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AN ENERGY-STABLE AND CONVERGENT FINITE-DIFFERENCE SCHEME FOR THE PHASE FIELD CRYSTAL EQUATION*

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Abstract. We present an unconditionally energy stable finite-difference scheme for the phase field crystal equation. The method is based on a convex splitting of a discrete energy and is semi-implicit. The equation at the implicit time level is nonlinear but represents the gradient of a strictly convex function and is thus uniquely solvable, regardless of time step size. We present local-in-time error estimates that ensure the convergence of the scheme. While this paper is primarily concerned with the phase field crystal equation, most of the theoretical results hold for the related Swift–Hohenberg equation as well.

Key words. phase field crystal, finite-difference methods, stability, nonlinear partial differential equations

AMS subject classifications. 35G25, 65M06, 65M12

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1. Introduction.

The phase field crystal (PFC) model was recently proposed in [7] as a new approach to simulating crystals at the atomic scale in space but on a coarse-grained diffusive time scale. The PFC model accounts for the periodic structure of a crystal lattice through a free energy functional of Swift–Hohenberg (SH) type [17] that is minimized by periodic functions. The model can account for elastic and plastic deformations of the lattice, dislocations, grain boundaries, and many other observable phenomena. See, for example, the recent review [15] that describes the variety of microstructures that can be modeled using the PFC approach. The idea is that the phase variable describes a coarse-grained temporal average of the number density of atoms, and the approach can be related to dynamic density functional theory [2, 13]. Consequently, this method represents a significant advantage over other atomistic methods, such as molecular dynamics, where the time steps are constrained by atomic-vibration time scales.

Presently, we introduce the PFC equation and the closely related SH equation and give an idea of the numerical schemes detailed in section 3. We also point out some of the previous theoretical and numerical work surrounding the SH and PFC equations.

1.1. Phase field crystal equation.

Herein we consider a dimensionless energy of the form [7, 17]

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

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where $\Omega \subset \mathbf{R}^D$, where $D = 2$ or 3, $\phi : \Omega \to \mathbf{R}$ is the density field, ϵ is a constant, and ∇ and Δ are the gradient and Laplacian operators, respectively. Suppose that $\Omega = (0, L_x) \times (0, L_y)$ and that ϕ and $\Delta\phi$ are periodic on Ω.

We consider two types of gradient dynamics on Ω: (i) nonconserved dynamics (SH) [17],

$$\partial_t \phi = -M\mu, \tag{1.2}$$

where $M > 0$ is a mobility, μ is the chemical potential defined as

$$\mu := \delta_\phi E = \phi^3 + (1-\epsilon)\,\phi + 2\Delta\phi + \Delta^2\phi, \tag{1.3}$$

and $\delta_\phi E$ denotes the variational derivative with respect to ϕ; and (ii) conserved dynamics (PFC) [7],

$$\partial_t \phi = \nabla \cdot (M(\phi)\nabla\mu)\,, \tag{1.4}$$

where $M(\phi) > 0$ is a mobility, and where we assume that μ is periodic on Ω. Because the dynamical equations are of gradient type, it is easy to see that the energy (1.1) is nonincreasing in time along the solution trajectories of either (1.2) or (1.4). Equation (1.4) is a mass conservation equation where the flux is proportional to the gradient of the chemical potential. This, along with the periodic boundary conditions, ensures that $\int_\Omega \partial_t\phi \; d\mathbf{x} = 0$.

Equation (1.2) is referred to as the Swift–Hohenberg (SH) equation [17] and is fourth-order in space. Equation (1.4) is the phase field crystal (PFC) equation and is a sixth-order equation. In this paper we wish to describe a practical computational scheme for solving the PFC equation primarily, though the theory will be applicable to the SH equation as well.

We wish to point out that while periodic boundary conditions are assumed herein, the theory and numerical analysis to follow also hold for homogeneous Neumann boundary conditions, as well as for mixed periodic-homogeneous Neumann boundary conditions.

1.2. Discrete-time, continuous-space schemes. To motivate the fully discrete methods that are to come, we first present related schemes at the discrete-time, continuous-space level. Here the discussion will be formal. However, in the next sections we develop a rigorous theory in the finite-dimensional framework.

The fundamental observation is that the energy E admits a (not necessarily unique) splitting into purely convex and concave energies, that is, $E = E_c - E_e$, where E_c and E_e are convex, though not necessarily strictly convex. Assuming that $\epsilon < 1$, the canonical splitting is

$$E_c = \int_\Omega \left\{ \frac{1}{4}\phi^4 + \frac{1-\epsilon}{2}\phi^2 + \frac{1}{2}\left(\Delta\phi\right)^2 \right\} d\mathbf{x}, \quad E_e = \int_\Omega \left|\nabla\phi\right|^2 \, d\mathbf{x}. \tag{1.5}$$

We note that the splitting is easy to modify in the case that $\epsilon > 1$. This observation about convex splitting was first exploited by Eyre [8] to craft energy-stable numerical schemes. We borrow the notation E_c and E_e from [8], where c refers to the contractive part of the energy, and e refers to the expansive part of the energy. The schemes we propose are of the type proposed by Eyre, but the theory to establish solvability and energy stability here is more direct and more complete. (We also point out that Eyre did not specifically consider the SH or PFC equations, though his framework was

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sufficiently general to do so.) In particular, we show that some of the assumptions made in [8] are unnecessary to prove energy (or gradient) stability. More importantly, we also establish solvability, convergence, and an error estimate for the numerical method for the conserved dynamics case (PFC), which were not pursued in [8].

Our approach is based upon the following simple, but fundamental, estimate that was not utilized in [8]. We will be primarily interested in its finite-dimensional counterpart in section 3.

THEOREM 1.1. *Suppose that* $\Omega = (0, L_x) \times (0, L_y)$ *and* ϕ, $\psi : \Omega \to \mathbf{R}$ *are periodic and sufficiently regular, and suppose that* $\Delta\phi$ *and* $\Delta\psi$ *are also periodic. Consider the canonical convex splitting of the energy* E *in* (1.1) *into* $E = E_c - E_e$ *given in* (1.5). *Then*

$$E(\phi) - E(\psi) \le \left(\delta_\phi E_c(\phi) - \delta_\phi E_e(\psi), \phi - \psi\right)_{L^2}, \tag{1.6}$$

where δ_ϕ *denotes the variational derivative.*

Proof. Let $E_c(\phi) = \int_\Omega e_c(\phi, \partial_x\phi, \partial_y\phi, \Delta\phi)\, d\mathbf{x}$. Since $e_c(\boldsymbol{\phi})$, where $\boldsymbol{\phi} = \big(\phi_1, \phi_2, \phi_3, \phi_4\big)$, is convex in all of its arguments we have the equivalent statement

$$e_c(\boldsymbol{\psi}) - e_c(\boldsymbol{\phi}) \ge \nabla_{\boldsymbol{\phi}} e_c(\boldsymbol{\phi}) \cdot (\boldsymbol{\psi} - \boldsymbol{\phi}) \tag{1.7}$$

for any $\boldsymbol{\phi}$, $\boldsymbol{\psi} \in \mathbf{R}^4$. Setting $\boldsymbol{\phi} = (\phi, \partial_x\phi, \partial_y\phi, \Delta\phi)$ and $\boldsymbol{\psi} = (\psi, \partial_x\psi, \partial_y\psi, \Delta\psi)$ and integrating (1.7) we get

$$\begin{aligned} E_c(\psi) - E_c(\phi) \ge \int_\Omega \Big\{ & \partial_\phi e_c(\phi, \partial_x\phi, \partial_y\phi, \Delta\phi)(\psi - \phi) \\ & + \partial_{\partial_x\phi} e_c(\phi, \partial_x\phi, \partial_y\phi, \Delta\phi)(\partial_x\psi - \partial_x\phi) \\ & + \partial_{\partial_y\phi} e_c(\phi, \partial_x\phi, \partial_y\phi, \Delta\phi)(\partial_y\psi - \partial_y\phi) \\ & + \partial_{\Delta\phi} e_c(\phi, \partial_x\phi, \partial_y\phi, \Delta\phi)(\Delta\psi - \Delta\phi) \Big\} d\mathbf{x}. \end{aligned} \tag{1.8}$$

Integration by parts leads to the inequality [6, Chap. 2]

$$E_c(\psi) - E_c(\phi) \ge \left(\delta_\phi E_c(\phi), \psi - \phi\right)_{L^2}. \tag{1.9}$$

By a similar analysis on E_e, but reversing the roles of $\boldsymbol{\phi}$ and $\boldsymbol{\psi}$, we have

$$E_e(\phi) - E_e(\psi) \ge \left(\delta_\phi E_e(\psi), \phi - \psi\right)_{L^2}. \tag{1.10}$$

Adding (1.9) and (1.10) yields

$$\begin{aligned} E(\psi) - E(\phi) &= E_c(\psi) - E_e(\psi) - (E_c(\phi) - E_e(\phi)) \\ &\ge \left(\delta_\phi E_c(\phi), \psi - \phi\right)_{L^2} + \left(\delta_\phi E_e(\psi), \phi - \psi\right)_{L^2} \\ &= \left(\delta_\phi E_c(\phi) - \delta_\phi E_e(\psi), \psi - \phi\right)_{L^2}. \qquad \square \end{aligned} \tag{1.11}$$

For nonconserved dynamics we propose the semi-implicit scheme

$$\phi^{k+1} - \phi^k = -sM\tilde{\mu}, \quad \tilde{\mu}\left(\phi^{k+1}, \phi^k\right) := \delta_\phi E_c(\phi^{k+1}) - \delta_\phi E_e(\phi^k), \tag{1.12}$$

where $s > 0$ is the time step size. Here $\delta_\phi E_c = \phi^3 + (1-\epsilon)\phi + \Delta^2\phi$, and $\delta_\phi E_e = -2\Delta\phi$. Setting $\phi = \phi^{k+1}$ and $\psi = \phi^k$ in (1.6) and using (1.12) we have

$$\begin{aligned} E(\phi^{k+1}) - E(\phi^k) &\le \left(\delta_\phi E_c(\phi^{k+1}) - \delta_\phi E_e(\phi^k), \phi^{k+1} - \phi^k\right)_{L^2} \\ &= \left(\tilde{\mu}, -sM\tilde{\mu}\right)_{L^2} = -sM \left\|\tilde{\mu}\right\|_{L^2}^2 \le 0. \end{aligned} \tag{1.13}$$

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Hence the energy is nonincreasing in time, regardless of time step size:

$$E(\phi^{k+1}) \le E(\phi^k). \tag{1.14}$$

In this case we say that the scheme is unconditionally energy stable. Note also that the scheme (1.12) is unconditionally solvable based on the convex structure of the equations, but is generally nonlinear.

