahn-Hilliard equation (1.2), it is typical that a discrete $L_s^\infty(0,T;L_h^2)$ error estimate is performed. See the related references [6–8, 17, 19–22, 26, 27, 29, 32, 33, 35, 40, 42]. However, such a classical error estimate does not work for the CHHS equation (1.3) – (1.6) due to the lack of control for the inner product of $\tilde{\phi}^{m+1}$ with the nonlinear error term associated with the convection part.

Instead, if an $L_s^\infty(0,T;H_h^1)\cap L_s^2(0,T;H_h^3)$ error estimate is pursued, as in the present analysis, we observe that the corresponding inner product associated with the nonlinear convection term is ensured to be non-positive, as given by (3.38). This fact is crucial to make the stability and convergence analysis go through.

The following bound can be derived for the growth coefficients appearing in Theorem 3.5.

Lemma 3.8. *With the same hypotheses as for Theorem* 3.5*, we have for any* $1 \le \ell \le M$*,*

$$s \sum_{m=0}^{\ell-1} \left(C_{10} D_1^{m+1} + C_{11} D_2^m + C_{12} D_3^{m+1} \right) \le C_{13}(t_\ell + 1) \le C_{13}(T+1) := C_{14}, \tag{3.42}$$

where $C_{13} > 0$ *is independent of* s *and* h*. Here* C_{13} *can depend upon* T*, since* C_{10}*,* C_{11}*,* C_{12} *can depend upon* T*.*

Proof. This is a direct consequence of the discrete $L_s^8(0,T)$ bound for $\alpha_m := \|\phi^m\|_\infty$, as given by (2.9), combined with the following simple result of Young's inequality:

$$\alpha_m^p \cdot \alpha_{m+1}^q \le C \left(\alpha_m^8 + \alpha_{m+1}^8 + 1 \right), \quad \forall\, p, q \in \mathbb{N} :\ 0 \le p + q \le 8. \tag{3.43}$$ □

Remark 3.9. We observe that the standard discrete Gronwall inequality cannot be applied directly to the error estimate (3.24) since the latter is implicit. To make the estimate explicit, we need to bound $sC_{10}D_1^{m+1}$ by a constant less than 1. Indeed, (3.42) implies that, for arbitrary $1 \le m \le M$,

$$sC_{10} D_1^m \le s \sum_{j=1}^{M} C_{10} D_1^j \le C_{14}. \tag{3.44}$$

No matter how small $s > 0$ is made, this inequality could only ensure that $sC_{10}D_1^m$ has a value bounded by C_{14}. Meanwhile, a direct point-wise bound (in m) for D_1^m is not available, as $s \to 0$, based on this inequality alone.

3.3. **The result of an *a priori* error assumption.** Since, as we mentioned, we are not able to use the discrete Gronwall inequality directly to derive an error estimate from the error stability (3.24), we use an induction argument to prove convergence. Specifically, we assume, as our induction hypothesis, that the desired error estimate holds at an arbitrary time step m ($0 \le m \le M-1$). We then use this *a priori* assumption to prove that $sC_{10}D_1^{m+1} < 1$, provided s is small enough. Then we conclude the induction argument by proving that the error estimate holds at the updated time step $m+1$.

First, we will need the following technical result, which is a direct result of Young's inequality. The proof is skipped for brevity.

Lemma 3.10. *For any* $a > 0$*,* $\delta > 0$ *and* $0 < q < 8$*, we have*

$$a \cdot \delta^q \le b\delta^8 + r(a,b,q), \quad \forall\, b > 0, \qquad \text{where} \qquad r(a,b,q) := \frac{a^{\frac{8}{8-q}}}{\frac{8}{8-q} \left(b \cdot \frac{8}{q} \right)^{\frac{q}{8-q}}}. \tag{3.45}$$

Theorem 3.11. *With the same hypotheses as for Theorem* 3.5*, suppose that* h *and* s *are sufficiently small and the following error estimate is valid up to the time step* $t_m := m \cdot s$*, for* $0 \le m \le M-1$*:*

$$\left\| \nabla_h \tilde{\phi}^m \right\|_2^2 + \varepsilon^2 s \sum_{j=1}^{m} \left\| \nabla_h \Delta_h \tilde{\phi}^j \right\|_2^2 \le C_{15} \exp\left(C_{16}(t_m + 1) \right) \left(s^2 + h^4 \right), \tag{3.46}$$

where $C_{15}, C_{16} > 0$ *may depend upon the final time* T *but are independent of* s *and* h. *Then*

$$sC_{10}D_1^{m+1} \le \frac{1}{2}. \tag{3.47}$$

Proof. As an application of (3.45), the terms after the two leading terms appearing on the right-hand side of (3.25) for the expansion of D_1^{m+1} can be bounded as follows:

$$\alpha_{m+1}^4 \le \frac{1}{16C_{10}C_4(T+1)}\alpha_{m+1}^8 + C, \tag{3.48}$$

$$\alpha_m^{\frac{16}{3}} \le \frac{1}{16C_{10}C_4(T+1)}\alpha_m^8 + C. \tag{3.49}$$

Then we get, for any $0 \le m \le M-1$,

$$\begin{aligned} sC_{11}\left(\alpha_m^{\frac{16}{3}} + \alpha_{m+1}^4 + 1\right) &\le \frac{s}{16C_4(T+1)}\alpha_{m+1}^8 + \frac{s}{16C_4(T+1)}\alpha_k^8 + sC_{17} \\ &\le \frac{1}{8} + sC_{17}, \end{aligned} \tag{3.50}$$

using the $L_s^8(0,T)$ bound for $\alpha_m := \|\phi^m\|_\infty$ in (2.9), where $C_{18} > 0$ is a constant that is independent of h and s.

