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AN H^2 CONVERGENCE OF A SECOND-ORDER CONVEX-SPLITTING, FINITE DIFFERENCE SCHEME FOR THE THREE-DIMENSIONAL CAHN–HILLIARD EQUATION*

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Abstract. In this paper we present an unconditionally solvable and energy stable second order numerical scheme for the three-dimensional (3D) Cahn–Hilliard (CH) equation. The scheme is a two-step method based on a second order convex splitting of the physical energy, combined with a centered difference in space. The equation at the implicit time level is nonlinear but represents the gradients of a strictly convex function and is thus uniquely solvable, regardless of time step-size. The nonlinear equation is solved using an efficient nonlinear multigrid method. In addition, a global in time H_h^2 bound for the numerical solution is derived at the discrete level, and this bound is independent on the final time. As a consequence, an unconditional convergence (for the time step s in terms of the spatial grid size h) is established, in a discrete $L_s^\infty(0,T;H_h^2)$ norm, for the proposed second order scheme. The results of numerical experiments are presented and confirm the efficiency and accuracy of the scheme.

Key words. Cahn–Hilliard equation, finite difference, second-order, energy stability, multigrid, global-in-time H^2 stability, $L_s^\infty(0,T;H^2)$ convergence analysis.

AMS subject classifications. 35K30, 65M12, 65M55.

1. Introduction

Suppose that $\Omega=(0,L_x)\times(0,L_y)\times(0,L_z)$. For any $\phi\in H_{\text{per}}^1(\Omega)$, we define an energy of the form

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

where ε is a positive constant. See [10] for a detailed derivation of E. The conserved gradient dynamics on Ω is given by

$$\partial_t\phi=\nabla\cdot(\mathcal{M}(\phi)\nabla\mu), \tag{1.2}$$

where $\mathcal{M}(\phi)>0$ is a mobility, and we take $\mathcal{M}(\phi)\equiv 1$ for simplicity. The chemical potential, μ, is defined as

$$\mu:=\delta_\phi E=\phi^3-\phi-\varepsilon^2\Delta\phi, \tag{1.3}$$

and $\delta_\phi E$ denotes the variational derivative with respect to ϕ. Both the phase field ϕ and the chemical potential, μ, are assumed to be Ω-periodic. Because the dynamical equations are of gradient type, it is easy to see that the energy (1.1) is non-increasing in time along the solution trajectories of (1.2). Equation (1.2) is a mass conservative equation where the flux is proportional to the gradient of the chemical potential. This, along with the periodic boundary conditions, ensures that $\int_\Omega\partial_t\phi\, d\mathbf{x}=0$.

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The convex-splitting scheme, which was originated by Eyre's pioneering work [26], treats the convex terms of μ implicitly and the concave terms explicitly, resulting in

$$\phi^{m+1}-\phi^m = s\Delta\mu^{m+1}, \quad \mu^{m+1} := \left(\phi^{m+1}\right)^3 - \phi^m - \varepsilon^2\Delta\phi^{m+1}, \tag{1.4}$$

where $s>0$ is the time step-size. See the related works for the phase field crystal (PFC) equation [35, 48], the modified phase field crystal (MPFC) equation [6, 7, 44, 45], epitaxial thin film growth models [12, 14, 41, 43], the Cahn–Hilliard–Hele–Shaw (CHHS) and related models [13, 18, 19, 30, 46]. All these convex splitting schemes have two important properties: unconditional energy stability and unconditionally unique solvability. These references describe both first and second order temporal splittings, the latter being an important extension of Eyre's general first-order framework. In particular, numerical experiments [6, 7, 12, 14, 33, 35, 41] have shown a great advantage of the second order splitting over the standard first order one in terms of numerical efficiency and accuracy.

In addition to the first order accurate (in time) schemes for the Cahn–Hilliard equation [3,5,21,23–25,27,29,31,32,34,37–40,47], there have also been extensive research works deriving and analyzing second order (in time) schemes [4, 20, 22, 31, 42]. Among the existing works, the secant-type algorithm [20, 31] is worthy of a detailed discussion. With the notation $\Psi(\phi) := \frac{1}{4}\phi^4 - \frac{1}{2}\phi^2$, the scheme may be formulated as

$$\phi^{m+1}-\phi^m = s\Delta\mu^{m+1/2}\ , \quad \mu^{m+1/2} := \frac{\Psi(\phi^{m+1})-\Psi(\phi^m)}{\phi^{m+1}-\phi^m} - \frac{\varepsilon^2}{2}\left(\Delta\phi^{m+1}+\Delta\phi^m\right), \tag{1.5}$$

where again we have taken $\mathcal{M}\equiv 1$ for simplicity. A straightforward calculation shows that this one-step scheme is unconditionally energy stable. In particular, $E(\phi^{m+1}) + s\left\|\nabla\mu^{m+1/2}\right\|_{L^2}^2 = E(\phi^m)$. However, this scheme is not expected to be unconditionally uniquely solvable with respect to the size of s (see [20, 22, 31] for the details.) Lack of solvability may be problematic, since coarsening studies using the CH equation may involve very large time scales, requiring potentially very large time steps for efficiency. Moreover, the scheme does not result as the gradient of a strictly convex function – in contrast to the first-order convex splitting scheme popularized by Eyre (1.4) and the second-order convex splitting schemes in [7, 35, 41]. This point can have significant implications for solver efficiency.

In this paper, we propose and analyze a new second order convex splitting scheme for the CH equation (1.2). We will show that our scheme is uniquely solvable, resulting as the gradient of strictly convex functional, and unconditionally energy stable. We additionally demonstrate a discrete version of an $L^\infty(0,T;H^2)$ bound of the numerical solution. (For the discrete norms we use notation of the form $L_s^\infty(0,T;H_h^2)$, where s and h are the time and space step-sizes.) We show that this bound can be obtained independent of the final time T, remarkably, but dependent polynomially on ε^{-1}. With the help of this global in time $L_s^\infty(0,T;H_h^2)$ bound, we also obtain a bound of the numerical solution in the discrete $L_s^2(0,T;H_h^4)$, the latter of which does depend upon the final time, T. We conclude the theoretical analyses, with an $L_s^\infty(0,T;H_h^2)\cap L_s^2(0,T;H_h^4)$ convergence of the numerical solution, which, to our knowledge, is the first such result of its kind in this area. It is observed that such a convergence is unconditional (for the time step s in terms of the spatial grid size h); the nonlinear error estimate is feasible because of the global in time H_h^2 bound for the numerical solution. A cut-off approach for the numerical solution is not needed in this paper, compared to a few existing works [42].

In Section 2 we define the scheme and present the unique solvability and discrete-energy stability analyses of the proposed numerical scheme. Leveraging the energy stabilities, refined $L_s^\infty\left(0,T;H_h^2\right)$ and $L_s^\infty(0,T;L_h^\infty)$ stabilities of the scheme are proven in Section 3. In Section 4 we present the primary results of the paper, namely, an $L_s^\infty(0,T;H_h^2)\cap L_s^2(0,T;H_h^4)$ convergence analysis for the scheme. Some 3D numerical results are presented in Section 5. In the appendices we prove discrete versions of some standard Sobolev embedding and elliptic regularity results for periodic grid functions.

2. The numerical scheme and its unique solvability and energy stability

First, we introduce the finite difference spatial discretization.

2.1. Discretization of space. Here we use the notation and results for some discrete functions and operators from [46, 48]. We begin with the definitions of grid functions and difference operators needed for our discretization of three-dimensional space. We consider the domain $\Omega=(0,\mathcal{L}_x)\times(0,\mathcal{L}_y)\times(0,\mathcal{L}_z)$ and assume that N_x, N_y and N_z are positive integers such that $h=\mathcal{L}_x/N_x=\mathcal{L}_y/N_y=\mathcal{L}_z/N_z$, for some $h>0$, which we refer to as the spatial step-size. For any positive integer N, consider the following sets

$$\mathcal{E}_N:=\{i\cdot h \mid i=0,\ldots,N\}, \qquad \mathcal{C}_N:=\{(i-1/2)\cdot h \mid i=1,\ldots,N)\}, \tag{2.1}$$

$$\mathcal{C}_{\overline{N}}:=\{(i-1/2)\cdot h \mid i=0,\ldots,N+1)\}. \tag{2.2}$$

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

$$\mathcal{C}_\Omega:=\{\phi:\mathcal{C}_{\overline{N}_x}\times\mathcal{C}_{\overline{N}_y}\times\mathcal{C}_{\overline{N}_z}\to\mathbb{R}\}, \qquad \mathcal{E}_\Omega^x:=\{\phi:\mathcal{E}_{N_x}\times\mathcal{C}_{N_y}\times\mathcal{C}_{N_z}\to\mathbb{R}\}, \tag{2.3}$$

$$\mathcal{E}_\Omega^y:=\{\phi:\mathcal{E}_{N_x}\times\mathcal{E}_{N_y}\times\mathcal{C}_{N_z}\to\mathbb{R}\}, \qquad \mathcal{E}_\Omega^z:=\{\phi:\mathcal{E}_{N_x}\times\mathcal{C}_{N_y}\times\mathcal{E}_{N_z}\to\mathbb{R}\}, \tag{2.4}$$

$$\vec{\mathcal{E}}_\Omega:=\mathcal{E}_\Omega^x\times\mathcal{E}_\Omega^y\times\mathcal{E}_\Omega^z. \tag{2.5}$$

The functions of $\mathcal{C}_\Omega$ are called *c*ell 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 $\mathcal{E}_\Omega^x$, *et cetera*, are called edge-centered functions. In component form, edge-centered functions are identified via $f_{i+\frac{1}{2},j,k}:=f(\xi_{i+1/2},\xi_j,\xi_k)$, *et cetera.*

A discrete function $\phi\in\mathcal{C}_\Omega$ is said to satisfy periodic boundary conditions if and only if at the ghost points ϕ satisfies

$$\phi_{N_x,j,k}=\phi_{0,j,k}, \quad \phi_{N_x+1,j,k}=\phi_{1,j,k}, \tag{2.6}$$

$$\phi_{i,N_y,k}=\phi_{i,0,k}, \quad \phi_{i,N_y+1,k}=\phi_{i,1,k}, \tag{2.7}$$

$$\phi_{i,j,N_z}=\phi_{i,j,0}, \quad \phi_{i,j,N_z+1}=\phi_{i,j,1}. \tag{2.8}$$

Subsequently, the discrete operators, inner products and norms could be defined in an appropriate way. We introduce the edge-to-center difference operator $d_x:\mathcal{E}_\Omega^x\to\mathcal{C}_\Omega$, defined component-wise via

$$d_x f_{i,j,k}:=\frac{1}{h}(f_{i+\frac{1}{2},j,k}-f_{i-\frac{1}{2},j,k}), \tag{2.9}$$

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

$$\nabla_h\cdot\boldsymbol{f}:=d_x f^x+d_y f^y+d_z f^z, \tag{2.10}$$

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

$$A_x\phi_{i+\frac{1}{2},j,k}:=\frac{1}{2}(\phi_{i,j,k}+\phi_{i+1,j,k}), \tag{2.11}$$

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

$$A_h\phi:=(A_x\phi,A_y\phi,A_z\phi)^T. \tag{2.12}$$

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

$$D_x\phi_{i+\frac{1}{2},j,k}:=\frac{1}{h}(\phi_{i+1,j,k}-\phi_{i,j,k}). \tag{2.13}$$

$D_y:\mathcal{C}_\Omega\to\mathcal{E}_\Omega^y$ 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

$$\nabla_h\phi:=(D_x\phi,D_y\phi,D_z\phi)^T. \tag{2.14}$$

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

$$\Delta_h\phi:=\nabla_h\cdot\nabla_h\phi. \tag{2.15}$$

We define the following inner products:

$$(\phi,\psi):=h^3\sum_{i=1}^{L}\sum_{j=1}^{M}\sum_{k=1}^{m}\phi_{i,j,k}\psi_{i,j,k}, \qquad \forall\ \phi,\psi\in\mathcal{C}_\Omega, \tag{2.16}$$

$$[f,g]_x:=\frac{1}{2}h^3\sum_{i=1}^{L}\sum_{j=1}^{M}\sum_{k=1}^{m}(f_{i+\frac{1}{2},j,k}g_{i+\frac{1}{2},j,k}+f_{i-\frac{1}{2},j,k}g_{i-\frac{1}{2},j,k}), \quad \forall\ f,g\in\mathcal{E}_\Omega^x. \tag{2.17}$$