For conserved dynamics we propose the semi-implicit scheme

$$\phi^{k+1} - \phi^k = s\nabla\cdot\left(M(\phi^k)\nabla\tilde{\mu}\right), \quad \tilde{\mu}\left(\phi^{k+1},\phi^k\right) := \delta_\phi E_c(\phi^{k+1}) - \delta_\phi E_e(\phi^k). \tag{1.15}$$

Again we set $\phi = \phi^{k+1}$ and $\psi = \phi^k$ in (1.6) and find

$$\begin{aligned} E(\phi^{k+1}) - E(\phi^k) &\le \left(\delta_\phi E_c(\phi^{k+1}) - \delta_\phi E_e(\phi^k), \phi^{k+1} - \phi^k\right)_{L^2} \\ &= s\left(\tilde{\mu}, \nabla\cdot\left(M(\phi^k)\nabla\tilde{\mu}\right)\right)_{L^2} \\ &= -s\left(\nabla\tilde{\mu}, M(\phi^k)\nabla\tilde{\mu}\right)_{L^2} \le 0, \end{aligned} \tag{1.16}$$

where we have dropped the boundary terms (coming from integration-by-parts) using the periodicity of $\tilde{\mu}$. As before, the energy is always nonincreasing in time,

$$E(\phi^{k+1}) \le E(\phi^k), \tag{1.17}$$

and thus the scheme is unconditionally energy stable. Moreover, we expect that it is unconditionally solvable based on convexity arguments. For both schemes, the global truncation error is first-order in time. We reiterate that schemes of this type were proposed by Eyre [8], primarily for solving the Cahn–Hilliard [4, 3] and Allen–Cahn [1] equations, but our analysis here is both more direct and more complete. We also note that the methodology herein is quite general and applicable to a broad class of gradient problems.

There has been some limited work developing stable schemes for the PFC equation recently. Cheng and Warren [5] and Mellenthin, Karma, and Plapp [14] describe linear spectral schemes for solving the PFC equation on periodic domains. Cheng and Warren's scheme is similar to one for the Cahn–Hilliard equation analyzed in [18] and depends upon a Fourier stability analysis of a linearized PFC equation, where, in particular, the nonlinear term ϕ^3 in the chemical potential is treated explicitly. Mellenthin et al. use an integrating factor approach. Neither method is a convex splitting scheme. The finite element method of Backofen, Rätz, and Voigt [2] employs what is essentially a standard backward Euler scheme, but where the nonlinear term ϕ^3 in the chemical potential is linearized via $(\phi^{k+1})^3 \approx 3(\phi^k)^2\phi^{k+1} - 2(\phi^k)^3$. No stability analysis is given, though they claim that relatively large step sizes can be achieved. None of the preceding works claim to propose rigorously (energy-)stable methods. The schemes mentioned above are linear, and consequently conditions on solvability are somewhat more accessible than in the nonlinear case. We point out that because Backofen et al. keep the $2\Delta\phi$ term implicit in the treatment of the chemical potential, their scheme is not expected to be unconditionally uniquely solvable.

We mention that an alternate approach to the nonlinear splitting scheme proposed here is a linear splitting scheme, as was suggested by Eyre [8] for the Cahn–Hilliard equation and by Xu and Tang [20] for a bistable epitaxial thin film equation. This would involve a splitting of the chemical potential such as

$$\tilde{\mu} = A\left(\phi^{k+1} - \phi^k\right) - B\left(\Delta\phi^{k+1} - \Delta\phi^k\right) + \Delta^2\phi^{k+1} + \left(\phi^k\right)^3 + (1-\epsilon)\,\phi^k + 2\Delta\phi^k\ ,$$

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where the splitting parameters $A, B \geq 0$ must be determined in order to ensure stability. Unconditional unique solvability is guaranteed, thanks to the linearity and positivity of the respective terms. It is expected that, as in [20], the energy will be nonincreasing in time, provided A and B are sufficiently large, but that such A and B will depend on the unknown ϕ^{k+1} [20, inequality (2.14)].

In what follows we demonstrate that the convex-splitting framework outlined in this section has an analogue in the finite-dimensional setting using difference operators. In section 2 we describe the two-dimensional finite-difference operators, summation-by-parts formulae, discrete norms, and discrete estimates that will facilitate the definition and analysis of our schemes. In section 3 we present the main results of our analysis, including the unique solvability, discrete-energy stability, and convergence of our schemes. We give some concluding remarks and suggest some future work in section 4.

2. Discretization of two-dimensional space. Our primary goal in this section is to define finite-difference operators and summation-by-parts formulae in two space dimensions needed to define and analyze the schemes. We begin by establishing some machinery in one space dimension.

2.1. One-dimensional difference operators and summation-by-parts formulae. Suppose $\Omega = (0, L)$. Let $h = L/n$, where $n \in \mathbf{Z}^+$. We define the function $x_r = x(r) := (r - 1/2) \cdot h$, where r takes on integer and half-integer values, and the following three sets: $E_n = \{x_{i+1/2} \mid i = 0, \ldots, n\}$, $C_n = \{x_i \mid i = 1, \ldots, n\}$, and $C_{\overline{n}} = \{x_i \mid i = 0, \ldots, n+1\}$. We define by $\mathcal{E}_n$ the space of functions whose domains equal E_n. The functions of $\mathcal{E}_n$ are called edge-centered functions, and we reserve the symbols f and g to denote them. In component form, these functions are identified via $f_{i+1/2} := f(x_{i+1/2})$ for $i = 0, \ldots, n$. By $\mathcal{C}_n$ we denote the vector space of functions whose domains are equal to C_n, and by $\mathcal{C}_{\overline{n}}$ we denote the space of functions whose domains equal $C_{\overline{n}}$. The functions of $\mathcal{C}_n$ and $\mathcal{C}_{\overline{n}}$ are called cell-centered functions, and we use the Greek symbols ϕ, ψ, and ζ to denote them. In component form, these functions are identified via $\phi_i := \phi(x_i)$, where $i = 1, \ldots, n$ if $\phi \in \mathcal{C}_n$, and $i = 0, \ldots, n+1$ if $\phi \in \mathcal{C}_{\overline{n}}$.

Let ϕ and ψ be cell-centered, and let f and g be edge-centered. We define the respective inner-products on $\mathcal{C}_n$ and $\mathcal{E}_n$:

$$(\phi|\psi) = \sum_{i=1}^{n} \phi_i \psi_i, \quad [f|g] = \frac{1}{2} \sum_{i=1}^{n} \left(f_{i-1/2} g_{i-1/2} + f_{i+1/2} g_{i+1/2} \right). \tag{2.1}$$

The edge-to-center difference operator $d : \mathcal{E}_n \to \mathcal{C}_n$; the center-to-edge average and difference operators, respectively, $A, D : \mathcal{C}_{\overline{n}} \to \mathcal{E}_n$; and the discrete Laplacian operator $\Delta_h : \mathcal{C}_{\overline{n}} \to \mathcal{C}_n$ are defined componentwise as

$$df_i = \frac{1}{h} \left(f_{i+1/2} - f_{i-1/2} \right), \ i = 1, \ldots, n, \tag{2.2}$$

$$A\phi_{i+1/2} = \frac{1}{2} \left(\phi_i + \phi_{i+1} \right), \ D\phi_{i+1/2} = \frac{1}{h} \left(\phi_{i+1} - \phi_i \right), \ i = 0, \ldots, n, \tag{2.3}$$

$$\Delta_h \phi_i = d \left(D\phi \right)_i = \frac{1}{h^2} \left(\phi_{i-1} - 2\phi_i + \phi_{i+1} \right), \ i = 1, \ldots, n. \tag{2.4}$$

The following summation-by-parts formulae are established straightforwardly.

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PROPOSITION 2.1. *Let ϕ, $\psi \in \mathcal{C}_{\overline{n}}$ and $f \in \mathcal{E}_n$. Then*

$$h\,[D\phi|f] = -h\,(\phi|df) - A\phi_{1/2}f_{1/2} + A\phi_{n+1/2}f_{n+1/2}, \tag{2.5}$$

$$h\,[D\phi|D\psi] = -h\,(\phi|\Delta_h\psi) - A\phi_{1/2}D\psi_{1/2} + A\phi_{n+1/2}D\psi_{n+1/2}, \tag{2.6}$$

$$\begin{aligned} h\,(\phi|\Delta_h\psi) = h\,(\Delta_h\phi|\psi) &+ A\phi_{n+1/2}D\psi_{n+1/2} - D\phi_{n+1/2}A\psi_{n+1/2} \\ &- A\phi_{1/2}D\psi_{1/2} + D\phi_{1/2}A\psi_{1/2}. \end{aligned} \tag{2.7}$$