Now, the leading terms appearing on the right-hand side of (3.25) in the expansion of D_1^{m+1} – namely, $\alpha_m^4\alpha_{m+1}^4$ and $\alpha_m^{\frac{16}{3}}\alpha_{m+1}^{\frac{8}{3}}$ – cannot be bounded in this way due to the fact that their exponents sum to exactly 8: $4+4=8$, $\frac{16}{3}+\frac{8}{3}=8$. We must, therefore, rely upon (3.46). This bound implies

$$\begin{aligned} \left\|\nabla_h\tilde{\phi}^m\right\|_2^2 &\le C_{15}\exp\left(C_{16}(T+1)\right)\left(s^2+h^4\right), \\ \left\|\nabla_h\Delta_h\tilde{\phi}^m\right\|_2^2 &\le \varepsilon^{-2}C_{15}\exp\left(C_{16}(T+1)\right)\left(s^2+h^4\right)s^{-1}. \end{aligned} \tag{3.51}$$

Using (3.22) and setting $C_{18} := C_{15}\exp\left(C_{16}(T+1)\right)$, we have

$$\begin{aligned} \left\|\tilde{\phi}^m\right\|_\infty^2 &\le 2C_9^2\left(\left\|\nabla_h\tilde{\phi}^m\right\|_2^{\frac{3}{2}}\left\|\nabla_h\Delta_h\tilde{\phi}^m\right\|_2^{\frac{1}{2}} + \left\|\nabla_h\tilde{\phi}^m\right\|_2^2 + h^4\right) \\ &\le 2C_9^2\left\{C_{18}\left(s^2+h^4\right)\left(\varepsilon^{-1/2}s^{-1/4}+1\right)+h^4\right\} \\ &= 2C_9^2\left\{C_{18}\varepsilon^{-1/2}s^{7/4} + C_{18}\varepsilon^{-1/2}h^4s^{-1/4} + C_{18}s^2 + (1+C_{18})\,h^4\right\}. \end{aligned} \tag{3.52}$$

Under the time and space step size constraint

$$C_{18}\varepsilon^{-1/2}s^{7/4} + C_{18}s^2 + (1+C_{18})\,h^4 \le \frac{1}{2C_9^2}, \tag{3.53}$$

the following bound is available:

$$\left\|\tilde{\phi}^m\right\|_\infty^2 \le 1 + 2C_9^2C_{18}\varepsilon^{-1/2}\frac{h^4}{s^{1/4}}. \tag{3.54}$$

Consequently, we see that

$$\alpha_m^2 := \|\phi^m\|_\infty^2 \le 2\|\Phi^m\|_\infty^2 + 2\left\|\tilde{\phi}^m\right\|_\infty^2 \le C_{19}\left(1+\frac{h^4}{s^{1/4}}\right), \tag{3.55}$$

where $C_{19} > 0$ is independent of s and h, but it does depend upon the final time T (at least exponentially) and the interface parameter ε. This shows that

$$\alpha_m^4 \alpha_{m+1}^4 \le C_{19}^2 \left(1 + \frac{h^4}{s^{1/4}}\right)^2 \alpha_{m+1}^4 \le 2C_{19}^2 \alpha_{m+1}^4 + 2C_{19}^2 \frac{h^8}{s^{1/2}} \alpha_{m+1}^4. \tag{3.56}$$

The first term on the right-hand side can be handled in the same way as (3.48):

$$2C_{19}^2 \alpha_{m+1}^4 \le \frac{1}{16 C_{10} C_4 (T+1)} \alpha_{m+1}^8 + C. \tag{3.57}$$

Hence

$$sC_{10} \left(2C_{19}^2 \alpha_{m+1}^4\right) \le \frac{1}{16} + sC_{20}, \tag{3.58}$$

where $C_{20} > 0$ is independent of s and h. The second term on the right-hand side of (3.56) can be analyzed as follows: using Cauchy's inequality and (2.9), we have

$$\begin{aligned} sC_{10} \left(2C_{19}^2 \frac{h^8}{s^{1/2}} \alpha_{m+1}^4\right) &\le C_{10} C_{19}^2 h^8 \left(s\alpha_{m+1}^8 + 1\right) \\ &\le C_{10} C_{19}^2 C_4 (T+1) h^8 + C_{10} C_{19}^2 h^8. \end{aligned} \tag{3.59}$$