$[\cdot,\cdot]_y$ and $[\cdot,\cdot]_z$ can be formulated analogously. For $\phi,\psi\in\mathcal{C}_\Omega$, a natural discrete inner product of their gradients is given by

$$(\nabla_h\phi,\nabla_h\psi):=[D_x\phi,D_x\psi]_x+[D_y\phi,D_y\psi]_y+[D_z\phi,D_z\psi]_z. \tag{2.18}$$

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

$$\|\phi\|_\infty:=\max_{i,j,k}|\phi_{i,j,k}|, \tag{2.19}$$

$$\|\phi\|_p:=(|\phi|^p,1)^{\frac{1}{p}}, \qquad 1\le p<\infty. \tag{2.20}$$

In addition, we define

$$\|\nabla_h\phi\|_p:=\left([|D_x\phi|^p,1]_x+[|D_y\phi|^p,1]_y+[|D_z\phi|^p,1]_z\right)^{\frac{1}{p}}. \tag{2.21}$$

In the case of $p=2$, it is clear that $(\nabla_h\phi,\nabla_h\phi)=\|\nabla_h\phi\|_2^2$. In addition, the discrete $\|\cdot\|_{H_h^1}$, $\|\cdot\|_{H_h^2}$ and $\|\cdot\|_{H_h^4}$ norms are defined as

$$\|f\|_{H_h^1}^2:=\|f\|_2^2+\|\nabla_h\phi\|_2^2, \tag{2.22}$$

$$\|f\|_{H_h^2}^2:=\|f\|_{H_h^1}^2+\|\Delta_h^x\phi\|_2^2+\|\Delta_h^y\phi\|_2^2+\|\Delta_h^z\phi\|_2^2+\|\Delta_h\phi\|_2^2, \tag{2.23}$$

$$\|f\|_{H_h^4}^2:=\|f\|_{H_h^2}^2+\|\nabla_h\Delta_h\phi\|_2^2+\left\|\Delta_h^2\phi\right\|_2^2. \tag{2.24}$$

It is observed that, for $\phi,\psi\in\mathcal{C}_\Omega$ satisfying the periodic boundary conditions, the following summation by parts formulas can be derived:

$$(\phi,\Delta_h\psi)=-(\nabla_h\phi,\nabla_h\psi), \quad \left(\phi,\Delta_h^2\psi\right)=(\Delta_h\phi,\Delta_h\psi). \tag{2.25}$$

2.2. The fully discrete numerical scheme. Let $M\in\mathbb{Z}^+$, and set $s:=T/M$, where T is the final time. Our second order convex splitting scheme can be formulated as follows: for $0\le m\le M-1$, given $\phi^m,\phi^{m-1}\in\mathcal{C}_\Omega$, find $\phi^{m+1},\mu^{m+1/2}\in\mathcal{C}_\Omega$ periodic such that

$$\phi^{m+1}-\phi^m=s\nabla_h\cdot\left(\mathcal{M}\left(A_h\tilde{\phi}^{m+1/2}\right)\nabla_h\mu^{m+1/2}\right), \tag{2.26}$$

where

$$\mu^{m+1/2}:=\chi\left(\phi^{m+1},\phi^m\right)-\tilde{\phi}^{m+1/2}-\varepsilon^2\Delta_h\hat{\phi}^{m+1/2}, \tag{2.27}$$

$$\chi\left(\phi^{m+1},\phi^m\right):=\frac{1}{4}\left(\phi^{m+1}+\phi^m\right)\left(\left(\phi^{m+1}\right)^2+\left(\phi^m\right)^2\right), \tag{2.28}$$

$$\tilde{\phi}^{m+1/2}:=\frac{3}{2}\phi^m-\frac{1}{2}\phi^{m-1}, \tag{2.29}$$

$$\hat{\phi}^{m+1/2}:=\frac{3}{4}\phi^{m+1}+\frac{1}{4}\phi^{m-1}. \tag{2.30}$$

We define $\phi^{-1}\equiv\phi^0$. The local truncation error of this scheme is second-order with respect to time, provided the time step-size s is invariant and $m\ge 1$. When $m=0$, the truncation error reduces to first-order, but this doesn't spoil the overall second-order accuracy of the scheme, as will be shown in later sections.

REMARK 2.1. We could, alternatively, define a different scheme for the first step. For example, the following has a second-order in time local truncation error and is also unconditionally energy stable and unconditionally uniquely solvable (over the single time step):

$$\phi^1-\phi^0=s\nabla_h\cdot\left(\mathcal{M}\left(A_h\tilde{\phi}^{1/2}\right)\nabla_h\mu^{1/2}\right), \tag{2.31}$$

$$\mu^{1/2}:=\chi\left(\phi^1,\phi^0\right)-\tilde{\phi}^{1/2}-\varepsilon^2\Delta_h\hat{\phi}^{1/2}, \tag{2.32}$$

$$\chi\left(\phi^1,\phi^0\right):=\frac{1}{4}\left(\phi^1+\phi^0\right)\left(\left(\phi^1\right)^2+\left(\phi^0\right)^2\right), \tag{2.33}$$

$$\tilde{\phi}^{1/2}:=\phi^0+\frac{s}{2}\nabla_h\cdot\left(\mathcal{M}\left(A_h\phi^0\right)\nabla_h\mu^0\right), \tag{2.34}$$

$$\mu^0:=(\phi^0)^3-\phi^0-\varepsilon^2\Delta_h\phi^0,\quad \hat{\phi}^{1/2}:=\frac{1}{2}\phi^1+\frac{1}{2}\phi^0. \tag{2.35}$$

Apart from its increased accuracy, this scheme has some other advantages over the simpler choice above – *i.e.*, the order reducing assignment $\phi^{-1}\equiv\phi^0$ – as we point out later. However, the choice $\phi^{-1}\equiv\phi^0$ simplifies the stability analyses greatly.

Because we use a convex splitting approach, it is easy to prove that the scheme is uniquely solvable for any time step.

THEOREM 2.2. *The second-order scheme* (2.26) *is uniquely solvable for any time step-size $s>0$, and, in particular, the scheme results from the minimization of a strictly convex functional. Moreover, it is discretely mass conserving,* i.e., $\left(\phi^{m+1}-\phi^m,1\right)=0$, *for all $0\le m\le M-1$.*

We now define a fully discrete energy that is consistent with the continuous space energy (1.1) as $h\to 0$. In particular, the discrete energy $F:\mathcal{C}_\Omega\to\mathbb{R}$ is

$$F(\phi):=\frac{1}{4}\|\phi\|_4^4-\frac{1}{2}\|\phi\|_2^2+\frac{\varepsilon^2}{2}\|\nabla_h\phi\|_2^2. \tag{2.36}$$

As in [46, 48], if $\phi \in \mathcal{C}_\Omega$ is periodic, then the energies $F_c(\phi) = \frac{1}{4}\|\phi\|_4^4 + \frac{\varepsilon^2}{2}\|\nabla_h \phi\|_2^2$ and $F_e(\phi) = \frac{1}{2}\|\phi\|_2^2$ are convex. Hence F, as defined in (2.36), admits the convex splitting $F = F_c - F_e$. We can not guarantee that the energy F is non-increasing in time, but, we can guarantee the dissipation of another modified energy. To be precise, for all $\psi, \phi \in \mathcal{C}_\Omega$, define an alternate numerical energy via

$$\widetilde{F}(\phi,\psi) := F(\phi) + \frac{1}{4}\|\phi - \psi\|_2^2 + \frac{\varepsilon^2}{8}\|\nabla_h(\phi - \psi)\|_2^2. \tag{2.37}$$

Note that this energy is consistent with the continuous space energy (1.1). For example, suppose that $u: \Omega \times [0,T] \to \mathbb{R}$ is a sufficiently regular, Ω-periodic function. Define – for our present and future use – the canonical grid projection operator $\mathsf{P}_h : C^0(\Omega) \to \mathcal{C}_\Omega$ via $[\mathsf{P}_h v]_{i,j,k} = v(\xi_i, \xi_j, \xi_k)$. Set $u_{h,s} := \mathsf{P}_h u(\cdot, t_0 + s)$. Then, clearly, $\widetilde{F}(u_{h,0}, u_{h,s}) \to E(u(\cdot, t_0))$, as $s \to 0$ and $h \to 0$.

Theorem 2.3. *Suppose that $\phi^{m+1}, \phi^m, \phi^{m-1} \in \mathcal{C}_\Omega$ are periodic solutions to (2.26). The second-order scheme (2.26) is unconditionally energy stable with respect to (2.37), meaning that for any time step-size $s > 0$ and any $0 \le m \le M-1$, $\widetilde{F}(\phi^{m+1}, \phi^m) \le \widetilde{F}(\phi^m, \phi^{m-1})$. More precisely,*

$$\widetilde{F}(\phi^{m+1},\phi^m) + s\left\|\sqrt{\mathcal{M}\left(A_h \tilde{\phi}^{m+1/2}\right)}\nabla_h \mu^{m+1/2}\right\|_2^2 + R\left(\widetilde{\Delta}_s \phi^m\right) = \widetilde{F}(\phi^m, \phi^{m-1}), \tag{2.38}$$

where the non-negative remainder term is

$$R\left(\widetilde{\Delta}_s \phi^m\right) := \frac{\varepsilon^2}{8}\left\|\nabla_h\left(\widetilde{\Delta}_s \phi^m\right)\right\|_2^2 + \frac{1}{4}\left\|\widetilde{\Delta}_s \phi^m\right\|_2^2, \tag{2.39}$$

with $\widetilde{\Delta}_s \phi^m := \phi^{m+1} - 2\phi^m + \phi^{m-1}$, and where

$$\begin{aligned}\left\|\sqrt{\mathcal{M}\left(A_h \tilde{\phi}^{m+1/2}\right)}\nabla_h \mu^{m+1/2}\right\|_2^2 := &\left[D_x \mu^{m+1/2}, \mathcal{M}\left(A_x \tilde{\phi}^{m+1/2}\right) D_x \mu^{m+1/2}\right]_x \\ &+ \left[D_y \mu^{k+1/2}, \mathcal{M}\left(A_y \tilde{\phi}^{m+1/2}\right) D_y \mu^{m+1/2}\right]_y \\ &+ \left[D_z \mu^{k+1/2}, \mathcal{M}\left(A_z \tilde{\phi}^{m+1/2}\right) D_z \mu^{m+1/2}\right]_z.\end{aligned} \tag{2.40}$$

Proof. The result follows readily by *(i)* testing (2.26) by $\mu^{m+1/2}$ and (2.27) by $\phi^{m+1} - \phi^m$, *(ii)* summing over the three-dimensional grid, *(iii)* adding the respective equations, and *(iv)* using the summation-by-parts formulas from Subsection 2.1 together with the periodic boundary conditions. We omit the details for the sake of brevity. □

From the energy stability – with respect to discrete energy (2.37) – we immediately obtain the following norm stabilities.

Corollary 2.4. *Suppose that $\psi \in C^4_{\text{per}}(\Omega)$, and $\phi^0 := \mathsf{P}_h \psi \in \mathcal{C}_\Omega$. Assume that there is some $\mathcal{M}_0 > 0$ such that $\mathcal{M}(s) \ge \mathcal{M}_0$, for all $s \in \mathbb{R}$. Then with the same hypotheses as in the last theorem, we have the following stabilities*

$$\|\nabla_h \phi\|^2_{L_s^\infty(0,T;L_h^2)} := \max_{0 \le m \le M} \|\nabla_h \phi^m\|_2^2 \le C_1, \tag{2.41}$$

$$\|\phi\|^2_{L^\infty_s(0,T;L^4_h)} := \max_{0\le m\le M} \|\phi^m\|_4^2 \le C_2, \tag{2.42}$$

$$\|\phi\|^2_{L^\infty_s(0,T;H^1_h)} := \max_{0\le m\le M} \|\phi^m\|_{H^1_h}^2 \le C_3, \tag{2.43}$$

$$\|\nabla_h\mu\|^2_{L^2_s(0,T;L^2_h)} := s\sum_{m=0}^{M-1} \left\|\nabla_h\mu^{m+1/2}\right\|_2^2 \le C_4, \tag{2.44}$$

where $C_1,\dots,C_4$ are positive constants independent of h, s, and T.