2.2. Two-dimensional difference operators and summation-by-parts formulae. Let $\Omega = (0, L_x) \times (0, L_y)$, where $L_x = m \cdot h$ and $L_y = n \cdot h$, where $h > 0$. As in the one-dimensional case, we define E_m, C_m, and $C_{\overline{m}}$ with respect to $(0, L_x)$ and E_n, C_n, and $C_{\overline{n}}$ with respect to $(0, L_y)$. Define the function spaces

$$\mathcal{C}_{m\times n} = \{\phi : C_m \times C_n \to \mathbf{R}\}, \quad \mathcal{C}_{\overline{m}\times\overline{n}} = \{\phi : C_{\overline{m}} \times C_{\overline{n}} \to \mathbf{R}\}, \tag{2.8}$$

$$\mathcal{C}_{\overline{m}\times n} = \{\phi : C_{\overline{m}} \times C_n \to \mathbf{R}\}, \quad \mathcal{C}_{m\times\overline{n}} = \{\phi : C_m \times C_{\overline{n}} \to \mathbf{R}\}, \tag{2.9}$$

$$\mathcal{E}^{\rm ew}_{m\times n} = \{f : E_m \times C_n \to \mathbf{R}\}, \quad \mathcal{E}^{\rm ns}_{m\times n} = \{f : C_m \times E_n \to \mathbf{R}\}. \tag{2.10}$$

The functions of $\mathcal{C}_{m\times n}$, $\mathcal{C}_{\overline{m}\times\overline{n}}$, $\mathcal{C}_{\overline{m}\times n}$, and $\mathcal{C}_{m\times\overline{n}}$ are called cell-centered functions, and we use the Greek symbols ϕ, ψ, and ζ to denote them. In component form these functions are identified via $\phi_{i,j} : \phi(x_i, y_j)$, where, like x_r, $y_r = (r - 1/2) \cdot h$. The functions of $\mathcal{E}^{\rm ew}_{m\times n}$ and $\mathcal{E}^{\rm ns}_{m\times n}$ are called east-west edge-centered functions and north-south edge-centered functions, respectively. We use the symbols f and g to denote these functions. In component form east-west edge-centered functions are identified via $f_{i+1/2,j} := f(x_{i+1/2}, y_j)$; north-south edge-centered functions are identified via $f_{i,j+1/2} := f(x_i, x_{j+1/2})$.

We define the following weighted inner-products:

$$(\phi\|\psi) = \sum_{i=1}^{m}\sum_{j=1}^{n} \phi_{i,j}\psi_{i,j}, \quad \phi,\, \psi \in \mathcal{C}_{m\times n} \cup \mathcal{C}_{\overline{m}\times n} \cup \mathcal{C}_{m\times\overline{n}} \cup \mathcal{C}_{\overline{m}\times\overline{n}}, \tag{2.11}$$

$$[f\|g]_{\rm ew} = \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{n} \left(f_{i+1/2,j}g_{i+1/2,j} + f_{i-1/2,j}g_{i-1/2,j}\right), \quad f,\, g \in \mathcal{E}^{\rm ew}_{m\times n}, \tag{2.12}$$

$$[f\|g]_{\rm ns} = \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{n} \left(f_{i,j+1/2}g_{i,j+1/2} + f_{i,j-1/2}g_{i,j-1/2}\right), \quad f,\, g \in \mathcal{E}^{\rm ns}_{m\times n}. \tag{2.13}$$

The edge-to-center differences, $d_x : \mathcal{E}^{\rm ew}_{m\times n} \to \mathcal{C}_{m\times n}$ and $d_y : \mathcal{E}^{\rm ns}_{m\times n} \to \mathcal{C}_{m\times n}$; the center-to-edge averages and differences, $A_x, D_x : \mathcal{C}_{\overline{m}\times n} \to \mathcal{E}^{\rm ew}_{m\times n}$ and $A_y, D_y : \mathcal{C}_{m\times\overline{n}} \to \mathcal{E}^{\rm ew}_{m\times n}$; and the two-dimensional discrete Laplacian, $\Delta_h : \mathcal{C}_{\overline{m}\times\overline{n}} \to \mathcal{C}_{m\times n}$, are defined componentwise via

$$d_x f_{i,j} = \frac{1}{h}\left(f_{i+1/2,j} - f_{i-1/2,j}\right),\ d_y f_{i,j} = \frac{1}{h}\left(f_{i,j+1/2} - f_{i,j-1/2}\right),\ {\scriptstyle i=1,\dots,m \atop j=1,\dots,n}, \tag{2.14}$$

$$A_x\phi_{i+1/2,j} = \frac{1}{2}\left(\phi_{i,j} + \phi_{i+1,j}\right),\ D_x\phi_{i+1/2,j} = \frac{1}{h}\left(\phi_{i+1,j} - \phi_{i,j}\right),\ {\scriptstyle i=0,\dots,m \atop j=1,\dots,n}, \tag{2.15}$$

$$A_y\phi_{i,j+1/2} = \frac{1}{2}\left(\phi_{i,j} + \phi_{i,j+1}\right),\ D_y\phi_{i,j+1/2} = \frac{1}{h}\left(\phi_{i,j+1} - \phi_{i,j}\right),\ {\scriptstyle i=1,\dots,m \atop j=0,\dots,n}, \tag{2.16}$$

$$\Delta_h\psi_{i,j} = d_x(D_x\psi)_{i,j} + d_y(D_y\psi)_{i,j},\ {\scriptstyle i=1,\dots,m \atop j=1,\dots,n}. \tag{2.17}$$

The following formulae follow directly.

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PROPOSITION 2.2. *If* $\phi,\,\psi \in \mathcal{C}_{\overline{m}\times\overline{n}}$*,* $f \in \mathcal{E}^{\rm ew}_{m\times n}$*, and* $g \in \mathcal{E}^{\rm ns}_{m\times n}$*, then*

$$h^2\,[D_x\phi\|f]_{\rm ew} = -h^2\,(\phi\|d_x f) - h\,\left(A_x\phi_{1/2,\star}\middle|f_{1/2,\star}\right) + h\,\left(A_x\phi_{m+1/2,\star}\middle|f_{m+1/2,\star}\right), \tag{2.18}$$

$$h^2\,[D_y\phi\|g]_{\rm ns} = -h^2\,(\phi\|d_y g) - h\,\left(A_y\phi_{\star,1/2}\middle|g_{\star,1/2}\right) + h\,\left(A_y\phi_{\star,n+1/2}\middle|g_{\star,n+1/2}\right), \tag{2.19}$$

where the $\star$ *indicates the direction along which the one-dimensional inner-product acts, and*

$$\begin{aligned} h^2\,[D_x\phi\|D_x\psi]_{\rm ew} + h^2\,[D_y\phi\|D_y\psi]_{\rm ns} &= -h^2\,(\phi\|\Delta_h\psi) \\ &\quad - h\,\left(A_x\phi_{1/2,\star}\middle|D_x\psi_{1/2,\star}\right) + h\,\left(A_x\phi_{m+1/2,\star}\middle|D_x\psi_{m+1/2,\star}\right) \\ &\quad - h\,\left(A_y\phi_{\star,1/2}\middle|D_y\psi_{\star,1/2}\right) + h\,\left(A_y\phi_{\star,n+1/2}\middle|D_y\psi_{\star,n+1/2}\right), \end{aligned} \tag{2.20}$$

$$\begin{aligned} h^2\,(\phi\|\Delta_h\psi) &= h^2\,(\Delta_h\phi\|\psi) \\ &\quad + h\,\left(A_x\phi_{m+1/2,\star}\middle|D_x\psi_{m+1/2,\star}\right) - h\,\left(D_x\phi_{m+1/2,\star}\middle|A_x\psi_{m+1/2,\star}\right) \\ &\quad - h\,\left(A_x\phi_{1/2,\star}\middle|D_x\psi_{1/2,\star}\right) + h\,\left(D_x\phi_{1/2,\star}\middle|A_x\psi_{1/2,\star}\right) \\ &\quad + h\,\left(A_y\phi_{\star,n+1/2}\middle|D_y\psi_{\star,n+1/2}\right) - h\,\left(D_y\phi_{\star,n+1/2}\middle|A_y\psi_{\star,n+1/2}\right) \\ &\quad - h\,\left(A_y\phi_{\star,1/2}\middle|D_y\psi_{\star,1/2}\right) + h\,\left(D_y\phi_{\star,1/2}\middle|A_y\psi_{\star,1/2}\right). \end{aligned} \tag{2.21}$$

2.3. Periodic boundary conditions. In this paper we use periodic grid functions. Specifically, we shall say the cell-centered function $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is periodic if and only if

$$\phi_{m+1,j} = \phi_{1,j}, \quad \phi_{0,j} = \phi_{m,j}, \quad j = 1,\dots,n, \tag{2.22}$$

$$\phi_{i,n+1} = \phi_{i,1}, \quad \phi_{i,0} = \phi_{i,n}, \quad i = 0,\dots,m+1. \tag{2.23}$$

For such functions, the center-to-edge averages and differences are periodic. For example, if $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is periodic, then $A_x\phi_{m+1/2,j} = A_x\phi_{1/2,j}$ and $D_x\phi_{m+1/2,j} = D_x\phi_{1/2,j}$ for all $j = 0,1,\dots,n+1$. We also note that the results for periodic functions that are to follow will also hold, in possibly slightly modified forms, when the boundary conditions are taken to be homogeneous Neumann,

$$\phi_{m+1,j} = \phi_{m,j}, \quad \phi_{0,j} = \phi_{1,j}, \quad j = 1,\dots,n, \tag{2.24}$$

$$\phi_{i,n+1} = \phi_{i,n}, \quad \phi_{i,0} = \phi_{i,1}, \quad i = 0,\dots,m+1, \tag{2.25}$$

or a mixture of homogeneous Neumann and periodic boundary conditions.