Under an additional constraint for the grid size

$$h^8 \le \min \left(\frac{1}{32 C_{10} C_{19}^2 C_4 (T+1)}, \frac{1}{32 C_{10} C_{19}^2} \right), \tag{3.60}$$

we arrive at

$$sC_{10} \left(2C_{19}^2 \frac{h^8}{s^{1/2}} \alpha_{m+1}^4\right) \le \frac{1}{16}. \tag{3.61}$$

A combination of (3.56), (3.58) and (3.61) yields

$$sC_{10} \alpha_m^4 \alpha_{m+1}^4 \le \frac{1}{8} + sC_{20}. \tag{3.62}$$

A similar analysis can be applied to the term $\alpha_m^{\frac{16}{3}} \alpha_{m+1}^{\frac{8}{3}}$ appearing in (3.25): under similar constraints as given in (3.60), we have

$$sC_{10} \alpha_m^{\frac{16}{3}} \alpha_{m+1}^{\frac{8}{3}} \le \frac{1}{8} + sC_{21}, \tag{3.63}$$

where $C_{21} > 0$ is independent of s and h. The details of the proof are skipped for the sake of brevity.

Therefore, a combination of (3.50), (3.62), and (3.63) leads to

$$sC_{10} D_1^{m+1} \le \frac{3}{8} + s(C_{17} + C_{20} + C_{21}), \tag{3.64}$$

and under the additional constraint for the time step

$$s \le \frac{1}{8(C_{17} + C_{20} + C_{21})}, \tag{3.65}$$

we get the desired result, estimate (3.47). □

Remark 3.12. The desired bound (3.47) holds under the constraints (3.53), (3.60), and (3.65), for time step s and grid size h. There is another bound, analogous to (3.60) required for (3.63) to hold. Observe that there is no CFL-like condition to be satisfied between s and h. In fact, all these constraints only depend on a few generic constants, the physical parameters, and final time T.

Remark 3.13. Under the *a priori* convergence assumption (3.46), we apply the discrete Gagliardo-Nirenberg inequality and obtain (3.52), with the only singular term being the one of the form $O\left(\frac{h^2}{s^{1/8}}\right)$. In turn, the $\|\cdot\|_\infty$ norm of the numerical error function has the bound (3.54). Consequently, in the more detailed expansion analysis (3.59), a term $s^{1/2}\alpha_m^4$ is involved in which the Cauchy inequality can be applied. In other words, this analysis is marginal in 3-D.

If, on the other hand, a naive application of inverse inequality,

$$\|f\|_\infty \le Ch^{-d/2}\|f\|_2 ,$$

is applied to the *a priori* convergence assumption (3.46), we obtain the $\|\cdot\|_\infty$ norm of the numerical error function as of order $O\left(\frac{s+h^2}{h^{3/2}}\right)$ in 3-D. Using this approach, it is not possible to get the desired estimates without having a CFL-like condition between s and h. Therefore, an application of the discrete Gagliardo-Nirenberg inequality (3.52) is crucial in the analysis.

3.4. **The main result: An error estimate.** The following theorem is the main result of this article. The basic idea is to extend the *a priori* error estimate (3.46) by an induction argument.

Theorem 3.14. *Given initial data $\phi_0 \in C^6(\overline{\Omega})$, with homogeneous Neumann boundary conditions, suppose the unique solution for the CHHS equation* (1.3) – (1.6) *is of regularity class $\mathcal{R}$. Then, provided s and h are sufficiently small, for all positive integers ℓ such that $s\cdot\ell\le T$, we have*

$$\left\|\nabla_h\tilde{\phi}^\ell\right\|_2^2 + \varepsilon^2 s\sum_{m=1}^{\ell}\left\|\nabla_h\Delta_h\tilde{\phi}^m\right\|_2^2 \le C\left(s^2+h^4\right), \tag{3.66}$$

where $C>0$ is independent of s and h.

Proof. Suppose that $m+1\le M$. By summing (3.24) we obtain

$$\begin{aligned}\left\|\nabla_h\tilde{\phi}^{m+1}\right\|_2^2 &+ \varepsilon^2 s\sum_{j=1}^{m+1}\left\|\nabla_h\Delta_h\tilde{\phi}^j\right\|_2^2\\ &\le \left\|\nabla_h\tilde{\phi}^0\right\|_2^2 + s\sum_{j=1}^{m+1}C_{10}D_1^j\left\|\nabla_h\tilde{\phi}^j\right\|_2^2\\ &\quad + s\sum_{j=0}^{m}C_{11}D_2^j\left\|\nabla_h\tilde{\phi}^j\right\|_2^2\\ &\quad + (s^2+h^4)s\sum_{j=1}^{m+1}\beta_j^2 + C_{12}h^4 s\sum_{j=1}^{m+1}D_3^j.\end{aligned} \tag{3.67}$$