Proof. By consistency,

$$F(\phi^0) \le E(\psi) + C =: C_0, \tag{2.45}$$

where $C>0$ is a constant that is independent of h. By the last theorem and the definition of the numerical energy (2.37), for any $1\le m\le M$, we have

$$F(\phi^m) \le \widetilde{F}(\phi^{m+1},\phi^m) \le \cdots \le \widetilde{F}(\phi^0,\phi^{-1}) = F(\phi^0) \le C_0, \tag{2.46}$$

where we have used $\phi^{-1}\equiv\phi^0$. Now, we use the fact that, for any $\phi\in\mathcal{C}_\Omega$,

$$\frac{1}{2}\|\phi\|_2^2 + \frac{\varepsilon^2}{2}\|\nabla_h\phi\|_2^2 - |\Omega| \le F(\phi), \tag{2.47}$$

to arrive at the norm stabilities (2.41)–(2.43). Summing (2.38) and using the positivity of the mobility and the non-negativity of the remainder term, we have

$$\widetilde{F}\left(\phi^M,\phi^{M-1}\right) + s\mathcal{M}_0\sum_{m=0}^{M-1}\left\|\nabla_h\mu^{m+1/2}\right\|_2^2 \le \widetilde{F}\left(\phi^0,\phi^{-1}\right) \le C_0, \tag{2.48}$$

from which we obtain (2.44). □

REMARK 2.5. The mobility function $\mathcal{M}(\cdot)$ may be truly degenerate in certain physical models, i.e., $\mathcal{M}(\cdot)\ge 0$ with $\mathcal{M}(\phi)=0$ for certain values of ϕ. The uniform in time $L^\infty_s(0,T;H^1_h)$ stability estimates (2.41), (2.43) and the $L^\infty_s(0,T;L^4_h)$ estimate (2.42) are still valid in this case. On the other hand, it is observed that the $L^2_s(0,T;L^2_h)$ estimate (2.44) for $\nabla_h\mu$ has to be derived under a non-degenerate condition for the mobility function: $\mathcal{M}(\phi)\ge\mathcal{M}_0>0$ at a point-wise level, for some positive number $\mathcal{M}_0$.

3. $L^\infty_s\left(0,T;H^2_h\right)$ and $L^\infty_s\left(0,T;L^\infty_h\right)$ stabilities of the scheme

We note that the $L^\infty_s(0,T;H^1_h)$ stability of the scheme obtained in the last section is not sufficient to recover an $L^\infty_s(0,T;L^\infty_h)$ bound of the numerical solution. We need an $L^\infty_s(0,T;H^2_h)$ bound to obtain point-wise control of the numerical approximation, and this is the goal of the present section. The following estimates are crucial to deriving the $L^\infty_s(0,T;H^2_h)$ stability and convergence analyses in this and later sections.

The proofs of the following estimates are contained in Section B.

LEMMA 3.1. *Suppose that $\phi\in\mathcal{C}_\Omega$. If ϕ and $\Delta_h\phi$ are periodic, as defined in* (2.6)–(2.8), *then we have*

$$\|\phi\|_{H^2_h} \le C_5\left(\|\phi\|_{H^1_h}^{\frac{2}{3}}\left\|\Delta_h^2\phi\right\|_2^{\frac{1}{3}} + \|\phi\|_{H^1_h}\right), \tag{3.1}$$

$$\|\phi\|_{H^2_h} \le C_6\left(\|\phi\|_2 + \|\Delta_h\phi\|_2\right), \tag{3.2}$$

$$\|\phi\|_{H^4_h} \le C_7\left(\|\phi\|_2 + \left\|\Delta_h^2\phi\right\|_2\right), \tag{3.3}$$

$$\left\|\phi-\bar{\phi}\right\|_{H_h^2} \leq C_8 \left\|\Delta_h \phi\right\|_2, \tag{3.4}$$

$$\|\phi\|_\infty \leq C_9 \|\phi\|_{H_h^2}, \tag{3.5}$$

$$\|\phi\|_\infty \leq C_{10} \left(\|\phi\|_{H_h^1}^{\frac{5}{6}} \left\|\Delta_h^2 \phi\right\|_2^{\frac{1}{6}} + \|\phi\|_{H_h^1} \right), \tag{3.6}$$

$$\|\nabla_h \phi\|_\infty \leq C_{11} \|\phi\|_{H_h^1}^{\frac{1}{2}} \left\|\Delta_h^2 \phi\right\|_2^{\frac{1}{2}}, \tag{3.7}$$

$$\|\nabla_h \phi\|_4 \leq C_{12} \|\phi\|_{H_h^2}, \tag{3.8}$$

$$\|\Delta_h \phi\|_2 \leq C_{13} \left\|\Delta_h^2 \phi\right\|_2, \tag{3.9}$$

where $C_i > 0$, $5 \leq i \leq 13$, are constants independent of h, and $\bar{\phi} := \frac{1}{|\Omega|}(\phi,1)$ is the discrete average.

THEOREM 3.2. *For simplicity, suppose that $\mathcal{M}(s) \equiv 1$. Assume that the hypotheses of Theorem 2.3 and Corollary 2.4 hold. Then, if $s \leq 176C_{13}^2/45\varepsilon^2$, we have*

$$\|\phi\|_{L_s^\infty(0,T;H_h^2)}^2 := \max_{0 \leq m \leq M} \|\phi^m\|_{H_h^2}^2 \leq C_{14}, \tag{3.10}$$

$$\|\phi\|_{L_s^2(0,T;H_h^4)}^2 := s \sum_{m=1}^{M} \|\phi^m\|_{H_h^4}^2 \leq C_{15}(T+1), \tag{3.11}$$

where $C_{14}, C_{15} > 0$ are constants independent of h, s, and T.

Proof. Since $\mathcal{M} \equiv 1$, the scheme (2.26) may be written as

$$\phi^{m+1} - \phi^m = s\Delta_h \left(\chi(\phi^{m+1},\phi^m) - \tilde{\phi}^{m+1/2} - \varepsilon^2 \Delta_h \hat{\phi}^{m+1/2} \right). \tag{3.12}$$

Taking the discrete inner product with (3.12) by $\Delta_h^2 \phi^{m+1}$ gives

$$\begin{aligned} &\left(\phi^{m+1} - \phi^m, \Delta_h^2 \phi^{m+1}\right) + s\left(\Delta_h^2 \phi^{m+1}, \Delta_h \tilde{\phi}^{m+1/2}\right) \\ &\quad - s\left(\Delta_h^2 \phi^{m+1}, \Delta_h \chi(\phi^{m+1},\phi^m)\right) + \varepsilon^2 s \left(\Delta_h^2 \phi^{m+1}, \Delta_h^2 \hat{\phi}^{m+1/2}\right) = 0. \end{aligned} \tag{3.13}$$

An application of summation-by-parts using periodic boundary conditions yields

$$\begin{aligned} \left(\phi^{m+1} - \phi^m, \Delta_h^2 \phi^{m+1}\right) &= \left(\Delta_h(\phi^{m+1} - \phi^m), \Delta_h \phi^{m+1}\right) \\ &= \frac{1}{2}\left(\left\|\Delta_h \phi^{m+1}\right\|_2^2 - \|\Delta_h \phi^m\|_2^2 \right) + \frac{1}{2}\left\|\Delta_h(\phi^{m+1} - \phi^m)\right\|_2^2. \end{aligned} \tag{3.14}$$

For the concave diffusion term, we have

$$\begin{aligned} -\left(\Delta_h^2 \phi^{m+1}, \Delta_h \tilde{\phi}^{m+1/2}\right) &\leq \alpha \left\|\Delta_h^2 \phi^{m+1}\right\|_2^2 + \frac{1}{4\alpha}\left\|\Delta_h \tilde{\phi}^{m+1/2}\right\|_2^2 \\ &\leq \alpha \left\|\Delta_h^2 \phi^{m+1}\right\|_2^2 + \frac{9}{8\alpha}\|\Delta_h \phi^m\|_2^2 + \frac{1}{8\alpha}\left\|\Delta_h \phi^{m-1}\right\|_2^2, \end{aligned} \tag{3.15}$$

for any $\alpha > 0$. Meanwhile, the quantities $\|\Delta_h \phi^m\|_2^2$, $\left\|\Delta_h \phi^{m-1}\right\|_2^2$ can be controlled by

$$\left\|\Delta_h \phi^\ell\right\|_2^2 \leq \frac{1}{4\alpha^2}\left\|\phi^\ell\right\|_2^2 + \alpha^2 \left\|\Delta_h^2 \phi^\ell\right\|_2^2 \leq \frac{C_3}{4\alpha^2} + \alpha^2 \left\|\Delta_h^2 \phi^\ell\right\|_2^2, \tag{3.16}$$

for any $\alpha > 0$, for $\ell = m, m-1$. A combination of (3.15) and (3.16) shows that

$$-\left(\Delta_h^2\phi^{m+1},\Delta_h\tilde{\phi}^{m+1/2}\right)\le\alpha\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{9\alpha}{8}\left\|\Delta_h^2\phi^m\right\|_2^2 \tag{3.17}$$

$$+\frac{\alpha}{8}\left\|\Delta_h^2\phi^{m-1}\right\|_2^2+\frac{5C_3}{16\alpha^3}, \tag{3.18}$$

which holds for any $\alpha>0$.

The bi-harmonic diffusion term can be analyzed as follows:

$$\begin{aligned}\left(\Delta_h^2\phi^{m+1},\Delta_h^2\hat{\phi}^{m+1/2}\right)&=\frac{3}{4}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{1}{4}\left(\Delta_h^2\phi^{m+1},\Delta_h^2\phi^{m-1}\right)\\&\ge\frac{3}{4}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2-\frac{1}{4}\left(\frac{1}{2}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{1}{2}\left\|\Delta_h^2\phi^{m-1}\right\|_2^2\right)\\&\ge\frac{5}{8}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2-\frac{1}{8}\left\|\Delta_h^2\phi^{m-1}\right\|_2^2.\end{aligned} \tag{3.19}$$

Regarding the nonlinear term, we begin with the following inequality:

$$\left(\Delta_h^2\phi^{m+1},\Delta_h\chi(\phi^{m+1},\phi^m)\right)\le\left\|\Delta_h^2\phi^{m+1}\right\|_2\cdot\left\|\Delta_h\chi(\phi^{m+1},\phi^m)\right\|_2. \tag{3.20}$$

The rest work is focused on obtaining a useful estimate for $\left\|\Delta_h\chi(\phi^{m+1},\phi^m)\right\|_2$. Detailed expansions and several applications of the discrete Hölder inequality yields

$$\begin{aligned}\|\Delta_h(fgh)\|_2\le C\Big(&\|f\|_\infty\cdot\|g\|_\infty\cdot\|h\|_{H_h^2}+\|f\|_\infty\cdot\|h\|_\infty\cdot\|g\|_{H_h^2}\\&+\|g\|_\infty\cdot\|h\|_\infty\cdot\|f\|_{H_h^2}+\|f\|_\infty\cdot\|\nabla_h g\|_\infty\cdot\|\nabla_h h\|_2\\&+\|g\|_\infty\cdot\|\nabla_h f\|_\infty\cdot\|\nabla_h h\|_2+\|h\|_\infty\cdot\|\nabla_h f\|_\infty\cdot\|\nabla_h g\|_2\Big).\end{aligned} \tag{3.21}$$