2.4. Norms. We define the following norms for cell-centered functions. If $\phi \in \mathcal{C}_{m\times n}$, then $\|\phi\|_2 := \sqrt{h^2\,(\phi\|\phi)}$, $\|\phi\|_4 := \sqrt{h^2\,(\phi^4\|\mathbf{1})}$, and $\|\phi\|_\infty := \max_{\substack{1\le i\le m\\ 1\le j\le n}} |\phi_{i,j}|$. We define $\|\nabla_h\phi\|_2$, where $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$, to mean

$$\|\nabla_h\phi\|_2 := \sqrt{h^2\,[D_x\phi\|D_x\phi]_{\rm ew} + h^2\,[D_y\phi\|D_y\phi]_{\rm ns}}\,. \tag{2.26}$$

We will use the following discrete Sobolev-type norms for grid functions $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$: $\|\phi\|_{0,2} := \|\phi\|_2$ and

$$\|\phi\|_{1,2} := \sqrt{\|\phi\|_2^2 + \|\nabla_h\phi\|_2^2}, \quad \|\phi\|_{2,2} := \sqrt{\|\phi\|_2^2 + \|\nabla_h\phi\|_2^2 + \|\Delta_h\phi\|_2^2}\,. \tag{2.27}$$

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2.5. Discrete Sobolev inequalities. Here we prove a discrete Sobolev-type inequality for two-dimensional grid functions that will be needed to prove pointwise stability. The primary result is Lemma 2.5. The two preliminary lemmas, Lemmas 2.3 and 2.4, are similar to results proved in [12, sec. 8.6], and we skip their proofs.

LEMMA 2.3. *Suppose that* $\phi \in \mathcal{C}_{\overline{n}}$. *Then, for any* $i \in \{1, 2, \dots, n\}$,

$$|\phi_i|^2 \leq \frac{2}{L} h\ (\phi|\phi) + 2Lh\ [D\phi|D\phi]\,. \tag{2.28}$$

LEMMA 2.4. *Suppose that* $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$. *Then, for any* $i \in \{1, 2, \dots, m\}$ *and any* $j \in \{1, 2, \dots, n\}$,

$$\begin{aligned} |\phi_{i,j}|^2 \leq{}& \frac{4}{L_x L_y} h^2\ (\phi\|\phi) + \frac{4L_x}{L_y} h^2\ [D_x\phi\|D_x\phi]_{\mathrm{ew}} + \frac{4L_y}{L_x} h^2\ [D_y\phi\|D_y\phi]_{\mathrm{ns}} \\ &+ 4L_x L_y h^2 \sum_{i'=0}^{m}\sum_{j'=0}^{n} w_{i'}^m w_{j'}^n \left| D_y\left(D_x\phi\right)_{i'+1/2,j'+1/2}\right|^2, \end{aligned} \tag{2.29}$$

where $w_k^n = 1$ *if* $k \in \{1, 2, \dots, n-1\}$ *and* $w_k^n = 1$ *if* $k \in \{0, n\}$.

LEMMA 2.5. *Suppose that* $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ *is periodic. Then, for any* $i \in \{1, 2, \dots, m\}$ *and any* $j \in \{1, 2, \dots, n\}$,

$$|\phi_{i,j}|^2 \leq 4 \max\left\{\frac{1}{L_x L_y}, \frac{L_x}{L_y}, \frac{L_y}{L_x}, \frac{L_x L_y}{2}\right\} \|\phi\|_{2,2}^2\,. \tag{2.30}$$

Hence $\|\phi\|_\infty \leq C\,\|\phi\|_{2,2}$, *where* C *depends only upon* L_x *and* L_y.

Proof. Using the previous lemma, this result will follow if we can show

$$S := h^2 \sum_{i'=0}^{m}\sum_{j'=0}^{n} w_{i'}^m w_{j'}^n \left| D_y\left(D_x\phi\right)_{i'+1/2,j'+1/2}\right|^2 \leq \frac{1}{2}\,\|\Delta_h\phi\|_2^2\,. \tag{2.31}$$

By definition of the edge inner-product $[\,\cdot\,|\,\cdot\,]$,

$$S = h \sum_{i'=0}^{m} w_{i'}^m h\ \left[D_y\left(D_x\phi\right)_{i'+1/2,\star} \middle| D_y\left(D_x\phi\right)_{i'+1/2,\star}\right]. \tag{2.32}$$

Using summation-by-parts Proposition 2.1 and dropping the boundary terms due to periodicity yields

$$S = -h \sum_{i'=0}^{m} w_{i'}^m h\ \left(\Delta_h^y\left(D_x\phi\right)_{i'+1/2,\star} \middle| D_x\phi_{i'+1/2,\star}\right), \tag{2.33}$$

where $\Delta_h^\square := d_\square D_\square$. Note the commutation of operators: $\Delta_h^y D_x = D_x \Delta_h^y$. Thus,

$$\begin{aligned} S &= -h \sum_{i'=0}^{m} w_{i'}^m h\ \left(D_x\left(\Delta_h^y\phi\right)_{i'+1/2,\star} \middle| D_x\phi_{i'+1/2,\star}\right) \\ &= -h \sum_{i'=0}^{m} w_{i'}^m h \sum_{j'=1}^{n} D_x\left(\Delta_h^y\phi\right)_{i'+1/2,j'} D_x\phi_{i'+1/2,j'} \\ &= -h \sum_{j'=1}^{n} h\ \left[D_x\left(\Delta_h^y\phi\right)_{\star,j'} \middle| D_x\phi_{\star,j'}\right]. \end{aligned} \tag{2.34}$$

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Again, using summation-by-parts Proposition 2.1 and dropping the boundary terms due to periodicity yields

$$\begin{aligned} S &= h\sum_{j'=1}^{n} h\ (\Delta_h^y \phi_{\star,j'} | \Delta_h^x \phi_{\star,j'}) = h^2\ (\Delta_h^y \phi \| \Delta_h^x \phi) \\ &\le h^2\ (\Delta_h^y \phi \| \Delta_h^x \phi) + \frac{h^2}{2}\ (\Delta_h^x \phi \| \Delta_h^x \phi) + \frac{h^2}{2}\ (\Delta_h^y \phi \| \Delta_h^y \phi) \\ &= \frac{h^2}{2}\ (\Delta_h^x \phi + \Delta_h^y \phi \| \Delta_h^x \phi + \Delta_h^y \phi) = \frac{h^2}{2}\ (\Delta_h \phi \| \Delta_h \phi) = \frac{1}{2}\ \|\Delta_h \phi\|_2^2 . \qquad (2.35) \end{aligned}$$

$\square$

3. Main results.

3.1. A convex splitting of the discrete energy.

We begin by defining a fully discrete energy that is consistent with the continuous space energy (1.1). In particular, define the discrete energy $F : \mathcal{C}_{\overline{m}\times\overline{n}} \to \mathbf{R}$ to be

$$F(\phi) := \frac{1}{4}\ \|\phi\|_4^4 + \frac{1-\epsilon}{2}\ \|\phi\|_2^2 - \|\nabla_h \phi\|_2^2 + \frac{1}{2}\ \|\Delta_h \phi\|_2^2 . \qquad (3.1)$$

Lemma 3.1 (existence of a convex splitting). *Suppose that $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is periodic and that $\Delta_h \phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is also periodic. Define the energies*

$$F_c(\phi) := \frac{1}{4}\ \|\phi\|_4^4 + \frac{1-\epsilon}{2}\ \|\phi\|_2^2 + \frac{1}{2}\ \|\Delta_h \phi\|_2^2 , \quad F_e(\phi) := \|\nabla_h \phi\|_2^2 . \qquad (3.2)$$

Then the gradients of the respective energies are $\delta_\phi F_c = \phi^3 + (1-\epsilon)\phi + \Delta_h^2 \phi$ and $\delta_\phi F_e = -2\Delta_h \phi$, and F_c and F_e are convex, provided $\epsilon < 1$. Hence F, as defined in (3.1)*, admits the convex splitting $F = F_c - F_e$.*

Proof. Suppose that $\psi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is periodic such that $\Delta_h \psi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is also periodic. Calculating the (discrete) variation of F_c and using summation-by-parts (Proposition 2.2, eq. (2.21)) shows

$$\left.\frac{dF_c}{ds}(\phi + s\psi)\right|_{s=0} = h^2\ \left(\phi^3 + (1-\epsilon)\phi + \Delta_h^2 \phi \middle\| \psi\right) , \qquad (3.3)$$

and the gradient formula follows. A calculation of the second variation reveals

$$\left.\frac{d^2F_c}{ds^2}(\phi + s\psi)\right|_{s=0} = h^2\ \left(3\phi^2\psi^2 + (1-\epsilon)\psi^2 + (\Delta_h \psi)^2 \middle\| \mathbf{1}\right) \ge 0 , \qquad (3.4)$$

which proves that F_c is convex. (In fact it is strictly convex.) For F_e, calculating the variation and using summation-by-parts (Proposition 2.2, eq. (2.20)) gives

$$\left.\frac{dF_e}{ds}(\phi + s\psi)\right|_{s=0} = -2h^2\ (\Delta_h \phi \| \psi) , \qquad (3.5)$$

which yields the gradient. Consider the second variation of the energy:

$$\frac{d^2F_D}{ds^2}(\phi + s\psi) = 2h^2\ [D_x\psi \| D_x\psi]_{\mathrm{ew}} + 2h^2\ [D_y\psi \| D_y\psi]_{\mathrm{ns}} . \qquad (3.6)$$

Hence, $\left.\frac{d^2F_e}{ds^2}(\phi + s\psi)\right|_{s=0} \ge 0$, which implies that F_e is convex. $\square$

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We now describe the fully discrete schemes in detail. Define the cell-centered chemical potential $\tilde{\mu} \in \mathcal{C}_{\overline{m}\times\overline{n}}$ to be

$$\begin{aligned} \tilde{\mu}\left(\phi^{k+1}, \phi^k\right) &:= \delta_\phi F_c(\phi^{k+1}) - \delta_\phi F_e(\phi^k) \\ &= \left(\phi^{k+1}\right)^3 + (1-\epsilon)\phi^{k+1} + 2\Delta_h \phi^k + \Delta_h \kappa, \end{aligned} \tag{3.7}$$

where $\kappa := \Delta_h \phi^{k+1}$. The semi-implicit scheme for nonconserved dynamics, i.e., the SH equation, is as follows: given $\phi^k \in \mathcal{C}_{\overline{m}\times\overline{n}}$ periodic, find ϕ^{k+1}, $\kappa \in \mathcal{C}_{\overline{m}\times\overline{n}}$ periodic such that

$$\phi^{k+1} - \phi^k = -sM\tilde{\mu}, \quad M > 0. \tag{3.8}$$

The scheme for conserved dynamics, i.e., the PFC equation, is the following: given $\phi^k \in \mathcal{C}_{\overline{m}\times\overline{n}}$ periodic, find ϕ^{k+1}, $\tilde{\mu}$, $\kappa \in \mathcal{C}_{\overline{m}\times\overline{n}}$ periodic such that

$$\phi^{k+1} - \phi^k = s\Big\{ d_x\left(M\left(A_x\phi^k\right) D_x\tilde{\mu}\right) + d_y\left(M\left(A_y\phi^k\right) D_y\tilde{\mu}\right)\Big\}, \quad M(\phi) > 0. \tag{3.9}$$

3.2. Unconditional unique solvability. We now show how the convexity translates into solvability for the schemes. We first need two lemmas that will help prove solvability for the mass-conserving scheme (3.9).