We proceed by induction. Namely, suppose that (3.46) holds. Then, if h and s are sufficiently small – as required in the proof of the last theorem – considering (3.47) and using $\tilde{\phi}^0 \equiv 0$, we have

$$\begin{aligned}\frac{1}{2}\left\|\nabla_h\tilde{\phi}^{m+1}\right\|_2^2 &+ \varepsilon^2 s\sum_{j=1}^{m+1}\left\|\nabla_h\Delta_h\tilde{\phi}^j\right\|_2^2 \\ &\le \left(1 - sC_{10}D_1^{m+1}\right)\left\|\nabla_h\tilde{\phi}^{m+1}\right\|_2^2 + \varepsilon^2 s\sum_{j=1}^{m+1}\left\|\nabla_h\Delta_h\tilde{\phi}^j\right\|_2^2 \\ &\le s\sum_{j=1}^{m}\left(C_{10}D_1^j + C_{11}D_2^j\right)\left\|\nabla_h\tilde{\phi}^j\right\|_2^2 \\ &\quad + (s^2+h^4)s\sum_{j=1}^{m+1}\beta_j^2 + C_{12}h^4 s\sum_{j=1}^{m+1}D_3^j. \end{aligned} \tag{3.68}$$

Hence

$$\begin{aligned}\left\|\nabla_h\tilde{\phi}^{m+1}\right\|_2^2 + 2\varepsilon^2 s\sum_{j=1}^{m+1}\left\|\nabla_h\Delta_h\tilde{\phi}^j\right\|_2^2 \le s\sum_{j=1}^{m}\left(2C_{10}D_1^j + 2C_{11}D_2^j\right)\left\|\nabla_h\tilde{\phi}^j\right\|_2^2 \\ + C_{22}(s^2+h^4), \end{aligned} \tag{3.69}$$

where $C_{22} > 0$ is a constant that is independent of s and h. Using the discrete Gronwall inequality and Lemma 3.8 gives

$$\begin{aligned}\left\|\nabla_h\tilde{\phi}^{m+1}\right\|_2^2 &+ 2\varepsilon^2 s\sum_{j=1}^{m+1}\left\|\nabla_h\Delta_h\tilde{\phi}^j\right\|_2^2 \\ &\le C_{22}(s^2+h^4)\exp\left(s\sum_{j=1}^{m}\left(2C_{10}D_1^j + 2C_{11}D_2^j\right)\right) \\ &\le C_{22}(s^2+h^4)\exp\left(2C_{13}(t_{m+1}+1)\right). \end{aligned} \tag{3.70}$$

Consequently, the *a priori* assumption (3.46) can be justified at time step t_{m+1} by taking $C_{15} = C_{22}$, $C_{16} = 2C_{13}$. This completes the induction argument, and the proof of Theorem 3.14 is finished. □

Remark 3.15. If the standard H^1 conforming piecewise-linear space was used for ϕ in a finite element approximation of (1.3) – (1.6) – which roughly corresponds to the centered difference approximation employed in this work – the standard estimate in the finite element space projection indicates an $O(h)$ accuracy in the H^1 norm. As a result, the global convergence for the fully discrete finite element scheme would be expected to be at best $O(h)$ in the $L^\infty(0,T;H^1)$ norm. Of course, the H^3 norm of the error would be undefined, since the approximation ϕ (and therefore the error) would be only globally H^1.

On the other hand, it is observed that an $O(h^2)$ convergence order has been established for the finite difference scheme over a uniform grid in the discrete $L_s^\infty(0,T;H_h^1) \cap L_s^2(0,T;H_h^3)$ norm. This might be regarded as a kind of super-convergence result and is due to the use of a uniform grid and spatially discrete norms. The detailed convergence analysis for a mixed conforming finite element approximation of the CHHS system (1.3) – (1.6) is currently being considered by the authors.

Remark 3.16. The convergence constant appearing in (3.66) (in Theorem 3.14) is independent of s and h. Of course this constant does depend on the final time T and on the interface parameter ε. A detailed calculation reveals it is of the order $\exp\left(\varepsilon^{-k}T\right)$ (k is some integer), which comes from the application of the discrete Gronwall inequality in the convergence analysis.

There have been existing works on the improved convergence constant for the pure Cahn-Hilliard equation (1.2). Specifically, Feng and Prohl [27] proved – for a first order in time, fully discrete finite element scheme – that the convergence constant is of order $O(e^{C_0 T}\varepsilon^{-m_0})$, for some positive integer m_0 and a constant C_0 independent of ε, instead of the singularly ε-dependent exponential growth. To the authors' knowledge, this result gives the sharpest convergence constant for the Cahn-Hilliard flow in the existing literature.

Such an elegant improvement was based on a subtle spectrum analysis for the linearized Cahn-Hilliard operator, provided in earlier publications [3, 4, 13–15]:

$$\lambda_{CH} := \inf_{\psi \in H^1, \psi \neq 0} \frac{\varepsilon^{-1}\left(\left(3\Phi^2(t) - 1\right)\psi, \psi\right) + \varepsilon \left\|\nabla \psi\right\|^2}{\left\|\psi\right\|_{H^{-1}}^2} \geq -C_0, \tag{3.71}$$

for any $t \geq 0$, $\varepsilon \in (0, \varepsilon_0)$, with $0 < \varepsilon_0 \ll 1$ and C_0 independent of ε, where Φ is the exact solution to the Cahn-Hilliard problem, with certain non-trivial structure assumptions in place.