An expansion of $\chi(\phi^{m+1},\phi^m)$, combined with the last inequality, results in

$$\begin{aligned}&\left\|\Delta_h\chi(\phi^{m+1},\phi^m)\right\|_2\\&\le C\left(\left\|\phi^{m+1}\right\|_\infty+\|\phi^m\|_\infty\right)\cdot\left(\left\|\nabla_h\phi^{m+1}\right\|_\infty+\|\nabla_h\phi^m\|_\infty\right)\cdot\left(\left\|\phi^{m+1}\right\|_{H_h^1}+\|\phi^m\|_{H_h^1}\right)\\&\quad+C\left(\left\|\phi^{m+1}\right\|_\infty^2+\|\phi^m\|_\infty^2\right)\cdot\left(\left\|\phi^{m+1}\right\|_{H_h^2}+\|\phi^m\|_{H_h^2}\right)\\&\le C_{16}\left(\left\|\phi^{m+1}\right\|_\infty+\|\phi^m\|_\infty\right)\cdot\left(\left\|\nabla_h\phi^{m+1}\right\|_\infty+\|\nabla_h\phi^m\|_\infty\right)\\&\quad+C_{17}\left(\left\|\phi^{m+1}\right\|_\infty^2+\|\phi^m\|_\infty^2\right)\cdot\left(\left\|\phi^{m+1}\right\|_{H_h^2}+\|\phi^m\|_{H_h^2}\right),\end{aligned} \tag{3.22}$$

where $C_{16},C_{17}>0$ are constants. The uniform in time H_h^1 estimate (2.43), combined with the 3D discrete Sobolev inequality (3.1), and the discrete Gagliardo–Nirenberg type inequalities (3.6) and (3.7), yields

$$\left\|\phi^\ell\right\|_{H_h^2}\le C_5\left(\left\|\phi^\ell\right\|_{H_h^1}^{\frac{2}{3}}\left\|\Delta_h^2\phi^\ell\right\|_2^{\frac{1}{3}}+\left\|\phi^\ell\right\|_{H_h^1}\right)\le C_5\left(C_3^{\frac{1}{3}}\cdot\left\|\Delta_h^2\phi^\ell\right\|_2^{\frac{1}{3}}+C_3^{\frac{1}{2}}\right), \tag{3.23}$$

$$\left\|\phi^\ell\right\|_\infty\le C_{10}\left(\left\|\phi^\ell\right\|_{H_h^1}^{\frac{5}{6}}\left\|\Delta_h^2\phi^\ell\right\|_2^{\frac{1}{6}}+\left\|\phi^\ell\right\|_{H_h^1}\right)\le C_{10}\left(C_3^{\frac{5}{12}}\cdot\left\|\Delta_h^2\phi^\ell\right\|_2^{\frac{1}{6}}+C_3^{\frac{1}{2}}\right), \tag{3.24}$$

$$\left\|\nabla_h\phi^\ell\right\|_\infty\le C_{11}\left\|\phi^\ell\right\|_{H_h^1}^{\frac{1}{2}}\left\|\Delta_h^2\phi^\ell\right\|_2^{\frac{1}{2}}\le C_{11}C_3^{\frac{1}{4}}\cdot\left\|\Delta_h^2\phi^\ell\right\|_2^{\frac{1}{2}}, \tag{3.25}$$

for $\ell=m,m+1$. Going back to (3.22), we arrive at

$$\begin{aligned}
&\left\|\Delta_h\chi(\phi^{m+1},\phi^m)\right\|_2\\
&\le C_{18}\left(\left\|\Delta_h^2\phi^{m+1}\right\|_2^{\frac{2}{3}}+\left\|\Delta_h^2\phi^m\right\|_2^{\frac{2}{3}}\right)+C_{19}\left(\left\|\Delta_h^2\phi^{m+1}\right\|_2^{\frac{1}{3}}+\left\|\Delta_h^2\phi^m\right\|_2^{\frac{1}{3}}\right)\\
&\qquad C_{20}\left(\left\|\Delta_h^2\phi^{m+1}\right\|_2^{\frac{1}{2}}+\left\|\Delta_h^2\phi^m\right\|_2^{\frac{1}{2}}\right)+C_{21},
\end{aligned}\tag{3.26}$$

where $C_{18},\ldots,C_{21}>0$ are constants that depend upon C_3, C_5, C_{10}, C_{11}, C_{16}, and C_{17}. The combination of this last estimate with (3.20) leads to

$$\begin{aligned}
&\left(\Delta_h^2\phi^{m+1},\Delta_h\chi(\phi^{m+1},\phi^m)\right)\\
&\le C_{18}\left(\left\|\Delta_h^2\phi^{m+1}\right\|_2^{\frac{5}{3}}+\left\|\Delta_h^2\phi^{m+1}\right\|_2\cdot\left\|\Delta_h^2\phi^m\right\|_2^{\frac{2}{3}}\right)\\
&\quad+C_{19}\left(\left\|\Delta_h^2\phi^{m+1}\right\|_2^{\frac{4}{3}}+\left\|\Delta_h^2\phi^{m+1}\right\|_2\cdot\left\|\Delta_h^2\phi^m\right\|_2^{\frac{1}{3}}\right)\\
&\quad+C_{20}\cdot\left(\left\|\Delta_h^2\phi^{m+1}\right\|_2^{\frac{3}{2}}+\left\|\Delta_h^2\phi^{m+1}\right\|_2\cdot\left\|\Delta_h^2\phi^m\right\|_2^{\frac{1}{2}}\right)+C_{21}\left\|\Delta_h^2\phi^{m+1}\right\|_2\\
&\le C_{22}(\alpha)+\alpha\left(\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\left\|\Delta_h^2\phi^m\right\|_2^2\right),
\end{aligned}\tag{3.27}$$

for all $\alpha>0$, where $C_{22}>0$ depends upon α and $C_{18},\ldots,C_{21}$.

A combination of (3.13), (3.14), (3.18), (3.19) and (3.27) results in

$$\begin{aligned}
&\left\|\Delta_h\phi^{m+1}\right\|_2^2-\left\|\Delta_h\phi^m\right\|_2^2+\left(\frac{5\varepsilon^2}{4}-4\alpha\right)s\left\|\Delta_h^2\phi^{m+1}\right\|_2^2\\
&\le\frac{17\alpha}{4}s\left\|\Delta_h^2\phi^m\right\|_2^2+\left(\frac{\varepsilon^2}{4}+\frac{\alpha}{4}\right)s\left\|\Delta_h^2\phi^{m-1}\right\|_2^2+\left(2C_{22}(\alpha)+\frac{5C_3}{8\alpha^3}\right)s.
\end{aligned}\tag{3.28}$$

Choosing $\alpha=\frac{1}{16}\varepsilon^2$ fixes C_{22} and yields

$$\left\|\Delta_h\phi^{m+1}\right\|_2^2-\left\|\Delta_h\phi^m\right\|_2^2+\varepsilon^2s\left\|\Delta_h^2\phi^{m+1}\right\|_2^2\le\frac{17\varepsilon^2}{64}s\left(\left\|\Delta_h^2\phi^m\right\|^2+\left\|\Delta_h^2\phi^{m-1}\right\|_2^2\right)+C_{23}s,\tag{3.29}$$

where $C_{23}>0$ is a constant. Now, adding $\frac{7\varepsilon^2}{16}\left\|\Delta_h^2\phi^m\right\|_2^2$ to both sides of the last inequality gives

$$\begin{aligned}
&\left\|\Delta_h\phi^{m+1}\right\|_2^2+\varepsilon^2s\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{7\varepsilon^2s}{16}\left\|\Delta_h^2\phi^m\right\|_2^2\\
&\le\left\|\Delta_h\phi^m\right\|_2^2+\frac{45\varepsilon^2s}{64}\left\|\Delta_h^2\phi^m\right\|_2^2+\frac{17\varepsilon^2s}{64}\left\|\Delta_h^2\phi^{m-1}\right\|_2^2+C_{23}s.
\end{aligned}\tag{3.30}$$

We define the "energy"

$$G^m:=\left\|\Delta_h\phi^m\right\|_2^2+\frac{45\varepsilon^2s}{64}\left\|\Delta_h^2\phi^m\right\|_2^2+\frac{17\varepsilon^2s}{64}\left\|\Delta_h^2\phi^{m-1}\right\|_2^2.\tag{3.31}$$

Then, it follows that

$$G^{m+1}+\frac{19\varepsilon^2s}{64}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{11\varepsilon^2s}{64}\left\|\Delta_h^2\phi^m\right\|_2^2\le G^m+C_{23}s.\tag{3.32}$$

Meanwhile, using estimate (3.9), we have

$$\begin{aligned}
&\frac{19\varepsilon^2}{64}s\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{11\varepsilon^2 s}{64}\left\|\Delta_h^2\phi^m\right\|_2^2\\
=&\frac{\varepsilon^2 s}{16}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{\varepsilon^2 s}{16}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{11\varepsilon^2 s}{64}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{11\varepsilon^2 s}{64}\left\|\Delta_h^2\phi^m\right\|_2^2\\
\geq&\frac{\varepsilon^2 s}{16}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{\varepsilon^2 s}{16C_{13}^2}\left\|\Delta_h\phi^{m+1}\right\|_2^2+\frac{11\varepsilon^2 s}{64}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{11\varepsilon^2 s}{64}\left\|\Delta_h^2\phi^m\right\|_2^2\\
=&\frac{\varepsilon^2 s}{16}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{\varepsilon^2 s}{16C_{13}^2}\left\{\left\|\Delta_h\phi^{m+1}\right\|_2^2+\frac{11C_{13}^2}{4}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{11C_{13}^2}{4}\left\|\Delta_h^2\phi^m\right\|_2^2\right\}\\
\geq&\frac{\varepsilon^2 s}{16}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{\varepsilon^2 s}{16C_{13}^2}\left\{\left\|\Delta_h\phi^{m+1}\right\|_2^2+\frac{45\varepsilon^2 s}{64}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{17\varepsilon^2 s}{64}\left\|\Delta_h^2\phi^m\right\|_2^2\right\}\\
=&\frac{\varepsilon^2 s}{16}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+\frac{\varepsilon^2 s}{16C_{13}^2}G^{m+1}, \qquad (3.33)
\end{aligned}$$

provided that

$$s\leq\frac{176C_{13}^2}{\varepsilon^2}\cdot\min\left(\frac{1}{45},\frac{1}{17}\right)=\frac{176C_{13}^2}{45\varepsilon^2}. \qquad (3.34)$$

Note that the condition in (3.34) is very easily satisfied, as the bound on the right-hand side will typically be greater than 1. As a result, we arrive at

$$\left(1+\frac{\varepsilon^2 s}{16C_{13}^2}\right)G^{m+1}+\frac{\varepsilon^2 s}{16}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2\leq G^m+C_{23}s. \qquad (3.35)$$

Applying an induction argument with the last estimate, we find

$$\left(1+\frac{\varepsilon^2 s}{16C_{13}^2}\right)^{m+1}G^{m+1}+\frac{\varepsilon^2 s}{16}\sum_{j=1}^{m+1}\left\|\Delta_h^2\phi^j\right\|_2^2\leq G^0+C_{23}s\sum_{j=0}^{m}\left(1+\frac{\varepsilon^2 s}{16C_{13}^2}\right)^j. \qquad (3.36)$$

Hence

$$\begin{aligned}
G^{m+1}&\leq\left(1+\frac{\varepsilon^2 s}{16C_{13}^2}\right)^{-(m+1)}G^0+C_{23}\frac{s\sum_{j=0}^m\left(1+\frac{\varepsilon^2 s}{16C_{13}^2}\right)^j}{\left(1+\frac{\varepsilon^2 s}{16C_{13}^2}\right)^{m+1}}\\
&=\left(1+\frac{\varepsilon^2 s}{16C_{13}^2}\right)^{-(m+1)}G^0+C_{23}\frac{\left(1+\frac{\varepsilon^2 s}{16C_{13}^2}\right)^{m+1}-1}{\frac{\varepsilon^2}{16C_{13}^2}\left(1+\frac{\varepsilon^2 s}{16C_{13}^2}\right)^{m+1}}\\
&\leq\left(1+\frac{\varepsilon^2 s}{16C_{13}^2}\right)^{-(m+1)}G^0+\frac{16C_{23}C_{13}^2}{\varepsilon^2}\\
&\leq G^0+\frac{16C_{23}C_{13}^2}{\varepsilon^2}. \qquad (3.37)
\end{aligned}$$

In particular, we have

$$\left\|\phi^{m+1}\right\|_2^2+\left\|\Delta_h\phi^{m+1}\right\|_2^2\leq C_3+G^0+\frac{16C_{23}C_{13}^2}{\varepsilon^2}\leq C_{24}, \qquad (3.38)$$

using $\phi^{-1} \equiv \phi^0$ and the fact that G^0 is bounded independently of h by consistency. Observe that C_{25} is independent of h and the final time T. An application of the discrete elliptic regularity (3.2) leads to the following result:

$$\|\phi^m\|_{H_h^2}^2 \le C_6^2 (\|\phi^m\|_2 + \|\Delta_h \phi^m\|_2)^2 =: 2C_6^2 C_{24} =: C_{14}, \tag{3.39}$$

where C_{14} is independent of s, h, and T. To finish up, summing (3.29) from $m=0$ to $m=M-1$, we have

$$\begin{aligned}\left\|\Delta_h \phi^M\right\|_2^2 - \left\|\Delta_h \phi^0\right\|_2^2 + \varepsilon^2 s \sum_{\ell=1}^{M} \left\|\Delta_h^2 \phi^\ell\right\|_2^2 \le \frac{17\varepsilon^2}{64} s \sum_{\ell=0}^{M-1} \left\|\Delta_h^2 \phi^\ell\right\|^2 \\ + \frac{17\varepsilon^2}{64} s \sum_{\ell=-1}^{M-2} \left\|\Delta_h^2 \phi^\ell\right\|_2^2 + C_{23} T.\end{aligned} \tag{3.40}$$

Hence,

$$\left\|\Delta_h \phi^M\right\|_2^2 + \frac{15\varepsilon^2}{32} s \sum_{\ell=1}^{M} \left\|\Delta_h^2 \phi^\ell\right\|^2 \le C_{23} T + \left\|\Delta_h \phi^0\right\|_2^2 + \frac{3 \cdot 17\varepsilon^2}{64} s \left\|\Delta_h^2 \phi^0\right\|_2^2. \tag{3.41}$$

Estimate (3.11) now follows by consistency, the stability estimate (2.43), and the discrete elliptic regularity result (3.3). □

REMARK 3.3. We observe that a global in time H_h^2 bound of the numerical approximation ϕ has been obtained. Indeed, a more detailed examination of (3.37) reveals an asymptotic decay of the contribution coming from the term G^0, which is essentially the H_h^2 norm of the initial data ϕ^0. In addition, the growth of the $L_s^2(0,T;H_h^4)$ norm of the numerical solution is, at worst, linear in time; no exponential growth occurs. These remarkable estimates will be important to the error analysis to follow.