LEMMA 3.2. *Suppose the edge-centered functions $M^{\mathrm{ew}} \in \mathcal{E}^{\mathrm{ew}}_{m\times n}$ and $M^{\mathrm{ns}} \in \mathcal{E}^{\mathrm{ns}}_{m\times n}$ are positive. For any $\phi \in \mathcal{C}_{m\times n}$, there exists a unique $\psi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ that solves*

$$L(\psi) := -d_x\left(M^{\mathrm{ew}} D_x\psi\right) - d_y\left(M^{\mathrm{ns}} D_y\psi\right) = \phi - \frac{1}{m\cdot n}\left(\phi\|\mathbf{1}\right), \tag{3.10}$$

$$\psi \textit{ is periodic and } (\psi\|\mathbf{1}) = 0. \tag{3.11}$$

Proof. Write $\hat{\phi} = \phi - (\phi\|\mathbf{1})/(m\cdot n)$ so that $\hat{\phi}$ has mean zero, i.e., $\left(\hat{\phi}\big\|\mathbf{1}\right) = 0$. Then (3.10) is $L(\psi) = \hat{\phi}$. Assuming that ψ is a periodic solution of the last equation, then the necessity of $\left(\hat{\phi}\big\|\mathbf{1}\right) = 0$ follows from

$$\begin{aligned} \left(\hat{\phi}\Big\|\mathbf{1}\right) &= -\left(d_x\left(M^{\mathrm{ew}} D_x\psi\right)\|\mathbf{1}\right) - \left(d_y\left(M^{\mathrm{ns}} D_y\psi\right)\|\mathbf{1}\right) \\ &= \left[M^{\mathrm{ew}} D_x\psi\|D_x\mathbf{1}\right]_{\mathrm{ew}} + \left[M^{\mathrm{ns}} D_y\psi\|D_y\mathbf{1}\right]_{\mathrm{ns}} = 0. \end{aligned} \tag{3.12}$$

We now show that L is symmetric and positive definite restricted to the subspace of mean-zero functions. Symmetry follows from the next calculation. Suppose ψ_1, $\psi_2 \in \mathcal{C}_{\overline{m}\times\overline{n}}$ are periodic. Then using summation-by-parts,

$$\begin{aligned} \left(\psi_1\|L(\psi_2)\right) &= \left(\psi_1\|-d_x\left(M^{\mathrm{ew}} D_x\psi_2\right) - d_y\left(M^{\mathrm{ns}} D_y\psi_2\right)\right) \\ &= \left[D_x\psi_1\|M^{\mathrm{ew}} D_x\psi_2\right]_{\mathrm{ew}} + \left[D_y\psi_1\|M^{\mathrm{ns}} D_y\psi_2\right]_{\mathrm{ns}} \\ &= \left[M^{\mathrm{ew}} D_x\psi_1\|D_x\psi_2\right]_{\mathrm{ew}} + \left[M^{\mathrm{ns}} D_y\psi_1\|D_y\psi_2\right]_{\mathrm{ns}} \\ &= \left(-d_x\left(M^{\mathrm{ew}} D_x\psi_1\right) - d_y\left(M^{\mathrm{ns}} D_y\psi_1\right)\|\psi_2\right) \\ &= \left(L(\psi_1)\|\psi_2\right), \end{aligned} \tag{3.13}$$

where the boundary terms vanish because of periodicity. Setting $\psi = \psi_1 = \psi_2$,

$$\left(\psi\|L(\psi)\right) = \left[M^{\mathrm{ew}} D_x\psi\|D_x\psi\right]_{\mathrm{ew}} + \left[M^{\mathrm{ns}} D_y\psi\|D_y\psi\right]_{\mathrm{ns}} \geq 0, \tag{3.14}$$

from which we get that L is positive semidefinite. Equality in the last line is achieved only when $D_x\psi = 0$ and $D_y\psi = 0$ at *every* edge-centered point. However, the only

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way that $D_x\psi = 0$ and $D_y\psi = 0$ at *every* edge point is if ψ is a constant function (as may be easily shown). With the restriction that ψ has mean zero, $(\psi\|\mathbf{1}) = 0$, this constant must be zero, which proves that L is positive definite. ∎

Suppose the edge-centered functions $M^{\rm ew} \in \mathcal{E}^{\rm ew}_{m\times n}$ and $M^{\rm ns} \in \mathcal{E}^{\rm ns}_{m\times n}$ are positive. Define the vector space

$$H := \{\phi \in \mathcal{C}_{m\times n} |\, (\phi\|\mathbf{1}) = 0\}\,, \tag{3.15}$$

and equip this space with the bilinear form

$$(\phi_1\|\phi_2)_{H,L} := [M^{\rm ew} D_x\psi_1\|D_x\psi_2]_{\rm ew} + [M^{\rm ns} D_y\psi_1\|D_y\psi_2]_{\rm ns} \tag{3.16}$$

for any ϕ_1, $\phi_2 \in H$, where $\psi_i \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is the unique solution to

$$L(\psi_i) = -d_x\left(M^{\rm ew} D_x\psi_i\right) - d_y\left(M^{\rm ns} D_y\psi_i\right) = \phi_i, \quad \psi_i \text{ periodic}, \quad (\psi_i\|\mathbf{1}) = 0. \tag{3.17}$$

If $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$, then we take $\phi \in H$ to mean that the restriction of ϕ to $C_m \times C_n$ is in H.

LEMMA 3.3. $(\phi_1\|\phi_2)_{H,L}$ *is an inner-product on the space* H. *Moreover,*

$$(\phi_1\|\phi_2)_{H,L} = \left(\phi_1\middle\|L^{-1}(\phi_2)\right) = \left(L^{-1}(\phi_1)\middle\|\phi_2\right). \tag{3.18}$$

Proof. Since L is symmetric and positive definite (SPD), it has an inverse, L^{-1}, and the inverse must also be SPD. The equality of the three bilinear forms follows from summation-by-parts, and $\left(\phi_1\middle\|L^{-1}(\phi_2)\right)$ is easily seen to be an inner-product. ∎

THEOREM 3.4 (unique solvability). *The nonconserved scheme* (3.8) *and the conserved scheme* (3.9) *are uniquely solvable for any time step size* $s > 0$. *Moreover, the scheme* (3.9) *is discretely mass conserving, i.e.,* $\left(\phi^{k+1} - \phi^k\middle\|\mathbf{1}\right) = 0$.

Proof. Unique solvability of the nonconserved scheme results from the fact that the functional

$$G(\phi) = \frac{h^2}{2}(\phi\|\phi) + sMF_c(\phi) - h^2\,\left(\phi\middle\|\phi^k + sM\delta_\phi F_e(\phi^k)\right) \tag{3.19}$$

is *strictly* convex with respect to ϕ, and its minimization is equivalent to solving (3.8).

Discrete mass conservation of (3.9) follows from

$$\begin{aligned}\left(\phi^{k+1} - \phi^k\middle\|\mathbf{1}\right) &= s\left(d_x\left(M\left(A_x\phi^k\right)D_x\tilde{\mu}\right) + d_y\left(M\left(A_y\phi^k\right)D_y\tilde{\mu}\right)\middle\|\mathbf{1}\right)\\ &= -s\left[M\left(A_x\phi^k\right)D_x\tilde{\mu}\middle\|D_x\mathbf{1}\right]_{\rm ew} - s\left[M\left(A_y\phi^k\right)D_y\tilde{\mu}\middle\|D_y\mathbf{1}\right]_{\rm ns}\\ &= 0.\end{aligned} \tag{3.20}$$

Thus, if (3.9) has a solution ϕ^{k+1}, then by necessity it must be that $\left(\phi^{k+1}\middle\|\mathbf{1}\right) = \left(\phi^k\middle\|\mathbf{1}\right)$; i.e., ϕ^{k+1} and ϕ^k have equal means.

