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

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Abstract. We present an unconditionally energy stable finite difference scheme for the Modified Phase Field Crystal equation, a generalized damped wave equation for which the usual Phase Field Crystal equation is a special degenerate case. The method is based on a convex splitting of a discrete pseudoenergy 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 a local-in-time error estimate that ensures the pointwise convergence of the scheme.

Key words. Phase Field Crystal, Modified 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 [4] 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 type [12] 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 [9] 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 [1, 8]. 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.

Recently, Stefanovic, Haataja, and Provatas [11] introduced an important extension of the PFC model known as the Modified Phase Field Crystal (MPFC) equation. This equation is designed to properly account for elastic interactions and includes a second-order time derivative:

$$\beta \partial_{tt}\phi + \partial_t \phi = \Delta\left(\phi^3 + \alpha\phi + 2\Delta\phi + \Delta^2\phi\right), \tag{1.1}$$

where $\beta \geq 0$ and $\alpha > 0$. Equation (1.1) is a generalized damped wave equation, though the parabolic PFC equation is recovered in the degenerate case when $\beta = 0$. The existence and uniqueness of global smooth solutions of the MPFC equation are established in our recent article [14], assuming that the initial data are smooth.

The MPFC approach introduces a separation of time scales that allows for the elastic relaxation of the crystal lattice on a rapid quasi-phononic time scale even

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while other processes evolve on the much slower diffusion time scale. While true elastic relaxation happens on a much faster time scale (i.e., the true phonon time scale) than can be captured in the MPFC model, it gives vastly superior predictions for dislocation dynamics, for example, than does the PFC equation [9, 11]. Because of the presence of elastic waves and the fast time scale, schemes for the MPFC equation may have stricter time step requirements than those for the PFC equation. Moreover, because the MPFC equation is a generalized damped wave equation and the PFC is parabolic, it is not clear that numerical methods that work for the latter will work for the former.

In the papers [7, 16] we described unconditionally stable, unconditionally uniquely solvable, and convergent schemes for the PFC equation based on convex-splitting methods. The method presented in [16] is a first-order in time second-order in space scheme. In [7] we described practical nonlinear multigrid methods for solving the first-order scheme from [16] and a new fully second-order convex-splitting scheme. We extended these methods to the thin film equations with and without slope selection in [3, 10, 13]. The goal of this paper is to extend the convex-splitting framework to develop a stable scheme for the MPFC equation. While some of the techniques that worked for the PFC and thin film schemes are appropriate, the analyses for stability and convergence, in particular, are quite different for the MPFC scheme mainly owing to the second-order time derivative. To the best of our knowledge no numerical analysis exists for the MPFC equation.

2. Properties and approximation of solutions.

2.1. Mass conservation and pseudoenergy dissipation. Consider a dimensionless spatial energy of the form [4, 12]

$$E(\phi) = \int_\Omega \left\{ \frac{1}{4}\phi^4 + \frac{\alpha}{2}\phi^2 - |\nabla\phi|^2 + \frac{1}{2}\left(\Delta\phi\right)^2 \right\} d\mathbf{x} \ , \tag{2.1}$$

where $\phi : \Omega \subset \mathbb{R}^2 \to \mathbb{R}$ is the "atom" density field, and $\alpha > 0$ is a constant. Suppose that $\Omega = (0, L_x) \times (0, L_y)$ and ϕ is periodic on Ω. Define μ to be the chemical potential with respect to E:

$$\mu := \delta_\phi E = \phi^3 + \alpha\phi + 2\Delta\phi + \Delta^2\phi \ , \tag{2.2}$$

where $\delta_\phi E$ denotes the variational derivative with respect to ϕ. The MPFC equation is the generalized damped wave equation [11]

$$\beta\partial_{tt}\phi + \partial_t\phi = \Delta\mu \ , \tag{2.3}$$

where $\beta \geq 0$. When $\beta = 0$ the ordinary PFC equation is recovered. See the discussion in [14] for some equations in the literature that are closely related to (1.1).

First, note that the energy (2.1) is not necessarily nonincreasing in time along the solution trajectories of (2.3). However, solutions of the MPFC equation do dissipate a pseudoenergy, as we show momentarily. Also observe that (2.3) is not precisely a mass conservation equation due to the term $\beta\partial_{tt}\phi$, unless one takes $\beta = 0$. However, with the introduction of a reasonable initial condition for $\partial_t\phi$, it is possible to show that $\int_\Omega \partial_t\phi \, d\mathbf{x} = 0$ for all time.