Using our discrete Sobolev inequalities, we immediately get the following:

COROLLARY 3.4. *With the same hypotheses as in the last theorem, we immediately have*

$$\|\phi^m\|_\infty \le C_9 \|\phi^m\|_{H_h^2} \le C_9 \sqrt{C_{14}}, \quad \|\nabla_h \phi^m\|_4 \le C_{12} \|\phi^m\|_{H_h^2} \le C_{12} \sqrt{C_{14}}, \tag{3.42}$$

for any $1 \le m \le M$. *We also note that, the constants* C_9, C_{12}, *and* C_{14} *are independents on* h, s *and the final time* T. *Regarding their dependence on* ε, *we observe that* C_9 *and* C_{12} *are* ε*-independent, while* C_{14} *depends polynomially on* ε^{-1}. *At worst,* $C_{14} = O(\varepsilon^{-m_0})$, *where* $m_0 = 26$.

REMARK 3.5. The reader will observe that the $\|\cdot\|_\infty$ bound for the numerical solution, namely $C_9\sqrt{C_{14}}$ in (3.42), is final time independent. There have been limited theoretical works to derive an L^∞ bound of the numerical solution for the Cahn–Hilliard equation; see [5] for the analysis of a first-order numerical scheme applied to the CH equation with a logarithmic energy. On the other hand, for a second-order scheme for the CH model with a nonlinear polynomial energy, our $\|\cdot\|_\infty$ estimate (3.42) is the first such result, to the authors' knowledge.

REMARK 3.6. The global-in-time $\|\cdot\|_\infty$ bound, $C_9\sqrt{C_{14}}$ in (3.42), depends singularly on ε, specifically, $C_9\sqrt{C_{14}} = O(\varepsilon^{-13})$. Meanwhile, a well-known theoretical analysis presented by L. Caffareilli [9] gives an ε-independent L^∞ bound for the CH equation, at the PDE level, provided that a cut-off is applied to the energy. For the standard CH energy (1.1), in which the polynomial part is given by $\frac{1}{4}\phi^4 - \frac{1}{2}\phi^2$ without a cut-off, the availability of an ε-independent L^∞ bound of the solution is still an open problem, at both the PDE and numerical levels.

REMARK 3.7. We note that, the second order (in time) numerical approximation to the linear bi-harmonic term, namely, $\frac{3}{4}\phi^{m+1} + \frac{1}{4}\phi^{m-1}$, is different from the standard Crank–Nicholson time stepping. In fact, a detailed analysis shows that, with the Crank–Nicholson temporal discretization applied to the linear bi-harmonic term, the unique solvability and unconditional energy stability are still valid for the resulting numerical scheme. However, an essential difficulty with Crank–Nicholson arises in the H_h^2 stability estimate and the convergence analysis, due to the lack of diffusion power at time-step t^{m+1}.

This subtle fact could also be explained by a linear stability domain argument. The temporal discretization applied to the linear bi-harmonic term, proposed in this paper, corresponds a much larger stability domain than the standard Crank–Nicholson one. In more detail, the stability domain for the Crank–Nicholson scheme is exactly the left half complex plane: $\{z : \mathrm{Re}(z) < 0\}$, while that for the proposed time stepping (in this paper) contains a large part on the right complex plane. In particular, if the nonlinear terms are involved, we believe that the proposed time stepping would bring a great deal of convenience in the stability and convergence analysis.

REMARK 3.8. The inequalities in Lemma 3.1 provide the elliptic regularity and the Sobolev embedding at the discrete level, which are required in the nonlinear analysis. Since the finite difference scheme defines the numerical solution on the collocation grid points, these inequalities can not be derived by a direct calculation. Instead, we have to establish a functional equivalence between the discrete and continuous norms, and apply the elliptic regularity and Sobolev embedding in the continuous functional space, so that these discrete inequalities are valid; see the details in Section B. Some related discussions could be found in the earlier works of mimetic difference methods (see [8, 11, 36], for example).

REMARK 3.9. Other than the standard second order centered difference approximation, other spatial discretizations with higher order accuracy could be applied to the proposed second order convex splitting scheme, with the numerical stability and convergence analysis expected to be available. For example, Fourier pseudo-spectral scheme could greatly improve the spatial accuracy, and the discrete Sobolev inequalities could be proven in a similar manner, so that a uniform in time H^2 bound is valid for the fully discrete numerical solution. As another example, the finite element approximation (with different polynomial degree order) could be chosen as the spatial discretization, and the discrete version of the Sobolev inequalities could be established in a modified way. These higher order approaches will be considered in our future works.

4. $L_s^\infty\left(0,T;H_h^2\right)$ and $L_s^\infty\left(0,T;L_h^\infty\right)$ convergence analysis of the scheme

For simplicity, we assume that $\mathcal{M}(\cdot) \equiv 1$. By ϕ_e we denote the exact solution to the original Cahn–Hilliard equation (1.2) with the initial data $\phi_e(\cdot, t=0) = \psi \in C^4_{\mathrm{per}}(\Omega)$. We assume that the exact solution has certain regularities. First we define the regularity class

$$\begin{aligned}\mathcal{R}_1 := H^3(0,T;C^0_{\mathrm{per}}(\Omega)) \cap H^2(0,T;C^4_{\mathrm{per}}(\Omega)) \\ \cap W^{2,\infty}(0,T;C^2_{\mathrm{per}}(\Omega)) \cap L^\infty(0,T;C^6_{\mathrm{per}}(\Omega)).\end{aligned} \tag{4.1}$$

For the error analysis over the first time-step, we will also need to assume additional regularity for a short time. For some $0<T^*\le T$ to be defined later, we define the enhanced regularity class

$$\mathcal{R}_2 := C^3([0,T^*];C^2_{\rm per}(\Omega))\cap C^2([0,T^*];C^6_{\rm per}(\Omega)) \\ \cap C^2([0,T^*];C^2_{\rm per}(\Omega))\cap C^0([0,T^*];C^8_{\rm per}(\Omega)). \tag{4.2}$$

We assume that $\phi_e\in\mathcal{R}:=\mathcal{R}_1\cap\mathcal{R}_2$.

THEOREM 4.1. *Given initial data $\psi\in C^4_{\rm per}(\Omega)$, suppose the unique solution $\phi_e(x,y,z,t)$ for the Cahn–Hilliard equation (1.2), with $\mathcal{M}(\phi)\equiv 1$, is of regularity class $\mathcal{R}$. Set $\Phi^m := \mathsf{P}_h\phi_e(\cdot,m\cdot s)$, for all $0\le m\le M$, and $\Phi^{-1}\equiv\Phi^0$. Define the error grid function $\breve{\phi}^\ell_{i,j,k} := \Phi^\ell_{i,j,k}-\phi^\ell_{i,j,k}$, where $\phi^\ell_{i,j,k}\in\mathcal{C}_\Omega$ is the ℓth periodic solution of the second order scheme (3.12). Then, provided s is sufficiently small, for all positive integers ℓ, such that $s\cdot\ell\le T$, we have*

$$\left\|\Delta_h\breve{\phi}^\ell\right\|_2^2+\varepsilon^2 s\sum_{m=1}^{\ell}\left\|\Delta_h^2\breve{\phi}^m\right\|_2^2\le C\left(s^2+h^2\right)^2, \tag{4.3}$$

where $C=C(\varepsilon,T)>0$ is independent of s and h.

The convergence analysis is carried out in three steps. First, in Section 4.1, we obtain an equation for the error function using a standard consistency analysis. In Section 4.2 we provide an estimate for the nonlinear error term. Finally, the stability and optimal rate error estimate is given by Section 4.3.

4.1. Consistency analysis and error equations. Detailed Taylor expansions for the exact solution shows that the grid function Φ, which represents the exact solution, satisfies the second order numerical scheme (3.12) with a truncation error: for $0\le m\le M-1$ we have

$$\frac{\Phi^{m+1}-\Phi^m}{s}=\Delta_h\left(\chi(\Phi^{m+1},\Phi^m)-\left(\frac{3}{2}\Phi^m-\frac{1}{2}\Phi^{m-1}\right)\right. \\ \left.-\varepsilon^2\Delta_h\left(\frac{3}{4}\Phi^{m+1}+\frac{1}{4}\Phi^{m-1}\right)\right)+\tau^{m+1/2}, \tag{4.4}$$

where $\tau^{m+1/2}\in\mathcal{C}_\Omega$ is the local truncation error grid function. The truncation error satisfies

$$\left\|\tau^{m+1/2}\right\|_2\le(s^2+h^2)\beta_{m+1/2},\quad s\sum_{\ell=1}^{M-1}\beta^2_{\ell+1/2}\le C_{25}, \tag{4.5}$$

where $s\cdot M=T$, and C_{25} is independent of h and s. The details are suppressed for brevity of presentation. The local truncation error is, however, only first-order accurate at the first time step. Using the increased regularity in the short-time frame, Taylor expansions reveal that

$$\left\|\Delta_h\tau^{1/2}\right\|_2\le(s+h^2)\beta_{1/2}, \tag{4.6}$$

where $\beta_{1/2}$ is bounded uniformly as $s\to 0$.

Subtracting (4.4) from the numerical scheme (3.12) yields

$$\frac{\breve{\phi}^{m+1}-\breve{\phi}^m}{s}=\Delta_h\Big(\chi(\Phi^{m+1},\Phi^m)-\chi(\phi^{m+1},\phi^m)-\Big(\frac{3}{2}\breve{\phi}^m-\frac{1}{2}\breve{\phi}^{m-1}\Big)$$
$$-\varepsilon^2\Delta_h\Big(\frac{3}{4}\breve{\phi}^{m+1}+\frac{1}{4}\breve{\phi}^{m-1}\Big)\Big)+\tau^{m+1/2}, \tag{4.7}$$

for all $0\le m\le M-1$. Observe that $\breve{\phi}^0\equiv\breve{\phi}^{-1}\equiv 0$, based on our constructions.

Remark 4.2. The Taylor expansion based on the regularity assumption (4.1) is straightforward. On the other hand, we remark that this assumption does not represent the optimal regularity requirement for the exact solution. For example, a reduced regularity assumption

$$\phi_e\in H^3(0,T;C^0_{\rm per}(\Omega))\cap H^2(0,T;H^4_{\rm per}(\Omega))$$
$$\cap W^{2,\infty}(0,T;H^2_{\rm per}(\Omega))\cap L^\infty(0,T;H^6_{\rm per}(\Omega)), \tag{4.8}$$

is sufficient for the $L^2_s(0,T;L^2_h)$ bound of the local truncation error τ in (4.5). In this case, the consistency analysis would be similar to that described in [7, 45]. The details are skipped in this paper for simplicity of presentation.

4.2. Preliminary estimates for the nonlinear error term. First, we prove a stability estimate for the discrete H^2_h norm of the error function.

Lemma 4.3. *Given initial data $\psi\in C^4_{\rm per}(\Omega)$, suppose the unique exact solution ϕ_e for the Cahn–Hilliard equation (1.2), with $\mathcal{M}(\phi)\equiv 1$, is of regularity class $\mathcal{R}$. Then, for any $1\le m\le M$,*

$$\left\|\breve{\phi}^m\right\|_{H^2_h}\le C_{26}\left(\left\|\Delta_h\breve{\phi}^m\right\|_2+h^2\right). \tag{4.9}$$

Proof. We observe the fact that

$$\begin{aligned}\left|\overline{\breve{\phi}^m}\right|&=\left|\overline{\Phi^m}-\overline{\phi^m}\right|=\left|\overline{\Phi^m}-\overline{\phi^0}\right|\\&=\left|\overline{\Phi^m}-|\Omega|^{-1}\int_\Omega\phi_e(\boldsymbol{x},t_m)\,d\boldsymbol{x}-\left(\overline{\phi^0}-|\Omega|^{-1}\int_\Omega\phi_e(\boldsymbol{x},t_0)\,d\boldsymbol{x}\right)\right|\\&\le\left|\overline{\Phi^m}-|\Omega|^{-1}\int_\Omega\phi_e(\boldsymbol{x},t_m)\,d\boldsymbol{x}\right|+\left|\overline{\phi^0}-|\Omega|^{-1}\int_\Omega\phi_e(\boldsymbol{x},t_0)\,d\boldsymbol{x}\right|\le Ch^2,\end{aligned} \tag{4.10}$$

owing to consistency. Here the overline refers only to the discrete average. As a result, the estimate (4.9) follows from the discrete elliptic regularity (3.4). ∎

In addition, a control of the error related to the nonlinear term in the second order scheme is needed in the convergence analysis.