Now, without loss of generality, we may suppose that $\phi^k \in H$, where H is the subspace of mean-zero functions in $\mathcal{C}_{m\times n}$ defined above. The appropriate space for solutions of (3.9) must necessarily be H. Now consider the following functional on H:

$$G(\phi) = \frac{h^2}{2}(\phi\|\phi)_{H,L} - h^2\,\left(\phi\middle\|\phi^k\right)_{H,L} + F_c(\phi) - h^2\,\left(\phi\middle\|\delta_\phi F_e(\phi^k)\right), \tag{3.21}$$

where the H inner-product is defined as

$$(\phi_1\|\phi_2)_{H,L} := \left[sM(A_x\phi^k)D_x\psi_1\middle\|D_x\psi_2\right]_{\rm ew} + \left[sM(A_y\phi^k)D_y\psi_1\middle\|D_y\psi_2\right]_{\rm ns}, \tag{3.22}$$

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and $\psi_i \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is the unique solution (by Lemma 3.2) to

$$L(\psi_i) = -sd_x\left(M(A_x\phi^k)D_x\psi_i\right) - sd_y\left(M(A_y\phi^k)D_y\psi_i\right) = \phi_i, \tag{3.23}$$

such that ψ_i is periodic and is mean-zero $(\psi_i\|\mathbf{1}) = 0$. By Lemma 3.3, G is equivalent to

$$G(\phi) = \frac{h^2}{2}\left(L^{-1}(\phi)\big\|\phi\right) - h^2\left(L^{-1}(\phi)\big\|\phi^k\right) + F_c(\phi) - h^2\left(\phi\big\|\delta_\phi F_e(\phi^k)\right), \tag{3.24}$$

and it is clear that this functional is strictly convex if ϕ is restricted to H. Moreover, it may be shown that $\phi^{k+1} \in H$ is the unique minimizer of G if and only if it solves

$$\delta_\phi G(\phi^{k+1}) = L^{-1}(\phi^{k+1} - \phi^k) + \delta_\phi F_c(\phi^{k+1}) - \delta F_e(\phi^k) - C = 0, \tag{3.25}$$

where C is a constant. Since $L^{-1}(\phi^{k+1} - \phi^k)$ has zero mean, it must be that $\delta_\phi F_c(\phi^{k+1}) - \delta F_e(\phi^k) - C$ has zero mean, in which case

$$C = \frac{1}{m\cdot n}\left(\delta_\phi F_c(\phi^{k+1}) - \delta F_e(\phi^k)\big\|\mathbf{1}\right). \tag{3.26}$$

Applying the invertible operator L to (3.25) we have

$$\phi^{k+1} - \phi^k = s\left\{d_x\left(M\left(A_x\phi^k\right)D_x\tilde{\mu}\right) + d_y\left(M\left(A_y\phi^k\right)D_y\tilde{\mu}\right)\right\} + L(C). \tag{3.27}$$

But, of course, $L(C) = 0$. Hence minimizing the strictly convex functional (3.24) is equivalent to solving (3.9). ∎

3.3. Unconditional stability. The following is a discrete version of Theorem 1.1.

THEOREM 3.5 (energy decay estimate). *Suppose that ϕ^{k+1}, $\phi^k \in \mathcal{C}_{\overline{m}\times\overline{n}}$ are periodic and that $\Delta_h\phi^{k+1} \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is also periodic. Assume that the discrete energy F is as given in* (3.1)*, and take the convex splitting $F = F_c - F_e$ in Lemma* 3.1*. Then*

$$F(\phi^{k+1}) - F(\phi^k) \le h^2\left(\delta_\phi F_c(\phi^{k+1}) - \delta_\phi F_e(\phi^k)\big\|\phi^{k+1} - \phi^k\right). \tag{3.28}$$

Proof. We have, by convexity,

$$F_c\left(\phi^k\right) - F_c\left(\phi^{k+1}\right) \ge h^2\left(\delta_\phi F_c\left(\phi^{k+1}\right)\big\|\phi^k - \phi^{k+1}\right), \tag{3.29}$$

$$F_e\left(\phi^{k+1}\right) - F_e\left(\phi^k\right) \ge h^2\left(\delta_\phi F_e\left(\phi^k\right)\big\|\phi^{k+1} - \phi^k\right). \tag{3.30}$$

Adding the inequalities and multiplying by -1 gives the result. ∎

The energy decay estimate readily yields the energy stability of the schemes.

THEOREM 3.6 (energy stability). *Both the nonconserved* (3.8) *and conserved* (3.9) *schemes are unconditionally (strongly) energy stable, meaning that for any time step size $s > 0$,*

$$F(\phi^{k+1}) \le F(\phi^k). \tag{3.31}$$

Proof. For the nonconserved case, using the energy decay estimate, we have

$$\begin{aligned} F(\phi^{k+1}) - F(\phi^k) &\le h^2\left(\delta_\phi F_c(\phi^{k+1}) - \delta_\phi F_e(\phi^k)\big\|\phi^{k+1} - \phi^k\right) \\ &= h^2\left(\tilde{\mu}\|-sM\tilde{\mu}\right) = -sMh^2\left(\tilde{\mu}\|\tilde{\mu}\right) \\ &\le 0. \end{aligned}$$

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For the conserved case, using the energy decay estimate and summation-by-parts, we have

$$\begin{aligned} F(\phi^{k+1}) - F(\phi^k) &\le h^2 \left(\delta_\phi F_c(\phi^{k+1}) - \delta_\phi F_e(\phi^k) \| \phi^{k+1} - \phi^k\right) \\ &= h^2 \left(\tilde{\mu} \| s \left\{ d_x \left(M \left(A_x \phi^k \right) D_x \tilde{\mu} \right) + d_y \left(M \left(A_y \phi^k \right) D_y \tilde{\mu} \right) \right\}\right) \\ &= -sh^2 \left\{ \left[D_x \tilde{\mu} \| M \left(A_x \phi^k \right) D_x \tilde{\mu} \right]_{\text{ew}} + \left[D_y \tilde{\mu} \| M \left(A_y \phi^k \right) D_y \tilde{\mu} \right]_{\text{ns}} \right\} \\ &\le 0. \qquad \square \end{aligned}$$

Using an idea from [9], we now show that energy stability leads to the uniform boundedness of the discrete solutions. First we need two lemmas.

LEMMA 3.7. *Suppose that* $\phi \in \mathcal{C}_{\overline{m} \times \overline{n}}$ *is periodic. Then*

$$F(\phi) \ge C \|\phi\|_{2,2}^2 - \frac{L_x L_y}{4}, \tag{3.32}$$

where $C > 0$ *is independent of* h.

Proof. First note that, using $(\alpha^2 - 1)^2 \ge 0$, we have

$$\frac{1}{4} \|\phi\|_4^4 \ge \frac{1}{2} \|\phi\|_2^2 - \frac{L_x L_y}{4}. \tag{3.33}$$

We also have the following from summation-by-parts and Cauchy's inequality:

$$\|\nabla_h \phi\|_2^2 = h^2 \left(-\phi \| \Delta_h \phi\right) \le \frac{1}{2\beta} \|\phi\|_2^2 + \frac{\beta}{2} \|\Delta_h \phi\|_2^2, \tag{3.34}$$

valid for any $\beta > 0$. Hence,

$$- \|\nabla_h \phi\|_2^2 + \frac{\beta}{2} \|\Delta_h \phi\|_2^2 \ge -\frac{1}{2\beta} \|\phi\|_2^2. \tag{3.35}$$

Set $a = 1 - \epsilon > 0$. Putting the above estimates together, we have

$$\begin{aligned} F(\phi) &= \frac{1}{4} \|\phi\|_4^4 + \frac{a}{2} \|\phi\|_2^2 - \|\nabla_h \phi\|_2^2 + \frac{1}{2} \|\Delta_h \phi\|_2^2 \\ &\ge \left(\frac{1}{2} + \frac{a}{2} - \frac{1}{2\beta} \right) \|\phi\|_2^2 + \left(\frac{1}{2} - \frac{\beta}{2} \right) \|\Delta_h \phi\|_2^2 - \frac{L_x L_y}{4}. \end{aligned} \tag{3.36}$$

We choose β such that $1/2 + a/2 - 1/2\beta > 0$ and $1/2 - \beta/2 > 0$. The last set of inequalities is equivalent to $1 + a > 1/\beta$ and $1 > \beta$, which always has a solution in the quadrant where β, $a > 0$. In particular, we take $\beta = \beta_0 := 1/\sqrt{1+a}$. Thus

$$F(\phi) \ge K \left(\|\phi\|_2^2 + \|\Delta_h \phi\|_2^2 \right) - \frac{L_x L_y}{4}, \tag{3.37}$$

where $K = \min\left(1/2 + a/2 - 1/2\beta_0, 1/2 - \beta_0/2\right) > 0$. Using inequality (3.34) again, but with $\beta = 1$, we have

$$F(\phi) \ge \frac{2K}{3} \left(\|\phi\|_2^2 + \|\nabla_h \phi\|_2^2 + \|\Delta_h \phi\|_2^2 \right) - \frac{L_x L_y}{4}, \tag{3.38}$$

and the desired result follows. $\square$

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LEMMA 3.8. *Suppose that* $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ *is periodic. Then*

$$F(\phi) \geq C \left\|\phi\right\|_\infty^2 - \frac{L_x L_y}{4}, \tag{3.39}$$

where $C > 0$ *is independent of* h.

Proof. This follows from the discrete Sobolev inequality of Lemma 2.5. ∎

Finally we can prove the uniform pointwise boundedness of the discrete solution of either the SH or PFC scheme.

THEOREM 3.9. *Let* $\Phi(x, y)$ *be a smooth, periodic function on* $\Omega = (0, L_x)\times(0\times L_y)$ *and* $\phi_{i,j}^0 := \Phi(x_i, y_j)$, *and suppose* E *is the continuous energy* (1.1). *Let* $\phi_{i,j}^k \in \mathcal{C}_{\overline{m}\times\overline{n}}$ *be the* k*th periodic solution of either of the schemes* (3.8) *or* (3.9). *Then*

$$\left\|\phi^k\right\|_\infty \leq \sqrt{C_1 E(\Phi) + C_2 L_x L_y}, \tag{3.40}$$

where $C_1, C_2 > 0$ *and neither* C_1 *nor* C_2 *depend on either* s *or* h.

Proof. From the energy stability Theorem 3.6 and the previous Lemma 3.8 we have

$$F(\phi^0) \geq F(\phi^k) \geq C \left\|\phi^k\right\|_\infty^2 - \frac{L_x L_y}{4}, \tag{3.41}$$

where $C > 0$ does not depend upon h. It is straightforward to show (e.g., [9, Cor. 1]) that

$$F(\phi^0) = E(\Phi) + \tau, \quad |\tau| \leq M h^2 \leq M L_x L_y, \tag{3.42}$$

where τ is an approximation error and M is some positive constant that does not depend upon h. Then

$$M L_x L_y + E(\Phi) \geq C \left\|\phi^k\right\|_\infty^2 - \frac{L_x L_y}{4}, \tag{3.43}$$

and the result follows. ∎

3.4. Error estimate for the PFC equation. We conclude this section with a local-in-time error estimate for the PFC equation. A similar result for the SH equation may be obtained without difficulty. For the PFC scheme we will need the following estimate showing control of the backward diffusion term.