We shall need a precise definition of the H_{per}^{-1} inner product to define an appropriate pseudoenergy for the MPFC equation. Define $\psi_f \in H_{per}^2(\Omega)$ to be the unique solution to the PDE problem

$$-\Delta\psi_f = f \quad \text{in } \Omega \ , \qquad \int_\Omega \psi_f \, d\mathbf{x} = 0 \ , \tag{2.4}$$

where $f \in L^2(\Omega)$ and $\int_\Omega f \, d\mathbf{x} = 0$. In this case we write $\psi_f = -\Delta^{-1} f$. Suppose that f and g are in $L^2(\Omega)$ and are of mean zero; then we define

$$(f, g)_{H^{-1}} := (\nabla\psi_f, \nabla\psi_g)_{L^2} \,. \tag{2.5}$$

Note that, via integration by parts, we have

$$(f, g)_{H^{-1}} = -\left(\Delta^{-1} f, g\right)_{L^2} = -\left(\Delta^{-1} g, f\right)_{L^2} = (g, f)_{H^{-1}} \ . \tag{2.6}$$

For every $f \in L^2(\Omega)$ that is of mean zero, i.e., $\int_\Omega f \, d\mathbf{x} = 0$, we define

$$\|f\|_{H^{-1}} = \sqrt{(f, f)_{H^{-1}}} \ . \tag{2.7}$$

We now recast the MPFC equation (2.3) as the following system of equations:

$$\beta\partial_t\psi = \Delta\mu - \psi \ , \quad \partial_t\phi = \psi \ . \tag{2.8}$$

And we introduce the pseudoenergy

$$\mathcal{E}(\phi, \psi) := E(\phi) + \frac{\beta}{2} \|\psi\|_{H^{-1}}^2 \ , \tag{2.9}$$

which, for well-definedness, requires that $\int_\Omega \psi \, d\mathbf{x} = 0$. This is the case as long as the initial condition $\int_\Omega \partial_t\phi(\mathbf{x}, 0) \, d\mathbf{x} = 0$ is satisfied. In what follows, we will use the initial data

$$\psi(\mathbf{x}, 0) = \partial_t\phi(\mathbf{x}, 0) \equiv 0 \quad \text{in } \Omega \ , \tag{2.10}$$

so that $\int_\Omega \partial_t\phi(\mathbf{x}, 0) \, d\mathbf{x} = 0$ is trivially satisfied. In any case, as long as $\psi = \partial_t\phi$ is of mean zero, a simple calculation shows that

$$d_t\mathcal{E} = -(\psi, \psi)_{H^{-1}} \leq 0 \ , \tag{2.11}$$

which guarantees that the pseudoenergy is nonincreasing in time.

2.2. A semidiscrete convex-splitting scheme. We now motivate our fully discrete scheme that will come in section 4 with a time-discrete space-continuous version. The scheme is based on the observation 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. The canonical splitting is

$$E_c = \frac{1}{4} \|\phi\|_{L^4}^4 + \frac{\alpha}{2} \|\phi\|_{L^2}^2 + \frac{1}{2} \|\Delta\phi\|_{L^2}^2 \ , \quad E_e = \|\nabla\phi\|_{L^2}^2 \ . \tag{2.12}$$

The idea to exploit a convex splitting of the energy for the construction of numerical schemes is generally attributed to Eyre [5]. We have used this idea to craft schemes for a number of gradient-flow equations [3, 10, 13, 16, 15]. However, the use of this idea for nongradient-flow equations, like (2.3), has not been pursued yet to the best of our knowledge. A direct application of convexity splitting is nonstandard, due to the presence of ψ in the pseudoenergy. However, note that $\frac{\beta}{2}\left\|\psi\right\|_{H^{-1}}^2$ is convex. This fact, together with [16, Thm. 1.1], immediately yields the following.

Lemma 2.1. *Suppose that $\Omega = (0, L_x) \times (0, L_y)$, ϕ_1, $\phi_2 \in H^2_{per}(\Omega)$, $\psi_1, \psi_2 \in L^2(\Omega)$, and $(\psi_1, 1)_{L^2} = (\psi_2, 1)_{L^2} = 0$. Consider the canonical convex splitting of the energy E in (2.1) into $E = E_c - E_e$ given in (2.12). Then*

$$\begin{aligned} \mathcal{E}(\phi_1,\psi_1) - \mathcal{E}(\phi_2,\psi_2) \le \left(\delta_\phi E_c(\phi_1) - \delta_\phi E_e(\phi_2), \phi_1 - \phi_2\right)_{L^2} \\ +\beta\left(\psi_1, \psi_1 - \psi_2\right)_{H^{-1}} \ , \end{aligned} \tag{2.13}$$

where δ_ϕ represents the variational derivative.