Lemma 4.4. *Suppose $\Phi^m,\Phi^{m+1},\phi^m,\phi^{m+1}\in\mathcal{C}_\Omega$ are periodic. Denote the differences by $\breve{\phi}^\ell:=\Phi^\ell-\phi^\ell$, for $\ell=m,m+1$. Then we have*

$$\left\|\Delta_h\left(\chi\left(\Phi^{m+1},\Phi^m\right)-\chi\left(\phi^{m+1},\phi^m\right)\right)\right\|_2$$
$$\le C_{26}\Big\{K_1^2\cdot\left(\left\|\breve{\phi}^{m+1}\right\|_{H^2_h}+\left\|\breve{\phi}^m\right\|_{H^2_h}\right)+\left(K_1K_3+K_4^2\right)\cdot\left(\left\|\breve{\phi}^{m+1}\right\|_\infty+\left\|\breve{\phi}^m\right\|_\infty\right)$$

$$+K_1K_4\left(\left\|\nabla_h\breve{\phi}^{m+1}\right\|_4+\left\|\nabla_h\breve{\phi}^{m}\right\|_4\right)+\left(K_5^2+K_1K_2\right)\cdot\left(\left\|\breve{\phi}^{m+1}\right\|_2+\left\|\breve{\phi}^{m}\right\|_2\right)\Big\}, \quad (4.11)$$

where C_{26} is a positive constant which is independent of h, and

$$\begin{aligned}
K_1 &:= \left\|\Phi^{m+1}\right\|_\infty+\|\Phi^m\|_\infty+\left\|\phi^{m+1}\right\|_\infty+\|\phi^m\|_\infty,\\
K_2 &:= \left\|\Delta_h^x\Phi^{m+1}\right\|_\infty+\|\Delta_h^x\Phi^m\|_\infty+\left\|\Delta_h^y\Phi^{m+1}\right\|_\infty+\|\Delta_h^y\Phi^m\|_\infty\\
&\quad+\left\|\Delta_h^z\Phi^{m+1}\right\|_\infty+\|\Delta_h^z\Phi^m\|_\infty,\\
K_3 &:= \left\|\phi^{m+1}\right\|_{H_h^2}+\|\phi^m\|_{H_h^2},\\
K_4 &:= \left\|\nabla_h\Phi^{m+1}\right\|_4+\|\nabla_h\Phi^m\|_4+\left\|\nabla_h\phi^{m+1}\right\|_4+\|\nabla_h\phi^m\|_4,\\
K_5 &:= \left\|\nabla_h\Phi^{m+1}\right\|_\infty+\|\nabla_h\Phi^m\|_\infty.
\end{aligned} \quad (4.12)$$

REMARK 4.5. A similar nonlinear error estimate has been established in the recent article [7], where an $L_s^\infty(0,T;H_h^3)$ convergence analysis for the second order numerical scheme for the modified phase field crystal (MPFC) model is undertaken in 2D. The present lemma represents an extension to the 3D case. Since the details are quite similar, we have omitted the proof.

LEMMA 4.6. *Given sufficiently regular initial data $\psi\in H_{\rm per}^m(\Omega)$, suppose the unique solution $\phi_e(x,y,z,t)$ for the Cahn–Hilliard equation* (1.2)*, with $\mathcal{M}(\phi)\equiv 1$, is of regularity class $\mathcal{R}$. Then, for any $1\le m\le M$,*

$$\left\|\Delta_h\left(\chi\left(\Phi^{m+1},\Phi^m\right)-\chi\left(\phi^{m+1},\phi^m\right)\right)\right\|_2\le C_{27}\left(\left\|\breve{\phi}^{k+1}\right\|_{H_h^2}+\left\|\breve{\phi}^{k}\right\|_{H_h^2}\right), \quad (4.13)$$

where $C_{27}>0$ is a constant that is independent of h and s.

Proof. The regularity assumptions for the exact solution (4.1) implies that, for any $1\le m\le M$,

$$\|\Phi^m\|_{W_h^{2,\infty}}\le C_{28}, \quad (4.14)$$

where the norm above denotes a discrete $W^{2,\infty}$ norm of Φ^m, *i.e.*, the maximum norm of Φ^m and all of its finite differences up to and including the second order ones. Consequently,

$$K_1,K_4\le C(C_{28}+C_9\sqrt{C_{14}}+C_{12}\sqrt{C_{14}}),\quad K_2,K_5\le CC_{28},\quad K_3\le C\sqrt{C_{14}}. \quad (4.15)$$

Using these estimates, combined with (4.11) and the discrete Sobolev inequalities (3.6) and (3.8), we get the result. ∎

COROLLARY 4.7. *Given initial data $\psi\in C_{\rm per}^4(\Omega)$, suppose the unique solution ϕ_e for the Cahn–Hilliard equation* (1.2)*, with $\mathcal{M}(\phi)\equiv 1$, is of regularity class $\mathcal{R}$. Then, for any $1\le m\le M$,*

$$\left\|\Delta_h\left(\chi\left(\Phi^{m+1},\Phi^m\right)-\chi\left(\phi^{m+1},\phi^m\right)\right)\right\|_2\le C_{14}C_{27}\left(\left\|\Delta_h\breve{\phi}^{m+1}\right\|_2+\left\|\Delta_h\breve{\phi}^{m}\right\|_2+2h^2\right). \quad (4.16)$$

4.3. Stability analysis for the error: proof of Theorem 4.1. In this section we prove Theorem 4.1.

Proof. Taking the inner product with the error equation (4.4) by $\Delta_h^2\breve{\phi}^{m+1}$, and using summation-by-parts, we have

$$\frac{1}{2}\left(\left\|\Delta_h\breve{\phi}^{m+1}\right\|_2^2-\left\|\Delta_h\breve{\phi}^{m}\right\|_2^2\right)+\frac{1}{2}\left\|\Delta_h(\breve{\phi}^{m+1}-\breve{\phi}^{m})\right\|_2^2$$
$$=-s\left(\Delta_h^2\breve{\phi}^{m+1},\Delta_h\left(\frac{3}{2}\breve{\phi}^{m}-\frac{1}{2}\breve{\phi}^{m-1}\right)\right)-\varepsilon^2 s\left(\Delta_h^2\breve{\phi}^{m+1},\Delta_h^2\left(\frac{3}{4}\breve{\phi}^{m+1}+\frac{1}{4}\breve{\phi}^{m-1}\right)\right)$$
$$+s\left(\Delta_h^2\breve{\phi}^{m+1},\Delta_h\left(\chi\left(\Phi^{m+1},\Phi^m\right)-\chi\left(\phi^{m+1},\phi^m\right)\right)\right)+s\left(\Delta_h^2\breve{\phi}^{m+1},\tau^{m+1/2}\right). \quad (4.17)$$

Notice that $\breve{\phi}^0\equiv\breve{\phi}^{-1}\equiv 0$. We need to analyze the error at the first time step separately, since the local truncation error is only first-order in time. Setting $m=0$ and using the Cauchy-Schwartz and Young's inequalities, we have

$$\left\|\Delta_h\breve{\phi}^{1}\right\|_2^2+\frac{3\varepsilon^2}{4}s\left\|\Delta_h^2\breve{\phi}^{1}\right\|_2^2$$
$$=s\left(\Delta_h^2\breve{\phi}^{1},\Delta_h\left(\chi\left(\Phi^1,\Phi^0\right)-\chi\left(\phi^1,\phi^0\right)\right)\right)+s\left(\Delta_h^2\breve{\phi}^{1},\tau^{1/2}\right)$$
$$\le s\left\|\Delta_h^2\breve{\phi}^{1}\right\|_2\left\|\Delta_h\left(\chi\left(\Phi^1,\Phi^0\right)-\chi\left(\phi^1,\phi^0\right)\right)\right\|_2+s\left(\Delta_h\breve{\phi}^{1},\Delta_h\tau^{1/2}\right)$$
$$\le sC_{14}C_{27}\left\|\Delta_h^2\breve{\phi}^{1}\right\|_2\left(\left\|\Delta_h\breve{\phi}^{1}\right\|_2+h^2\right)+\left\|\Delta_h\breve{\phi}^{1}\right\|_2 s\left\|\Delta_h\tau^{1/2}\right\|_2$$
$$\le\frac{2sh^4C_{14}^2C_{27}^2}{3\varepsilon^2}+\left(\frac{3\varepsilon^2 s}{8}+s^2C_{14}^2C_{27}^2\right)\left\|\Delta_h^2\breve{\phi}^{1}\right\|_2^2+\frac{1}{2}\left\|\Delta_h\breve{\phi}^{1}\right\|_2^2+s^2\left\|\Delta_h\tau^{1/2}\right\|_2^2. \quad (4.18)$$

Hence,

$$\frac{1}{2}\left\|\Delta_h\breve{\phi}^{1}\right\|_2^2+\left(\frac{3\varepsilon^2 s}{8}-s^2C_{14}^2C_{27}^2\right)\left\|\Delta_h^2\breve{\phi}^{1}\right\|_2^2\le\frac{2sh^4C_{14}^2C_{27}^2}{3\varepsilon^2}+\beta_{1/2}s^2\left(s^2+h^4\right), \quad (4.19)$$

where, recall, $0\le\beta_{1/2}$ is bounded uniformly as $s\to 0$. Now, provided the time step-size satisfies

$$s\le\frac{\varepsilon^2}{4C_{14}^2C_{27}^2}=:s_1^*, \quad (4.20)$$

then it follows that

$$\left\|\Delta_h\breve{\phi}^{1}\right\|_2^2+\frac{\varepsilon^2 s}{4}\left\|\Delta_h^2\breve{\phi}^{1}\right\|_2^2\le C_{29}\varepsilon^{-2}\left(s^2+h^2\right)^2, \quad (4.21)$$

where $C_{29}>0$ is independent of s, h, ε, and T.

Now we go back to the typical case, where $1\le m\le M$ in (4.17). The term associated with the local truncation error can be bounded in the standard way:

$$\left(\tau^{m+1/2},\Delta_h^2\breve{\phi}^{m+1}\right)\le C(s^2+h^2)\beta_{m+1/2}\cdot\left\|\Delta_h^2\breve{\phi}^{m+1}\right\|_2$$
$$\le C\varepsilon^{-2}(s^2+h^2)^2\beta_{m+1/2}^2+\frac{\varepsilon^2}{8}\left\|\Delta_h^2\breve{\phi}^{m+1}\right\|_2^2. \quad (4.22)$$

For the concave diffusion error term we have

$$-\left(\Delta_h^2\breve{\phi}^{k+1},\Delta_h\left(\frac{3}{2}\breve{\phi}^{k}-\frac{1}{2}\breve{\phi}^{k-1}\right)\right)\le\frac{\varepsilon^2}{8}\left\|\Delta_h^2\breve{\phi}^{k+1}\right\|^2+\frac{1}{\varepsilon^2}\left(9\left\|\Delta_h\breve{\phi}^{k}\right\|_2^2+\left\|\Delta_h\breve{\phi}^{k-1}\right\|_2^2\right).$$

(4.23)

The analysis for the bi-harmonic diffusion error term follows that of (3.19):

$$\frac{5}{8}\left\|\Delta_h^2\breve{\phi}^{m+1}\right\|_2^2-\frac{1}{8}\left\|\Delta_h^2\breve{\phi}^{m-1}\right\|_2^2\leq\left(\Delta_h^2\breve{\phi}^{m+1},\Delta_h^2\left(\frac{3}{4}\breve{\phi}^{m+1}+\frac{1}{4}\breve{\phi}^{m-1}\right)\right). \tag{4.24}$$

The term associated with the nonlinear error can be analyzed as follows: using estimates (4.13), (4.9), for any $1\leq m\leq M$,

$$\begin{aligned}&\left(\Delta_h^2\phi^{m+1},\Delta_h\left(\chi\left(\Phi^{m+1},\Phi^m\right)-\chi\left(\phi^{m+1},\phi^m\right)\right)\right)\\ &\leq\left\|\Delta_h^2\phi^{m+1}\right\|_2\cdot\left\|\Delta_h\left(\chi\left(\Phi^{m+1},\Phi^m\right)-\chi\left(\phi^{m+1},\phi^m\right)\right)\right\|_2\\ &\leq C_{14}\left\|\Delta_h^2\phi^{m+1}\right\|_2\left(\left\|\breve{\phi}^{m+1}\right\|_{H_h^2}+\left\|\breve{\phi}^{m}\right\|_{H_h^2}\right)\\ &\leq C_{14}C_{27}\left\|\Delta_h^2\phi^{m+1}\right\|_2\left(\left\|\Delta_h\breve{\phi}^{m+1}\right\|_2+\left\|\Delta_h\breve{\phi}^{m}\right\|_2+2h^2\right)\\ &\leq\frac{\varepsilon^2}{8}\left\|\Delta_h^2\phi^{m+1}\right\|_2^2+C_{30}\varepsilon^{-2}\left(\left\|\Delta_h\breve{\phi}^{m+1}\right\|_2^2+\left\|\Delta_h\breve{\phi}^{m}\right\|_2^2+h^4\right),\end{aligned} \tag{4.25}$$

where $C_{30}>0$ is independent of s, h, and ε.