LEMMA 3.10. *Suppose that* $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ *is periodic and that* $\Delta_h\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ *is also periodic. Then*

$$\left\|\Delta_h\phi\right\|_2^2 \leq \frac{1}{3\alpha^2}\left\|\phi\right\|_2^2 + \frac{2\alpha}{3}\left\|\nabla_h\left(\Delta_h\phi\right)\right\|_2^2, \tag{3.44}$$

valid for arbitrary $\alpha > 0$.

Proof. Using summation-by-parts (Proposition 2.2, eq. (2.20)) and Cauchy's inequality,

$$\begin{aligned}
\left\|\Delta_h\phi\right\|_2^2 = h^2\left(\Delta_h\phi\|\Delta_h\phi\right) &= h^2\left[-D_x\phi\|D_x\left(\Delta_h\phi\right)\right]_{\mathrm{ew}} + h^2\left[-D_y\phi\|D_y\left(\Delta_h\phi\right)\right]_{\mathrm{ns}} \\
&\leq \frac{h^2}{2\alpha}\left[D_x\phi\|D_x\phi\right]_{\mathrm{ew}} + \frac{h^2\alpha}{2}\left[D_x\left(\Delta_h\phi\right)\|D_x\left(\Delta_h\phi\right)\right]_{\mathrm{ew}} \\
&\quad + \frac{h^2}{2\alpha}\left[D_y\phi\|D_y\phi\right]_{\mathrm{ns}} + \frac{h^2\alpha}{2}\left[D_y\left(\Delta_h\phi\right)\|D_y\left(\Delta_h\phi\right)\right]_{\mathrm{ns}} \\
&= \frac{1}{2\alpha}\left\|\nabla_h\phi\right\|_2^2 + \frac{\alpha}{2}\left\|\nabla_h\left(\Delta_h\phi\right)\right\|_2^2. \qquad (3.45)
\end{aligned}$$

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Again, using summation-by-parts and Cauchy's inequality, we have the estimate

$$\|\nabla_h\phi\|_2^2 = h^2\ [D_x\phi\|D_x\phi]_{\rm ew} + h^2\ [D_y\phi\|D_y\phi]_{\rm ns} = h^2\ (-\phi\|\Delta_h\phi)$$

$$\leq \frac{h^2}{2\alpha}(\phi\|\phi) + \frac{h^2\alpha}{2}(\Delta_h\phi\|\Delta_h\phi) = \frac{1}{2\alpha}\|\phi\|_2^2 + \frac{\alpha}{2}\|\Delta_h\phi\|_2^2. \tag{3.46}$$

Putting the two estimates together, we find

$$\|\Delta_h\phi\|_2^2 \leq \frac{1}{2\alpha}\left(\frac{1}{2\alpha}\|\phi\|_2^2 + \frac{\alpha}{2}\|\Delta_h\phi\|_2^2\right) + \frac{\alpha}{2}\|\nabla_h(\Delta_h\phi)\|_2^2$$

$$= \frac{1}{4\alpha^2}\|\phi\|_2^2 + \frac{1}{4}\|\Delta_h\phi\|_2^2 + \frac{\alpha}{2}\|\nabla_h(\Delta_h\phi)\|_2^2. \tag{3.47}$$

Equivalently,

$$\frac{3}{4}\|\Delta_h\phi\|_2^2 \leq \frac{1}{4\alpha^2}\|\phi\|_2^2 + \frac{\alpha}{2}\|\nabla_h(\Delta_h\phi)\|_2^2, \tag{3.48}$$

and the desired result follows. ∎

The existence and uniqueness of a smooth, periodic solution to the PFC equation may be established using standard techniques. See Remark 3.12. In the following pages we denote this PDE solution by Φ, and in the next theorem we establish an error estimate for the fully discrete approximation to Φ.

THEOREM 3.11 (error estimate). *For simplicity, assume that $M(\phi) = 1$ in* (1.4), *and let $\Omega = (0, L_x) \times (0 \times L_y)$. Given smooth, periodic initial data $\Phi(x, y, t = 0)$, suppose the unique, smooth, periodic solution for the PFC equation* (1.4) *is given by $\Phi(x, y, t)$ on Ω for $0 < t \leq T$, for some $T < \infty$. Define $\Phi_{i,j}^k := \Phi(x_i, y_j, ks)$, and $e_{i,j}^k := \Phi_{i,j}^k - \phi_{i,j}^k$, where $\phi_{i,j}^k \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is kth periodic solution of* (3.9) *with $\phi_{i,j}^0 := \Phi_{i,j}^0$. Then, where $\ell \cdot s = T$,*

$$\left\|e^\ell\right\|_2 \leq C\left(h^2 + s\right), \tag{3.49}$$

provided s is sufficiently small, for some $C > 0$ that is independent of h and s.

Proof. The continuous function Φ solves the discrete equations

$$\Phi^{k+1} - \Phi^k = s\Delta_h\tilde{\mu}\left(\Phi^{k+1}, \Phi^k\right) + s\tau^{k+1}, \tag{3.50}$$

where τ^{k+1} is the local truncation error, which satisfies

$$\left|\tau_{i,j}^{k+1}\right| \leq M_1\left(h^2 + s\right) \tag{3.51}$$

for all i, j, and k for some $M_1 \geq 0$ that depends only on T, L_x, and L_y. In particular, we have

$$\left|\tau_{i,j}^{k+1}\right| \leq C\left(s\|\Phi\|_{C^2(0,T;C^4(\Omega))} + h^2\left(\|\Phi\|_{L^\infty(0,T;C^6(\Omega))}^3 + \|\Phi\|_{L^\infty(0,T;C^8(\Omega))}\right)\right). \tag{3.52}$$

Hence,

$$M_1 \leq \|\Phi\|_{C^2(0,T;C^4(\Omega))} + \|\Phi\|_{L^\infty(0,T;C^6(\Omega))}^3 + \|\Phi\|_{L^\infty(0,T;C^8(\Omega))}. \tag{3.53}$$

Subtracting (3.9) from (3.50) yields

$$e^{k+1} - e^k = s\Delta_h\left(\tilde{\mu}\left(\Phi^{k+1}, \Phi^k\right) - \tilde{\mu}\left(\phi^{k+1}, \phi^k\right)\right) + s\tau^{k+1}. \tag{3.54}$$

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Multiplying by $2h^2 e^{k+1}$, summing over i and j, and applying Green's second identity (Proposition 2.2, eq. (2.21)) we have

$$\begin{aligned}
\left\|e^{k+1}\right\|_2^2 - \left\|e^k\right\|_2^2 + \left\|e^{k+1} - e^k\right\|_2^2 &= 2h^2 s \left(\tilde{\mu}\left(\Phi^{k+1}, \Phi^k\right) - \tilde{\mu}\left(\phi^{k+1}, \phi^k\right) \middle\| \Delta_h e^{k+1}\right) \\
&\quad + 2h^2 s \left(\tau^{k+1} \middle\| e^{k+1}\right) \\
&= 2h^2 s \left(\left(\Phi^{k+1}\right)^3 - \left(\phi^{k+1}\right)^3 \middle\| \Delta_h e^{k+1}\right) \\
&\quad + 2h^2 s (1-\epsilon) \left(e^{k+1} \middle\| \Delta_h e^{k+1}\right) \\
&\quad + 4h^2 s \left(\Delta_h e^k \middle\| \Delta_h e^{k+1}\right) + 2h^2 s \left(\Delta_h^2 e^{k+1} \middle\| \Delta_h e^{k+1}\right) \\
&\quad + 2h^2 s \left(\tau^{k+1} \middle\| e^{k+1}\right). \qquad (3.55)
\end{aligned}$$

Dropping the nonnegative term $\left\|e^{k+1} - e^k\right\|_2^2$ and using summation-by-parts we have

$$\begin{aligned}
\left\|e^{k+1}\right\|_2^2 - \left\|e^k\right\|_2^2 &\le 2h^2 s \left(\left(\Phi^{k+1}\right)^3 - \left(\phi^{k+1}\right)^3 \middle\| \Delta_h e^{k+1}\right) \\
&\quad - 2s(1-\epsilon) \left\|\nabla_h e^{k+1}\right\|_2^2 + 4h^2 s \left(\Delta_h e^k \middle\| \Delta_h e^{k+1}\right) \\
&\quad - 2s \left\|\nabla_h \left(\Delta_h^2 e^{k+1}\right)\right\|_2^2 + 2h^2 s \left(\tau^{k+1} \middle\| e^{k+1}\right). \qquad (3.56)
\end{aligned}$$

Using Cauchy's inequality and the pointwise boundedness of both ϕ^{k+1} and Φ^{k+1} we have the following estimate:

$$\begin{aligned}
2h^2 s \left(\left(\Phi^{k+1}\right)^3 - \left(\phi^{k+1}\right)^3 \middle\| \Delta_h e^{k+1}\right) &\le \frac{2s}{2} \left\|\left(\Phi^{k+1}\right)^3 - \left(\phi^{k+1}\right)^3\right\|_2^2 + \frac{2s}{2} \left\|\Delta_h e^{k+1}\right\|_2^2 \\
&\le sC_1 \left\|e^{k+1}\right\|_2^2 + s \left\|\Delta_h e^{k+1}\right\|_2^2, \qquad (3.57)
\end{aligned}$$

where C_1 is independent of s and h. Two more applications of Cauchy's inequality yield

$$4h^2 s \left(\Delta_h e^k \middle\| \Delta_h e^{k+1}\right) \le 2s \left\|\Delta_h e^k\right\|_2^2 + 2s \left\|\Delta_h e^{k+1}\right\|_2^2 \qquad (3.58)$$

and

$$2h^2 s \left(\tau^{k+1} \middle\| e^{k+1}\right) \le sM_2 \left(h^2 + s\right)^2 + s \left\|e^{k+1}\right\|_2^2, \qquad (3.59)$$

where $M_2 := M_1^2 L_x L_y$. Putting these together and dropping the nonpositive term $-2s(1-\epsilon)\left\|\nabla_h e^{k+1}\right\|_2^2$ yields

$$\begin{aligned}
\left\|e^{k+1}\right\|_2^2 - \left\|e^k\right\|_2^2 &\le s\left(C_1 + 1\right) \left\|e^{k+1}\right\|_2^2 + 2s \left\|\Delta_h e^k\right\|_2^2 + 3s \left\|\Delta_h e^{k+1}\right\|_2^2 \\
&\quad - 2s \left\|\nabla_h \left(\Delta_h^2 e^{k+1}\right)\right\|_2^2 + sM_2 \left(h^2 + s\right)^2. \qquad (3.60)
\end{aligned}$$