On the other hand, such a linearized spectrum estimate is not (yet) available for the CHHS equation (1.3) – (1.6) due to the highly nonlinear convection term. In turn, an improvement of the convergence constant reported in (3.66) cannot be applied straightforwardly. This issue will be explored in the authors' future work.

Remark 3.17. In the numerical approximation of any nonlinear PDE, the convergence constant in the error analysis usually always contains an exponential growth term (in the final time) when the discrete Gronwall inequality is utilized; see the details of Remark 3.16. As a result, a theoretical analysis based on the discrete Gronwall inequality would not likely justify the long time accuracy of the numerical simulation. On the other hand, one can go a different route in the analysis. See, for example, [5], where the authors establish an error constant that is only linear in final time, T, for a numerical scheme approximating the Navier-Stokes equation. They do not use the discrete Gronwall inequality, but a more intricate analysis that requires the assumption of sufficiently small PDE solutions. The general analysis without assumptions on the solutions or initial data is usually always difficult for fully nonlinear equations.

The value of the energy stable schemes for long time numerical simulation is not realized in terms of the convergence order at a fixed final time. Instead, the energy stable schemes are expected to lead to a numerical accuracy in terms of the long time average quantities via a recently developed technique of statistical convergence; see the related works for two-dimensional incompressible Navier-Stokes equations [30] and the epitaxial thin film growth model [43], to cite a couple of examples.

The statistical convergence properties and the numerical accuracy in terms of long time average for the convex splitting scheme applied to the CHHS equation (1.3) – (1.6) and other Cahn-Hilliard flow models are expected to involve many more technical details, and such analyses will be the subject of future works.

Remark 3.18. The numerical scheme (2.1) – (2.3) is only first order accurate in time. Meanwhile, higher order energy stable schemes, such as a second order convex splitting, is also available for the CHHS equation (1.3) – (1.6). For the second order convex splitting scheme, the unique solvability, unconditional energy stability and full order convergence analysis are all expected, though the analyses are somewhat more complicated. We plan to report our results in future works.

Appendix A. Discretization of space

A.1. **Basic definitions.** Here we use the notation and results for some discrete functions and operators from [47]. We begin with definitions of grid functions and difference operators needed for our discretization of three-dimensional space. We consider the domain $\Omega = (0, L_x) \times (0, L_y) \times (0, L_z)$ and assume that N_x, N_y and N_z are positive integers such that $h = L_x/N_x = L_y/N_y = L_z/N_z$, for some $h > 0$, which is called the spatial step size. Consider, for any positive integer N, the following sets:

$$\mathcal{E}_N := \{i \cdot h \mid i = 0, \ldots, N\}, \qquad \mathcal{C}_N := \{(i - 1/2) \cdot h \mid i = 1, \ldots, N)\}, \tag{A.1}$$

$$\mathcal{C}_{\overline{N}} := \{(i - 1/2) \cdot h \mid i = 0, \ldots, N + 1)\}. \tag{A.2}$$

The two points belonging to $\mathcal{C}_{\overline{N}} \backslash \mathcal{C}_N$ are the so-called *ghost points*. Define the function spaces

$$\mathcal{C}_\Omega := \{\phi : \mathcal{C}_{\overline{N}_x} \times \mathcal{C}_{\overline{N}_y} \times \mathcal{C}_{\overline{N}_z} \to \mathbb{R}\}, \qquad \mathcal{E}^x_\Omega := \{\phi : \mathcal{E}_{N_x} \times \mathcal{C}_{N_y} \times \mathcal{C}_{N_z} \to \mathbb{R}\}, \tag{A.3}$$

$$\mathcal{E}^y_\Omega := \{\phi : \mathcal{C}_{N_x} \times \mathcal{E}_{N_y} \times \mathcal{C}_{N_z} \to \mathbb{R}\}, \qquad \mathcal{E}^z_\Omega := \{\phi : \mathcal{C}_{N_x} \times \mathcal{C}_{N_y} \times \mathcal{E}_{N_z} \to \mathbb{R}\}, \tag{A.4}$$

$$\vec{\mathcal{E}}_\Omega := \mathcal{E}^x_\Omega \times \mathcal{E}^y_\Omega \times \mathcal{E}^z_\Omega. \tag{A.5}$$

The functions of $\mathcal{C}_\Omega$ are called *cell-centered functions*. In component form, cell-centered functions are identified via $\phi_{i,j,k} := \phi(\xi_i, \xi_j, \xi_k)$, where $\xi_i := (i - 1/2) \cdot h$. The functions of $\mathcal{E}^x_\Omega$, *etc.*, are called face-centered functions. In component form, face-centered functions are identified via $f_{i+\frac{1}{2},j,k} := f(\xi_{i+1/2}, \xi_j, \xi_k)$, *etc.*