A combination of (4.17), (4.22), (4.23), (4.24) and (4.25) leads to

$$\begin{aligned}&\left\|\Delta_h\breve{\phi}^{m+1}\right\|_2^2-\left\|\Delta_h\breve{\phi}^{m}\right\|_2^2+\frac{\varepsilon^2}{2}s\left\|\Delta_h^2\breve{\phi}^{m+1}\right\|_2^2-\frac{\varepsilon^2}{4}s\left\|\Delta_h^2\breve{\phi}^{m-1}\right\|_2^2\\ &\leq C_{31}\varepsilon^{-2}s\left(\left\|\Delta_h\breve{\phi}^{m+1}\right\|_2^2+\left\|\Delta_h\breve{\phi}^{m}\right\|_2^2+\left\|\Delta_h\breve{\phi}^{m-1}\right\|_2^2\right)+C_{32}\varepsilon^{-2}s(s^2+h^2)^2(\beta_{m+1/2}^2+1).\end{aligned} \tag{4.26}$$

for any $1\leq m\leq M-1$, where $C_{31},C_{32}>0$ are independent of s, h, and ε. Summing from $m=1$ to $m=\ell-1$, with $1\leq\ell\leq M$, and rearranging terms, we have

$$\begin{aligned}&\left\|\Delta_h\breve{\phi}^{\ell}\right\|_2^2+\frac{\varepsilon^2}{4}s\sum_{m=1}^{\ell}\left\|\Delta_h^2\breve{\phi}^{m}\right\|_2^2\\ &\leq 3C_{31}\varepsilon^{-2}s\sum_{m=1}^{\ell}\left\|\Delta_h\breve{\phi}^{m}\right\|_2^2+C_{32}\varepsilon^{-2}(s^2+h^2)^2(C_{25}+T)+\left\|\Delta_h\breve{\phi}^{1}\right\|_2^2+\frac{\varepsilon^2 s}{4}\left\|\Delta_h^2\breve{\phi}^{1}\right\|_2^2\\ &\leq 3C_{31}\varepsilon^{-2}s\sum_{m=1}^{\ell}\left\|\Delta_h\breve{\phi}^{m}\right\|_2^2+C_{33}(T+1)\varepsilon^{-2}(s^2+h^2)^2,\end{aligned} \tag{4.27}$$

where $C_{33}:=\max(C_{32}C_{25}+C_{29},C_{32})$. Note, we have used (4.21) in the last step, assuming $s\leq s_1^*$. If the step-size additionally satisfies

$$s\leq\frac{\varepsilon^2}{4C_{31}}=:s_2^*, \tag{4.28}$$

then it follows that

$$\left\|\Delta_h\breve{\phi}^{\ell}\right\|_2^2+\varepsilon^2 s\sum_{m=1}^{\ell}\left\|\Delta_h^2\breve{\phi}^{m}\right\|_2^2\leq 12C_{31}\varepsilon^{-2}s\sum_{m=1}^{\ell-1}\left\|\Delta_h\breve{\phi}^{m}\right\|_2^2+4C_{33}\varepsilon^{-2}(s^2+h^2)^2. \tag{4.29}$$

Invoking the Discrete Gronwall Lemma A.1, we have

$$\left\|\Delta_h \breve{\phi}^\ell\right\|_2^2 + \varepsilon^2 s \sum_{n=1}^{\ell} \left\|\Delta_h^2 \breve{\phi}^m\right\|_2^2 \le 4C_{33}(T+1)\varepsilon^{-2}\exp\left(12C_{31}\varepsilon^{-2}T\right)(s^2+h^2)^2, \tag{4.30}$$

provided that $s \le \min(s_1^*, s_2^*)$. The proof of Theorem 4.1 is complete. □

Remark 4.8. The convergence constant appearing in (4.30) is independent of s and h. Of course this constant does depend on the final time T and on the interface parameter ε. Indeed, our detailed calculation reveals its dependence on $\exp\left(\varepsilon^{-2}T\right)$, which comes from the application of discrete Gronwall inequality in the convergence analysis.

There have been some existing works on the improved convergence constant for the CH equation (1.2). Specifically, Feng and Prohl [29] 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 on ε, instead of the singularly ε-dependent exponential growth predicted here. Such an elegant improvement was based on a subtle spectrum analysis for the linearized Cahn–Hilliard operator (with certain given structure assumptions of the solution), provided in earlier literatures [1, 2, 15–17].

These numerical analysis techniques have been recently applied to the convergence of a first-order in time convex splitting scheme for the Allen–Cahn equation by Feng and Li [28]. The authors used a discontinuous Galerkin discretization of space. These techniques may also be applied to analyze our second order convex splitting scheme (3.12). On the other hand, such an analysis is expected be highly non-trivial, due to the complicated form of the nonlinear error terms. This issue will be explored in the future work.

Remark 4.9. The unconditional convergence is proven in the sense that the constant in (4.30) is independent on s and h. Meanwhile, there are two restriction conditions for the time step, namely (4.20) and (4.28), for the estimates to hold. A more careful analysis shows that, these two conditions correspond to a bound of $s \le C^* \varepsilon^{-k_0}$, with k_0 an integer and C^* independent of the final time T and ε.

Our various numerical experiments indicates that, these restriction condition comes from certain technical difficulties in the theoretical analysis, and this severe restriction is not needed in the practical numerical simulation. A further theoretical improvement of these two restriction conditions is possible, and it is left to interested readers.

In addition, we observe that another restriction condition, namely $s \le {}^{176 C_{13}^2}/_{45\varepsilon^2}$, is needed in the uniform in time H_h^2 stability estimate, established in Theorem 3.2. However, we note that this condition is trivial for small ε, and it will not pose a numerical challenge in the practical computations.

Remark 4.10. For the second order numerical scheme (2.26) combined with the trivial initial extrapolation formula $\phi^{-1} \equiv \phi^0$, the first time step is first order accurate while the rest time steps are of second order accuracy. This leads to an additional time step restriction (4.20), which is needed to assure the second order convergence at the first step. Meanwhile, an alternate initialization (2.31)–(2.35) was presented in Remark 2.1, which turns out to be the second order accurate at the first time step. As a result, for this alternate approach, we only need the second time step restriction condition (4.28) to assure the convergence analysis, and the first restriction (4.20) could be dropped, since the second order convergence at the first step could be derived by a direct Taylor expansion.

Similar to the last remark, the trivial time step condition, $s \le {}^{176C_{13}^2}/_{45\varepsilon^2}$, is also needed in the uniform in time H_h^2 bound in Theorem 3.2, since the derivation of this condition is independent on the initialization. Again, this condition is easily satisfied for small ε, and it does not pose any practical challenge.

5. Numerical results

5.1. Numerical accuracy check. In this subsection we perform a numerical accuracy check for the unconditionally energy stable, fully discrete, second order scheme (3.12). The computational domain is set to be $\Omega = (0,L)^3$, with $L = 3.2$, and the exact profile for the phase variable is set to be

$$\phi_e(x,y,z,t) = \cos(2\pi x/L)\cos(2\pi y/L)\cos(2\pi z/L)\cos(t). \tag{5.1}$$

To make ϕ_e satisfy the original PDE (1.2), we have to add an artificial, time-dependent forcing term. The proposed second order scheme (3.12) (with centered difference approximation in space) is implemented via an efficient nonlinear multigrid solver. The details of the nonlinear multigrid solver are similar to those of the solvers for the phase-field crystal equation given in [6,35] and the CHHS equation [46]. We compute solutions with grid sizes $N = 16$ to $N = 96$ in increments of 8, where $N := N_x = N_y = N_z$ – and we solve up to the final time $T = 1.0$. The errors are reported at this final time only. The interface parameter is given by $\varepsilon = 0.5$. The time step s is determined by the linear refinement path $s = 0.5h$, where h is the spatial grid size. Figure 5.1 shows the discrete L_h^2 and H_h^2 norms of the errors between the numerical and exact solutions. A clear second order accuracy is observed.

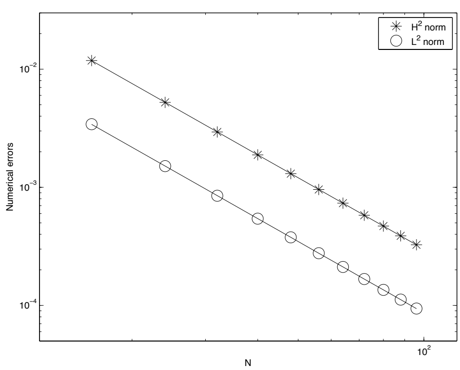

FIG. 5.1. *Discrete L_h^2 and H_h^2 numerical errors for ϕ at $T = 1.0$, plotted versus $N = 16:8:96$, the number of spatial grid point, for the fully discrete scheme (3.12). $\varepsilon = 0.5$. The time step-size is taken as $s = \frac{1}{2}h$. The slope for the linear least squares fit for the L_h^2 errors is -2.00405, that for the H_h^2 errors is -2.00474.*

5.2. 3D spinodal decomposition and 3D multigrid solver efficiency. In this subsection we present a numerical simulation with random initial data on a square domain $\Omega = (0,L)^3$, with $L = 3.2$ and $N := N_x = N_y = N_z$. In particular, we take $\phi_{i,j,k}^0 = \eta_{i,j,k}$, $1 \le i,j,k \le N$, where $\eta_{i,j,k}$ is a spatially random number uniformly distributed on the interval $-0.05 \le \eta_{i,j,k} \le 0.05$. The interface parameter is set to be $\varepsilon = 0.05$. The spatial resolution is given by $h = 0.05 = L/64$. In Figure 5.2 we present the isosurface plots of $\phi = 0$ at the intermediate time $t = 20.0$ and the final time $t = T = 110$. These plots are based on the numerical simulation with the time step $s = 0.001$. The dynamics show a clear coarsening behavior, which is the hallmark of the late stages of spinodal decomposition. As a side note, we typically observe that the energy (2.36) is decreasing during the simulation, using three different time step-sizes: $s=0.01$, $s=0.005$, and $s=0.001$; see the energy plot (vs. time) in Figure 5.3. Keep in mind that only the alternate numerical energy (2.37) is guaranteed to decrease at each time step.