We propose the convex-splitting scheme

$$\beta\left(\psi^{k+1} - \psi^k\right) = s\Delta\mu^{k+1} - s\psi^{k+1} \ , \tag{2.14}$$

$$\mu^{k+1} = \delta_\phi E_c\left(\phi^{k+1}\right) - \delta_\phi E_e\left(\phi^k\right) \ , \tag{2.15}$$

$$\phi^{k+1} - \phi^k = s\psi^{k+1} \ , \tag{2.16}$$

where $s > 0$ is the time step-size, ϕ^{k+1} and μ^{k+1} are periodic, and $\psi^0 \equiv 0$. It is straightforward to see that this first-order scheme is mass conserving since $\int_\Omega \psi^0 \, d\mathbf{x} = 0$. Let us now show that (2.14)–(2.16) is unconditionally energy stable. By Lemma 2.1 with the proper replacements we have immediately that

$$\begin{aligned} \mathcal{E}\left(\phi^{k+1},\psi^{k+1}\right) - \mathcal{E}\left(\phi^k,\psi^k\right) \le \left(\delta_\phi E_c\left(\phi^{k+1}\right) - \delta_\phi E_e\left(\phi^k\right), \phi^{k+1} - \phi^k\right)_{L^2} \\ -\beta\left(\Delta^{-1}\psi^{k+1}, \psi^{k+1} - \psi^k\right)_{L^2} \ . \end{aligned} \tag{2.17}$$

Now, let $C := \frac{1}{L_x L_y}\int_\Omega \mu^{k+1}\, d\mathbf{x}$, and using (2.14)–(2.16) in the right-hand side of inequality (2.17) we find

$$\begin{aligned} \mathcal{E}\left(\phi^{k+1},\psi^{k+1}\right) - \mathcal{E}\left(\phi^k,\psi^k\right) &\le \left(\mu^{k+1}, s\psi^{k+1}\right)_{L^2} - \beta\left(\psi^{k+1}, \Delta^{-1}\left(\psi^{k+1} - \psi^k\right)\right)_{L^2} \\ &= \left(\psi^{k+1}, s\left(\mu^{k+1} - C\right) - \beta\Delta^{-1}\left(\psi^{k+1} - \psi^k\right)\right)_{L^2} \\ &\quad + \left(\psi^{k+1}, s\,C\right)_{L^2} \\ &= \left(\psi^{k+1}, \Delta^{-1}\left\{s\Delta\mu^{k+1} - s\Delta C - \beta\left(\psi^{k+1} - \psi^k\right)\right\}\right)_{L^2} \\ &= -s\left(\psi^{k+1},\psi^{k+1}\right)_{H^{-1}} = -s\left\|\psi^{k+1}\right\|_{H^{-1}}^2 \le 0 \ . \end{aligned} \tag{2.18}$$

Thus, thanks to the estimate (2.13), we have shown that the scheme is energy stable, not with respect to the spatial energy E, but with respect to the modified energy $\mathcal{E}$.

2.3. Outline of this paper. In the following sections we demonstrate that the preliminary calculations of this section can be carried out in a finite-dimensional setting using difference operators. The main goal in what follows is to define a first-order in time, second-order in space scheme that is unconditionally discrete-energy stable, discretely mass conserving, and unconditionally solvable. In section 3 we define some discrete norms and some estimates that will be used to define and analyze our scheme. In section 4 we define the scheme for the MPFC equation and present the main results of our analyses, including the unique solvability, discrete-energy stability, and convergence of our scheme. We give some concluding remarks and suggest some future work in section 5.

3. Tools for cell-centered finite differences. Our primary goal in this section is to define the summation-by-parts formulae, discrete norms, and estimates in two space dimensions that are used to define and analyze our finite difference scheme. With some exceptions, the theory will extend straightforwardly to three-dimensions. Here we use the same notation and results for 2D cell-centered functions as from [16, sect. 2]. The reader is directed there for all of the missing details.