A discrete function $\phi \in \mathcal{C}_\Omega$ is said to satisfy homogeneous Neumann boundary conditions, and we write $\boldsymbol{n} \cdot \nabla_h \phi = 0$ iff at the ghost points ϕ satisfies

$$\phi_{0,j,k} = \phi_{1,j,k}, \quad \phi_{N_x,j,k} = \phi_{N_x+1,j,k}, \tag{A.6}$$

$$\phi_{i,0,k} = \phi_{i,1,k}, \quad \phi_{i,N_y,k} = \phi_{i,N_y+1,k}, \tag{A.7}$$

$$\phi_{i,j,0} = \phi_{i,j,1}, \quad \phi_{i,j,N_z} = \phi_{i,j,N_z+1}. \tag{A.8}$$

A discrete function $\boldsymbol{f} = (f^x, f^y, f^z)^T \in \vec{\mathcal{E}}_\Omega$ is said to satisfy the homogeneous boundary conditions $\boldsymbol{n} \cdot \boldsymbol{f} = 0$ iff we have

$$f^x_{1/2,j,k} = 0, \quad f^x_{N_x+1/2,j,k} = 0, \tag{A.9}$$

$$f^y_{i,1/2,k} = 0, \quad f^y_{i,N_y+1/2,k} = 0, \tag{A.10}$$

$$f^z_{i,j,1/2} = 0, \quad f^z_{i,j,N_z+1/2} = 0. \tag{A.11}$$

This staggered grid is also known as the marker and cell (MAC) grid and was first proposed in [31] to deal with the incompressible Navier-Stokes equations. Also see [38] for related applications to the 3-D primitive equations.

A.2. **Discrete operators, inner products, and norms.** We introduce the face-to-center difference operator $d_x : \mathcal{E}^x_\Omega \to \mathcal{C}_\Omega$, defined component-wise via

$$d_x f_{i,j,k} := \frac{1}{h}(f_{i+\frac{1}{2},j,k} - f_{i-\frac{1}{2},j,k}), \tag{A.12}$$

with $d_y : \mathcal{E}_\Omega^y \to \mathcal{C}_\Omega$ and $d_z : \mathcal{E}_\Omega^z \to \mathcal{C}_\Omega$ formulated analogously. Define $\nabla_h \cdot : \vec{\mathcal{E}}_\Omega \to \mathcal{C}_\Omega$ via

$$\nabla_h \cdot \boldsymbol{f} := d_x f^x + d_y f^y + d_z f^z, \tag{A.13}$$

where $\boldsymbol{f} = (f^x, f^y, f^z)^T$. Define $A_x : \mathcal{C}_\Omega \to \mathcal{E}_\Omega^x$ component-wise via

$$A_x \phi_{i+\frac{1}{2},j,k} := \frac{1}{2}(\phi_{i,j,k} + \phi_{i+1,j,k}), \tag{A.14}$$

with $A_y : \mathcal{C}_\Omega \to \mathcal{E}_\Omega^y$ and $A_z : \mathcal{C}_\Omega \to \mathcal{E}_\Omega^z$ formulated analogously. Define $A_h : \mathcal{C}_\Omega \to \vec{\mathcal{E}}_\Omega$ via

$$A_h \phi := (A_x \phi, A_y \phi, A_z \phi)^T. \tag{A.15}$$

Define $D_x : \mathcal{C}_\Omega \to \mathcal{E}_\Omega^x$ component-wise via

$$D_x \phi_{i+\frac{1}{2},j,k} := \frac{1}{h}(\phi_{i+1,j,k} - \phi_{i,j,k}). \tag{A.16}$$

$D_y : \mathcal{C}_\Omega \to \mathcal{E}_\Omega^y$ and $D_z : \mathcal{C}_\Omega \to \mathcal{E}_\Omega^z$ are similarly evaluated. Define $\nabla_h : \mathcal{C}_\Omega \to \vec{\mathcal{E}}_\Omega$ via

$$\nabla_h \phi := (D_x \phi, D_y \phi, D_z \phi)^T. \tag{A.17}$$

The standard discrete Laplace operator $\Delta_h : \mathcal{C}_\Omega \to \mathcal{C}_\Omega$ is just

$$\Delta_h \phi := \nabla_h \cdot \nabla_h \phi. \tag{A.18}$$

We define the following inner-products:

(A.19)

$$(\phi, \psi) := h^3 \sum_{i=1}^{L} \sum_{j=1}^{M} \sum_{m=1}^{N} \phi_{i,j,k} \psi_{i,j,k}, \qquad \forall\ \phi, \psi \in \mathcal{C}_\Omega,$$

(A.20)

$$[f, g]_x := \frac{1}{2} h^3 \sum_{i=1}^{L} \sum_{j=1}^{M} \sum_{m=1}^{N} (f_{i+\frac{1}{2},j,k} g_{i+\frac{1}{2},j,k} + f_{i-\frac{1}{2},j,k} g_{i-\frac{1}{2},j,k}), \quad \forall\ f, g \in \mathcal{E}_\Omega^x.$$