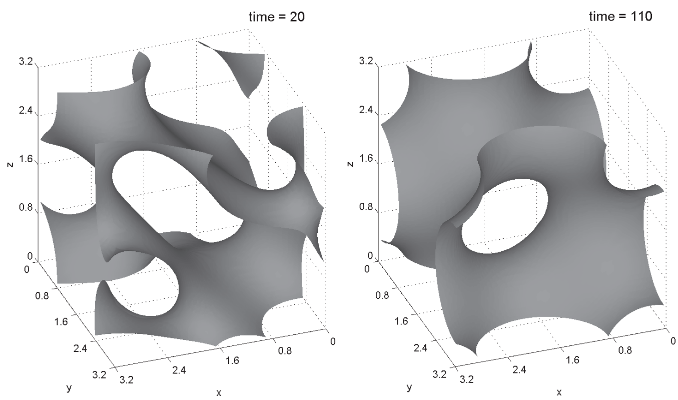

FIG. 5.2. *Isosurface plots of $\phi=0$ at the indicated times. These snapshots are from a simulation of spinodal decomposition, where the initial state is a random perturbation of the state $\phi=0$. The parameters for the simulation are as follows: $L=3.2$; $N=64$; $\varepsilon=0.05$; $h=0.05=3.2/64$; $s=0.001$.*

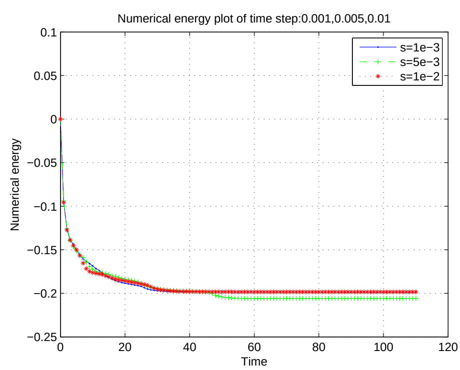

FIG. 5.3. *Time history of the alternate energy* (2.37) *of the numerical simulation, using three different time step-sizes: $s=0.01$, $s=0.005$ and $s=0.001$.*

We conclude the subsection with a test that demonstrates the efficiency of the multigrid solver. The parameters for the test are similar to those for the spinodal decomposition simulation above: $L=3.2$; $\varepsilon=0.05$; $h=3.2/N$; $s=0.001$. We use random initial data and vary the spatial resolution using the values $N=32,64,96,128$. The convergence rates of the solver are reported in Figure 5.4 after precisely 10 time steps, or, in other words, at the time $t=10\cdot s=0.01$. Using the smoothing parameter $\lambda=2$, we observe that the rate of decrease of the residual, and therefore the error as well, is nearly constant, and nearly h independent. This implies that, essentially, the amount of work required to yield a predefined error tolerance depends only on the number of degrees of freedom. Roughly speaking, only 5 v-cycle iterations are required to yield an

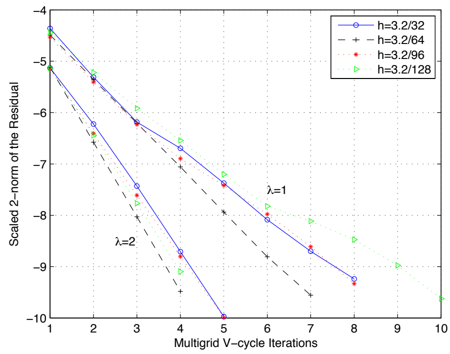

FIG. 5.4. *Nonlinear multigrid v-cycle convergence rates. The stopping tolerance for the multigrid solver in* $\tau = 10^{-9}$. *For* $\lambda = 2$ *pre- and post-smoothing steps we observe a nearly h-independent convergence rate of the solver. The parameters for the simulation are as follows:* $L = 3.2$; $N = 32, 64, 96, 128$; $\varepsilon = 0.05$; $h = 3.2/N$; $s = 0.001$. *The convergence rates are reported after precisely 10 time steps, or, in other words, at the time* $t = 20 \cdot s = 0.01$.

error tolerance of $\tau = 10^{-9}$.

Appendix A. Discrete Gronwall inequality. We use the following discrete Gronwall inequality in the proof of Theorem 4.1:

LEMMA A.1. *Fix* $T > 0$, *and suppose* $\{a^m\}_{m=1}^M$, $\{b^m\}_{m=1}^M$ *and* $\{c^m\}_{m=1}^{M-1}$ *are nonnegative sequences such that* $\tau \sum_{m=1}^{M-1} c^m \le C_1$, *where* C_1 *is independent of* τ *and* M, *with* $M\tau = T$. *Suppose that, for all* $\tau > 0$,

$$a^M + \tau \sum_{m=1}^{M} b^m \le C_2 + \tau \sum_{m=1}^{M-1} a^m c^m, \tag{A.1}$$

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

$$a^M + \tau \sum_{m=1}^{M} b^m \le C_2 \exp\left(\tau \sum_{m=1}^{M-1} c^m \right) \le C_2 \exp(C_1). \tag{A.2}$$

Note that the sum on the right-hand side of (A.1) must be explicit.

Appendix B. Proof of Lemma 3.1. 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 a similar manner to what follows but with a few more technical details involved.

Proof. Denote $N = 2K + 1$. Due to the periodic boundary conditions for ϕ and its cell-centered representation, it has a corresponding discrete Fourier transformation:

$$\phi_{i,j,k} = \sum_{\ell,m,n=-K}^{K} \hat{\phi}^N_{\ell,m,n} \mathrm{e}^{2\pi i(\ell x_i + m y_j + n z_k)/L}, \tag{B.1}$$

where $x_i = (i - \frac{1}{2})h$, $y_j = (j - \frac{1}{2})h$, $z_k = (k - \frac{1}{2})h$, and $\hat{\phi}^N_{\ell,m,n}$ are coefficients. Then we make its extension to a continuous function:

$$\phi_{\mathbf{F}}(x,y,z) = \sum_{\ell,m,n=-K}^{K} \hat{\phi}^N_{\ell,m,n} \mathrm{e}^{2\pi i(\ell x + my + nz)/L}. \tag{B.2}$$

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

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

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

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

$$\|\phi\|_2^2 = \|\phi_{\mathbf{F}}\|_{L^2}^2 = L^3 \sum_{\ell,m,n=-K}^{K} |\hat{\phi}_{\ell,m,n}^N|^2. \tag{B.5}$$

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

$$\begin{aligned}(D_x\phi)_{i+1/2,j,k} &= \frac{\phi_{i+1,j,k} - \phi_{i,j,k}}{h} \\ &= \sum_{\ell,m,n=-K}^{K} \mu_\ell \hat{\phi}_{\ell,m,n}^N \mathrm{e}^{2\pi i(\ell x_{i+1/2} + m y_j + n z_k)/L},\end{aligned} \tag{B.6}$$

$$\partial_x \phi_{\mathbf{F}}(x,y,z) = \sum_{\ell,m,n=-K}^{K} \nu_\ell \hat{\phi}_{\ell,m,n}^N \mathrm{e}^{2\pi i(\ell x + m y + n z)/L}, \tag{B.7}$$

with

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

In turn, an application of Parseval's identity yields

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

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

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

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

This indicates that

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

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

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

It can be proved analogously that

$$\frac{4}{\pi^2}\|\Delta\phi_{\mathbf{F}}\|_{L^2} \le \|\Delta_h\phi\|_2 \le \|\Delta\phi_{\mathbf{F}}\|_{L^2}, \tag{B.14}$$
$$\frac{8}{\pi^3}\|\nabla\Delta\phi_{\mathbf{F}}\|_{L^2} \le \|\nabla_h\Delta_h\phi\|_2 \le \|\nabla\Delta\phi_{\mathbf{F}}\|_{L^2}, \tag{B.15}$$
$$\frac{16}{\pi^4}\|\Delta^2\phi_{\mathbf{F}}\|_{L^2} \le \|\Delta_h^2\phi\|_2 \le \|\Delta^2\phi_{\mathbf{F}}\|_{L^2}. \tag{B.16}$$

Subsequently, the following estimates are valid:

$$\gamma_1\|\phi_{\mathbf{F}}\|_{H^1} \le \|\phi\|_{H_h^1} \le \gamma_2\|\phi_{\mathbf{F}}\|_{H^1}, \quad \gamma_1\|\phi_{\mathbf{F}}\|_{H^2} \le \|\phi\|_{H_h^2} \le \gamma_2\|\phi_{\mathbf{F}}\|_{H^2}, \tag{B.17}$$
$$\gamma_1\|\phi_{\mathbf{F}}\|_{H^4} \le \|\phi\|_{H_h^4} \le \gamma_2\|\phi_{\mathbf{F}}\|_{H^4}, \tag{B.18}$$

in which the elliptic regularity for $\phi_{\mathbf{F}}$ has been recalled in the derivation:

$$\|\phi_{\mathbf{F}}\|_{H^2} \le M_1\left(\|\phi_{\mathbf{F}}\|_{L^2} + \left\|\Delta^2\phi_{\mathbf{F}}\right\|_{L^2}\right), \quad \|\phi_{\mathbf{F}}\|_{H^4} \le M_2\left(\|\phi_{\mathbf{F}}\|_{L^2} + \left\|\Delta^2\phi_{\mathbf{F}}\right\|_{L^2}\right). \tag{B.19}$$

The discrete Sobolev inequality (3.1) comes from the norm equivalence estimates (B.14), (B.17), and the following inequalities in the continuous function space:

$$\begin{aligned}\|\phi_{\mathbf{F}}\|_{H^2} &\le C\|\phi_{\mathbf{F}}\|_{H^1}^{\frac{2}{3}} \cdot \|\phi_{\mathbf{F}}\|_{H^4}^{\frac{1}{3}} \le C\|\phi_{\mathbf{F}}\|_{H^1}^{\frac{2}{3}} \cdot \left(\|\phi_{\mathbf{F}}\|_{L^2} + \left\|\Delta^2\phi_{\mathbf{F}}\right\|_{L^2}\right)^{\frac{1}{3}} \\ &\le C\left(\|\phi_{\mathbf{F}}\|_{H^1}^{\frac{2}{3}}\left\|\Delta^2\phi_{\mathbf{F}}\right\|_{L^2}^{\frac{1}{3}} + \|\phi_{\mathbf{F}}\|_{H^1}\right).\end{aligned} \tag{B.20}$$

Similarly, the discrete elliptic regularity (3.3) comes from a combination of (B.5), (B.13)–(B.16), (B.17)–(B.18), and (B.19).

An alternate form of the discrete elliptic regularity (3.4) can be derived in the same manner, with the estimate in the continuous function space recalled:

$$\|\phi_{\mathbf{F}}\|_{H^2} \le C\left(\overline{\phi_{\mathbf{F}}} + \left\|\Delta^2\phi_{\mathbf{F}}\right\|_{L^2}\right), \quad \text{with } \overline{\phi_{\mathbf{F}}} := \frac{1}{|\Omega|}\int_\Omega \phi_{\mathbf{F}}(\boldsymbol{x})\,d\boldsymbol{x}; \tag{B.21}$$

combined with a subtle fact that the discrete average of ϕ and the continuous average of $\phi_{\mathbf{F}}$ are identical:

$$\bar{\phi} := \frac{h^3}{|\Omega|}\sum_{i,j,k=1}^{N}\phi_{i,j,k} = \hat{\phi}_{0,0,0}^N = \frac{1}{|\Omega|}\int_\Omega \phi_{\mathbf{F}}(\boldsymbol{x})\,d\boldsymbol{x} = \overline{\phi_{\mathbf{F}}}. \tag{B.22}$$

The discrete Sobolev embedding (3.5) from H_h^2 into ℓ^∞ can be derived as follows:

$$\|\phi\|_\infty \le \|\phi_{\mathbf{F}}\|_{L^\infty} \le C\|\phi_{\mathbf{F}}\|_{H^2} \le C\|\phi\|_{H_h^2}, \tag{B.23}$$

in which the continuous embedding was applied in the second step, and the norm equivalence estimate (B.17) was recalled at the last step.

For the discrete Gagliardo–Nirenberg type inequality (3.6), we have the following observation:

$$\begin{aligned}\|\phi\|_\infty \le \|\phi_{\mathbf{F}}\|_{L^\infty} &\le C\left(\|\phi_{\mathbf{F}}\|_{H^1}^{\frac{5}{6}}\left\|\Delta^2\phi_{\mathbf{F}}\right\|_{L^2}^{\frac{1}{6}} + \|\phi_{\mathbf{F}}\|_{L^6}\right) \\ &\le C\left(\|\phi_{\mathbf{F}}\|_{H^1}^{\frac{5}{6}}\left\|\Delta^2\phi_{\mathbf{F}}\right\|_{L^2}^{\frac{1}{6}} + \|\phi_{\mathbf{F}}\|_{H^1}\right)\end{aligned}$$

$$\leq C\left(\|\phi\|_{H_h^1}^{\frac{5}{6}}\left\|\Delta_h^2\phi\right\|_2^{\frac{1}{6}}+\|\phi\|_{H_h^1}\right), \tag{B.24}$$

in which the 3D Gagliardo–Nirenberg inequality and Sobolev embedding were applied, and the equivalence estimates (B.15), (B.17), and (B.18) were recalled in the derivation.

The second discrete Gagliardo–Nirenberg type inequality (3.7) can be derived in a similar manner. The details are skipped for the sake of brevity.

Finally, the discrete Sobolev embedding (3.8) from H_h^2 into $W^{1,4}$ is based on the following fact:

$$\|\nabla_h\phi\|_4 \leq C\|\nabla\phi_{\mathbf{F}}\|_{L^4} \leq C\|\phi_{\mathbf{F}}\|_{H^2} \leq C\|\phi\|_{H_h^2}, \tag{B.25}$$

in which a detailed Fourier expansion was analyzed in the first step, the continuous embedding was applied in the third step, and the norm equivalence estimate (B.17) was recalled at the last step.

Completing the proof of Lemma 3.1. □

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