We assume that $L_x = m \times h_x$ and $L_y = n \times h_y$, for some mesh sizes $h_x > 0$, $h_y > 0$ and some positive integers m and n. We take $h_x = h_y = h$ for simplicity of presentation.[1] The linear spaces $\mathcal{C}_{m\times n}$, $\mathcal{C}_{\overline{m}\times n}$, $\mathcal{C}_{m\times\overline{n}}$, and $\mathcal{C}_{\overline{m}\times\overline{n}}$ contain *cell-centered* grid functions. We generally use the Greek symbols ϕ, ψ, and ζ to denote such functions. In component form cell-centered functions are identified via $\phi_{i,j} := \phi(p_i, p_j)$, where $p_r = (r - 1/2)\cdot h$ and r can take on integer and half-integer values. The functions of $\mathcal{E}^{\rm ew}_{m\times n}$ and $\mathcal{E}^{\rm ns}_{m\times n}$ are called *east-west edge-centered* grid functions and *north-south edge-centered* grid functions, respectively. We generally reserve the symbols f and g to denote these functions. In component form east-west edge-centered functions are identified via $f_{i+1/2,j} := f(p_{i+1/2}, p_j)$; north-south edge-centered functions are identified via $f_{i,j+1/2} := f(p_i, p_{j+1/2})$. The summation-by-parts formula we need from [16] is the following.

PROPOSITION 3.1 (summation-by-parts). *If $\phi \in \mathcal{C}_{\overline{m}\times n} \cup \mathcal{C}_{\overline{m}\times\overline{n}}$ and $f \in \mathcal{E}^{\rm ew}_{m\times n}$, then*

$$\begin{aligned} h^2\,[D_x\phi\|f]_{\rm ew} = &-h^2\,(\phi\|d_x f)\\ &-h\,\left(A_x\phi_{1/2,\star}\middle|f_{1/2,\star}\right) + h\,\left(A_x\phi_{m+1/2,\star}\middle|f_{m+1/2,\star}\right), \end{aligned} \tag{3.1}$$

and if $\phi \in \mathcal{C}_{m\times\overline{n}} \cup \mathcal{C}_{\overline{m}\times\overline{n}}$ and $f \in \mathcal{E}^{\rm ns}_{m\times n}$, then

$$\begin{aligned} h^2\,[D_y\phi\|f]_{\rm ns} = &-h^2\,(\phi\|d_y f)\\ &-h\,\left(A_y\phi_{\star,1/2}\middle|f_{\star,1/2}\right) + h\,\left(A_y\phi_{\star,n+1/2}\middle|f_{\star,n+1/2}\right). \end{aligned} \tag{3.2}$$

PROPOSITION 3.2 (discrete Green's identities). *Let ϕ, $\psi \in \mathcal{C}_{\overline{m}\times\overline{n}}$. Then*

$$\begin{aligned} &h^2\,[D_x\phi\|D_x\psi]_{\rm ew} + h^2\,[D_y\phi\|D_y\psi]_{\rm ns}\\ &= -h^2\,(\phi\|\Delta_h\psi) - h\,\left(A_x\phi_{1/2,\star}\middle|D_x\psi_{1/2,\star}\right) + h\,\left(A_x\phi_{m+1/2,\star}\middle|D_x\psi_{m+1/2,\star}\right)\\ &\qquad -h\,\left(A_y\phi_{\star,1/2}\middle|D_y\psi_{\star,1/2}\right) + h\,\left(A_y\phi_{\star,n+1/2}\middle|D_y\psi_{\star,n+1/2}\right)\ , \end{aligned} \tag{3.3}$$

and

$$\begin{aligned} h^2\,(\phi\|\Delta_h\psi) = h^2\,(\Delta_h\phi\|\psi)&\\ &+h\,\left(A_x\phi_{m+1/2,\star}\middle|D_x\psi_{m+1/2,\star}\right) - h\,\left(D_x\phi_{m+1/2,\star}\middle|A_x\psi_{m+1/2,\star}\right)\\ &-h\,\left(A_x\phi_{1/2,\star}\middle|D_x\psi_{1/2,\star}\right) + h\,\left(D_x\phi_{1/2,\star}\middle|A_x\psi_{1/2,\star}\right)\\ &+h\,\left(A_y\phi_{\star,n+1/2}\middle|D_y\psi_{\star,n+1/2}\right) - h\,\left(D_y\phi_{\star,n+1/2}\middle|A_y\psi_{\star,n+1/2}\right)\\ &-h\,\left(A_y\phi_{\star,1/2}\middle|D_y\psi_{\star,1/2}\right) + h\,\left(D_y\phi_{\star,1/2}\middle|A_y\psi_{\star,1/2}\right)\ . \end{aligned} \tag{3.4}$$