$[\cdot,\cdot]_y$ and $[\cdot,\cdot]_z$ can be formulated analogously. For $\boldsymbol{f} = (f^x, f^y, f^z)^T$, $\boldsymbol{g} = (g^x, g^y, g^z)^T$ $\in \vec{\mathcal{E}}_\Omega$ we define the natural inner product

$$(\boldsymbol{f}, \boldsymbol{g}) := [f^x, g^x]_x + [f^y, g^y]_y + [f^y, g^y]_z, \tag{A.21}$$

which gives the associated norm $\|\boldsymbol{f}\|_2 = \sqrt{(\boldsymbol{f}, \boldsymbol{f})}$. Analogously, for $\phi, \psi \in \mathcal{C}_\Omega$, a natural discrete inner product of their gradients is given by

$$(\nabla_h \phi, \nabla_h \psi) := [D_x \phi, D_x \psi]_x + [D_y \phi, D_y \psi]_y + [D_z \phi, D_z \psi]_z. \tag{A.22}$$

We also introduce the following norms for cell-centered functions $\phi \in \mathcal{C}_\Omega$:

$$\|\phi\|_\infty := \max_{i,j,k} |\phi_{i,j,k}|, \tag{A.23}$$

$$\|\phi\|_p := (|\phi|^p, 1)^{\frac{1}{p}}, \qquad 1 \le p < \infty. \tag{A.24}$$

In addition, we define

$$\|\nabla_h \phi\|_p := \left([|D_x \phi|^p, 1]_x + [|D_y \phi|^p, 1]_y + [|D_z \phi|^p, 1]_z \right)^{\frac{1}{p}}. \tag{A.25}$$

In the case of $p = 2$, it is clear that $(\nabla_h \phi, \nabla_h \phi) = \|\nabla_h \phi\|_2^2$.

A.3. **Summation by parts formulas.** For $\phi, \psi \in \mathcal{C}_\Omega$ and a velocity vector field $\boldsymbol{u} \in \vec{\mathcal{E}}_\Omega$, the following summation by parts formulas can be derived. If ψ satisfies the homogeneous Neumann boundary conditions, we have

$$(\phi, \Delta_h \psi) = -\left(\nabla_h \phi, \nabla_h \psi\right). \tag{A.26}$$

If $\boldsymbol{u} \cdot \boldsymbol{n} = 0$ on the boundary, we get

$$(\phi, \nabla_h \cdot \boldsymbol{u}) = -\left(\nabla_h \phi, \boldsymbol{u}\right). \tag{A.27}$$

Appendix B. Proof of the Gagliardo-Nirenberg inequality in Lemma 2.2

For simplicity of presentation, we assume $N_x = N_y = N_z =: N$ is odd and $L_x = L_y = L_z =: L$. The general case can be analyzed in the same manner, with more technical details involved.

Proof. Due to the discrete Neumann boundary conditions for ϕ and its cell-centered representation, it has a corresponding discrete Fourier cosine transformation in quarter wave sequence:

$$\phi_{i,j,k} = \sum_{\ell,m,n=0}^{N-1} \alpha_{\ell,m,n} \hat{\phi}^N_{\ell,m,n} \cos\frac{\ell\pi x_i}{L} \cos\frac{m\pi y_j}{L} \cos\frac{n\pi z_k}{L}, \tag{B.1}$$

$$\text{with} \qquad \alpha_{\ell,m,n} = \begin{cases} 1, & \text{if } \ell \neq 0,\ m \neq 0,\ n \neq 0, \\ \sqrt{\frac{1}{2}}, & \text{if one among } \ell, m, n \text{ is } 0, \\ \sqrt{\frac{1}{4}}, & \text{if two among } \ell, m, n \text{ are } 0, \\ \sqrt{\frac{1}{8}}, & \text{if } \ell = m = n = 0, \end{cases}$$

where $x_i = (i - \frac{1}{2})h, y_j = (j - \frac{1}{2})h, z_k = (k - \frac{1}{2})h$. Then we make its extension to a continuous function:

$$\phi_{\mathbf{F}}(x,y,z) = \sum_{\ell,m,n=0}^{N-1} \alpha_{\ell,m,n} \hat{\phi}^N_{\ell,m,n} \cos\frac{\ell\pi x}{L} \cos\frac{m\pi y}{L} \cos\frac{n\pi z}{L}. \tag{B.2}$$

Parseval's identity (at both the discrete and continuous levels) implies that

$$\sum_{i,j,k=1}^{N} |\phi_{i,j,k}|^2 = \frac{1}{8} N^3 \sum_{\ell,m,n=0}^{N-1} |\hat{\phi}^N_{\ell,m,n}|^2, \tag{B.3}$$

$$\|\phi_{\mathbf{F}}\|_{L^2}^2 = \frac{1}{8} L^3 \sum_{\ell,m,n=0}^{N-1} |\hat{\phi}^N_{\ell,m,n}|^2. \tag{B.4}$$

Based on the fact that $hN = L$, this in turn results in

$$\|\phi\|_2^2 = h^3 \sum_{i,j,k=1}^{N} |\phi_{i,j,k}|^2 = \|\phi_{\mathbf{F}}\|_{L^2}^2 = \frac{1}{8} L^3 \sum_{\ell,m,n=0}^{N-1} |\hat{\phi}^N_{\ell,m,n}|^2. \tag{B.5}$$