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Summing over k and using $e^0 = \mathbf{0}$, we obtain

$$\begin{aligned}
\left\|e^{\ell}\right\|_2^2 &= \sum_{k=0}^{\ell-1}\left\{\left\|e^{k+1}\right\|_2^2 - \left\|e^{k}\right\|_2^2\right\} \\
&\le \sum_{k=0}^{\ell-1}\Big\{s\left(C_1+1\right)\left\|e^{k+1}\right\|_2^2 + 2s\left\|\Delta_h e^{k}\right\|_2^2 + 3s\left\|\Delta_h e^{k+1}\right\|_2^2 \\
&\quad - 2s\left\|\nabla_h\left(\Delta_h^2 e^{k+1}\right)\right\|_2^2 + sM_2\left(h^2+s\right)^2\Big\}, \\
&= s\left(C_1+1\right)\sum_{k=1}^{\ell}\left\|e^{k}\right\|_2^2 + 5s\sum_{k=1}^{\ell}\left\|\Delta_h e^{k}\right\|_2^2 - 2s\left\|\Delta_h e^{\ell}\right\|_2^2 \\
&\quad - 2s\sum_{k=1}^{\ell}\left\|\nabla_h\left(\Delta_h e^{k}\right)\right\|_2^2 + \left(h^2+s\right)^2 M_2 T \\
&\le s\left(C_1+1\right)\sum_{k=1}^{\ell}\left\|e^{k}\right\|_2^2 + 5s\sum_{k=1}^{\ell}\left\|\Delta_h e^{k}\right\|_2^2 \\
&\quad - 2s\sum_{k=1}^{\ell}\left\|\nabla_h\left(\Delta_h e^{k}\right)\right\|_2^2 + \left(h^2+s\right)^2 M_2 T,
\end{aligned} \tag{3.61}$$

where we assume $\ell \cdot s = T$. We now use Lemma 3.10 with e^k to obtain

$$\begin{aligned}
\left\|e^{\ell}\right\|_2^2 &\le s\left(C_1+1+\frac{5}{3\alpha^2}\right)\sum_{k=1}^{\ell}\left\|e^{k}\right\|_2^2 + s\left(\frac{10\alpha}{3}-2\right)\sum_{k=1}^{\ell}\left\|\nabla_h\left(\Delta_h e^{k}\right)\right\|_2^2 \\
&\quad + \left(h^2+s\right)^2 M_2 T,
\end{aligned} \tag{3.62}$$

where $\alpha > 0$ is arbitrary. Choosing $\alpha = 3/10$ yields

$$\begin{aligned}
\left\|e^{\ell}\right\|_2^2 &\le s\left(C_1+\frac{527}{27}\right)\sum_{k=1}^{\ell}\left\|e^{k}\right\|_2^2 - s\sum_{k=1}^{\ell}\left\|\nabla_h\left(\Delta_h e^{k}\right)\right\|_2^2 \\
&\quad + \left(h^2+s\right)^2 M_2 T.
\end{aligned} \tag{3.63}$$

Dropping the nonpositive term $-s\sum_{k=1}^{\ell}\left\|\nabla_h\left(\Delta_h e^{k}\right)\right\|_2^2$ and setting $C_2 := (C_1 + 527/27)$ yields

$$\left\|e^{\ell}\right\|_2^2 \le sC_2\sum_{k=1}^{\ell}\left\|e^{k}\right\|_2^2 + \left(h^2+s\right)^2 M_2 T. \tag{3.64}$$

Manipulating, we have

$$\left\|e^{\ell}\right\|_2^2 \le \frac{sC_2}{1-sC_2}\sum_{k=1}^{\ell-1}\left\|e^{k}\right\|_2^2 + \frac{TM_2}{1-sC_2}\left(h^2+s\right)^2. \tag{3.65}$$

Provided $s < 1/C_2$, the discrete Gronwall inequality guarantees that

$$\left\|e^{\ell}\right\|_2^2 \le \frac{TM_2}{1-sC_2}\left(1+\frac{sC_2}{1-sC_2}\right)^{\ell-1}\left(h^2+s\right)^2. \tag{3.66}$$

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The coefficient

$$\frac{TM_2}{1-sC_2}\left(1+\frac{sC_2}{1-sC_2}\right)^{\ell-1} \tag{3.67}$$

may be bounded by a positive constant that is dependent on T (exponentially), but otherwise independent of h and s. This proves the theorem. □

Remark 3.12. Energy estimates to the semidiscrete scheme (1.15) (at the continuous-space level) can be applied to establish the well-posedness of the PFC model. The limit of the numerical solution (as time step $s \to 0$) is a solution of the PDE system. The nonincreasing property of the physical energy (1.17) indicates a bound in the $L^\infty\left(0,T;H^2\left(\Omega\right)\right)$ norm. Moreover, by testing the numerical scheme with $-\Delta\phi^{k+1}$, we can derive an $L^2\left(0,T;H^4\left(\Omega\right)\right)$ bound of the numerical solution (independent of s), with the help of the L^∞ estimate of ϕ^{k+1}. This in turn gives a weak solution of the PFC model by taking the limit of $s \to 0$, with the regularity $\phi \in L^\infty\left(0,T;H^2\left(\Omega\right)\right) \cap L^2\left(0,T;H^4\left(\Omega\right)\right)$.

Similar energy estimate techniques can be applied to analyze the higher-order derivatives of the numerical solution. By testing the numerical scheme with $(-\Delta)^m\phi^{k+1}$ ($m \geq 3$), we obtain a higher-order regularity of the numerical solution, with a uniform (s-independent) bound for $\phi \in L^\infty\left(0,T;H^m\left(\Omega\right)\right) \cap L^2\left(0,T;H^{m+3}\left(\Omega\right)\right)$. The analysis of the nonlinear term can be handled in the same way as in the derivation of the weak solution. As a result, a unique global (in time) strong solution (with $m = 3$) can be proven for the PFC model, since passing to the limit as $s \to 0$ does not cause any difficulty. A unique global smooth solution can also be derived for any smooth initial data by taking a higher value of m.

4. Conclusions.

In this paper, we have developed and proven convergence of an unconditionally energy-stable finite-difference scheme for the sixth-order phase field crystal (PFC) equation. The method is based on a convex splitting of a discrete energy and is semi-implicit. The equation at the implicit time level is nonlinear but is uniquely solvable for any time step. The algorithm is first-order accurate in time and second-order accurate in space, as is demonstrated in an error estimate.

Our scheme is based on a generalization of the convex-splitting methodology proposed by Eyre [8] for solving bistable gradient-flow equations. Herein, we put the framework on a sound, complete theoretical footing, which was missing in [8]. In particular, Theorem 3.5, which is the centerpiece of our work, facilitates the energy stability of both conserved and nonconserved schemes in a general way. Indeed, the theory herein applies to a very broad class of bistable gradient flows and, as we show in [19], to certain equations of nongradient-flow type as well.

In a companion paper [11], we develop an efficient nonlinear multigrid method to solve the unconditionally energy-stable algorithm presented here. In fact we demonstrate therein that the nonlinearity of the schemes is not a difficulty. We compare solutions of our first-order scheme with those of a new, fully second-order accurate multistep numerical scheme (also given in [11]). In this new scheme, the discrete energy is bounded by its initial value, for any time step, but may not be strictly decreasing from one time step to the next. This weak energy stability is still sufficient to guarantee pointwise stability of the scheme, and the convergence analysis given here can be modified to apply to this new scheme. It remains an open question, however, whether one can obtain a fully second-order accurate numerical scheme that is both (i) unconditionally (strongly) energy stable (i.e., the discrete energy is nonincreasing from one time step to the next) and (ii) unconditionally solvable.

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Herein we have utilized periodic boundary conditions. This usage is for simplicity, but it is in no ways a fundamental constraint. All of our results hold, though in perhaps slightly modified forms, assuming homogeneous Neumann boundary conditions and also boundary conditions of mixed periodic-homogeneous Neumann type. Indeed, in [11] we perform a computation with the latter type of boundary conditions.

There are a number of other interesting problems we plan to address in the future. These include the development of adaptive time step algorithms. Such algorithms can be very effective in accelerating PFC simulations since the dynamics typically involves a slowly evolving microstructure punctuated by a few rapid events. An accelerated algorithm would make it possible to increase the range of scales capable of being simulated by the PFC model. The role of adaptive spatial mesh refinement is less clear due to the periodic oscillations of the phase field variable that characterize the spatial extent of the crystal phase.

Finally, we mention that the convex-splitting framework can be extended to deal with an important generalization of the PFC equation. In forthcoming papers [10, 19] we analyze and test numerically convex-splitting schemes for the modified phase field crystal (MPFC) equation, which was proposed in [16]. The MPFC equation is designed to account for elastic interactions and includes a second-order time derivative, which adds a quasiphononic time scale on top of the diffusive time scale in the PFC equation [15, 16]. Specifically, the MPFC equation is

$$\beta\partial_{tt}\phi + \partial_t\phi = \nabla\cdot(M(\phi)\nabla\mu)\,, \tag{4.1}$$

which is a generalized damped wave equation. In the MPFC approach, atomic positions relax at early times consistent with elasticity theory, and the evolution on long time scales is dissipative. Because of the presence of elastic waves, the MPFC equation can have stricter time step requirements than the PFC, and thus the design of efficient algorithms for the MPFC is very important.

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