For the comparison between the discrete and continuous gradient, we start with the following Fourier expansions:

$$(D_x\phi)_{i+1/2,j,k} = \frac{\phi_{i+1,j,k} - \phi_{i,j,k}}{h}$$

$$= \sum_{\ell,m,n=0}^{N-1} \alpha_{\ell,m,n}\mu_\ell \hat{\phi}^N_{\ell,m,n} \sin\frac{\ell\pi x_{i+1/2}}{L}\cos\frac{m\pi y_j}{L}\cos\frac{n\pi z_k}{L}, \tag{B.6}$$

$$\partial_x\phi_{\mathbf{F}}(x,y,z) = \sum_{\ell,m,n=0}^{N-1} \alpha_{\ell,m,n}\nu_\ell \hat{\phi}^N_{\ell,m,n} \sin\frac{\ell\pi x}{L}\cos\frac{m\pi y}{L}\cos\frac{n\pi z}{L}, \tag{B.7}$$

with

$$\mu_\ell = -\frac{2\sin\frac{\ell\pi h}{2L}}{h}, \quad \nu_\ell = -\frac{\ell\pi}{L}. \tag{B.8}$$

In turn, an application of Parseval's identity yields

$$\|D_x\phi\|_2^2 = \frac{1}{8}L^3 \sum_{\ell,m,n=0}^{N-1} |\mu_\ell|^2 |\hat{\phi}^N_{\ell,m,n}|^2, \tag{B.9}$$

$$\|\partial_x\phi_{\mathbf{F}}\|_{L^2}^2 = \frac{1}{8}L^3 \sum_{\ell,m,n=0}^{N-1} |\nu_\ell|^2 |\hat{\phi}^N_{\ell,m,n}|^2. \tag{B.10}$$

The comparison of Fourier eigenvalues between $|\mu_\ell|$ and $|\nu_\ell|$ shows that

$$\frac{2}{\pi}|\nu_\ell| \le |\mu_\ell| \le |\nu_\ell|, \quad \text{for} \quad 0 \le \ell \le \mathrm{N}-1. \tag{B.11}$$

This indicates that

$$\frac{2}{\pi}\left\|\partial_x\phi_{\mathbf{F}}\right\|_{L^2} \le \|D_x\phi\|_2 \le \left\|\partial_x\phi_{\mathbf{F}}\right\|_{L^2}. \tag{B.12}$$

Similar comparison estimates can be derived in the same manner to reveal

$$\frac{2}{\pi}\|\nabla\phi_{\mathbf{F}}\|_{L^2} \le \|\nabla_h\phi\|_2 \le \|\nabla\phi_{\mathbf{F}}\|_{L^2}. \tag{B.13}$$

It can be proved analogously that

$$\frac{4}{\pi^2}\|\Delta\phi_{\mathbf{F}}\|_{L^2} \le \|\Delta_h\phi\|_2 \le \|\Delta\phi_{\mathbf{F}}\|_{L^2}, \tag{B.14}$$

$$\frac{8}{\pi^3}\|\nabla\Delta\phi_{\mathbf{F}}\|_{L^2} \le \|\nabla_h\Delta_h\phi\|_2 \le \|\nabla\Delta\phi_{\mathbf{F}}\|_{L^2}. \tag{B.15}$$

Meanwhile, we observe that the discrete average of ϕ and the continuous average of $\phi_{\mathbf{F}}$ are identical:

$$\bar{\phi} := \frac{h^3}{|\Omega|}\sum_{i,j,k=1}^{N} \phi_{i,j,k} = \alpha_{0,0,0}\hat{\phi}^N_{0,0,0} = \frac{1}{|\Omega|}\int_\Omega \phi_{\mathbf{F}}(\boldsymbol{x})\,d\boldsymbol{x} =: \overline{\phi_{\mathbf{F}}}. \tag{B.16}$$

As a result, we see that

$$
\begin{aligned}
\left\|\phi-\bar{\phi}\right\|_{\infty} &\le \left\|\phi_{\mathbf{F}}-\bar{\phi}\right\|_{L^\infty} \\
&\le C\left(\|\phi_{\mathbf{F}}-\bar{\phi}\|_{L^6}^{\frac{3}{4}}\|\nabla\Delta\phi_{\mathbf{F}}\|_{L^2}^{\frac{1}{4}}+\|\phi_{\mathbf{F}}-\bar{\phi}\|_{L^6}\right) \\
&\le C\left(\|\nabla\phi_{\mathbf{F}}\|_{L^2}^{\frac{3}{4}}\|\nabla\Delta\phi_{\mathbf{F}}\|_{L^2}^{\frac{1}{4}}+\|\nabla\phi_{\mathbf{F}}\|_{L^2}\right) \\
&\le C_1\left(\|\nabla_h\phi\|_2^{\frac{3}{4}}\|\nabla_h\Delta_h\phi\|_2^{\frac{1}{4}}+\|\nabla_h\phi\|_2\right),
\end{aligned}
\tag{B.17}
$$

in which the 3-D Gagliardo-Nirenberg inequality, Sobolev embedding (see [1] for more details) and Poincaré inequality were applied, and the equivalence estimates (B.13), (B.15) were recalled in the derivation. The proof of Lemma 2.2 is complete. □

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