The symbols $(\cdot\|\cdot)$, $[\cdot\|\cdot]_{\rm ns}$, $[\cdot\|\cdot]_{\rm ew}$ are 2D inner products, and $(\cdot|\cdot)$ is a 1D inner product. The symbols D_x, d_x, A_x, etc. are difference and average operators. By Δ_h we denote the standard five-point stencil. See [16, sect. 2] for the complete details.

[1] The extension to the more general case for which $h_x \neq h_y$ may be obtained by replacing instances of h^2 by $h_x h_y$ and instances of h by h_x or h_y, as appropriate, in what follows.

In this paper we are interested in 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

$$\phi_{m+1,j} = \phi_{1,j}, \quad \phi_{0,j} = \phi_{m,j}, \quad j = 1,\ldots,n, \tag{3.5}$$

$$\phi_{i,n+1} = \phi_{i,1}, \quad \phi_{i,0} = \phi_{i,n}, \quad i = 0,\ldots,m+1. \tag{3.6}$$

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 also $D_x\phi_{m+1/2,j} = D_x\phi_{1/2,j}$ for all $j = 0,1,\ldots,n+1$. We note that the results for periodic functions that are to follow will also hold, in a possibly slightly modified form, when the boundary conditions are taken to be homogeneous Neumann.

We define the following norms for cell-centered functions. If $\phi \in \mathcal{C}_{m\times n}$, then $\|\phi\|_2 := \sqrt{h^2\,(\phi\|\phi)}$, and we define $\|\nabla_h\phi\|_2$, where $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$, to mean

$$\|\nabla_h\phi\|_2 := \sqrt{h^2\ [D_x\phi\|D_x\phi]_{\mathrm{ew}} + h^2\ [D_y\phi\|D_y\phi]_{\mathrm{ns}}}\ . \tag{3.7}$$

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

$$\|\phi\|_{1,2} := \sqrt{\|\phi\|_2^2 + \|\nabla_h\phi\|_2^2}\ , \quad \|\phi\|_{2,2} := \sqrt{\|\phi\|_2^2 + \|\nabla_h\phi\|_2^2 + \|\Delta_h\phi\|_2^2}\ . \tag{3.8}$$

In addition, we introduce the following discrete L^4 and L^∞ norms: for any $\phi \in \mathcal{C}_{m\times n}$ define

$$\|\phi\|_4 := \left(h^2\ \left(\phi^4\|\mathbf{1}\right)\right)^{1/4} \quad \text{and} \quad \|\phi\|_\infty = \max_{\substack{i=1,\ldots,m\\ j=1,\ldots,n}} |\phi_{i,j}|\,. \tag{3.9}$$

And for $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ define

$$\|\nabla_h\phi\|_4 := \left(h^2\ \left[(D_x\phi)^4\middle\|\mathbf{1}\right]_{\mathrm{ew}} + h^2\ \left[(D_y\phi)^4\middle\|\mathbf{1}\right]_{\mathrm{ns}}\right)^{1/4}\ . \tag{3.10}$$

We will need some discrete Sobolev-type inequalities for 2D grid functions that will be used to prove the pointwise stability of our scheme.

LEMMA 3.3. *Suppose that $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$. Then, for any $i \in \{1,2,\ldots,m\}$ and any $j \in \{1,2,\ldots,n\}$,*

$$|\phi_{i,j}|^2 \le \frac{2}{L_x}h\sum_{i'=1}^{m}(\phi_{i',j})^2 + 2L_xh\sum_{i'=0}^{m}w_{i'}^m\left(D_x\phi_{i'+1/2,j}\right)^2 =: Q_j\ , \tag{3.11}$$

$$|\phi_{i,j}|^2 \le \frac{2}{L_y}h\sum_{j'=1}^{n}(\phi_{i,j'})^2 + 2L_yh\sum_{j'=0}^{n}w_{j'}^n\left(D_y\phi_{i,j'+1/2}\right)^2 =: R_i\ , \tag{3.12}$$

where

$$w_k^\ell := \begin{cases} 1 & \text{if} \quad k \in \{1,2,\ldots,\ell-1\}\ , \\ 1/2 & \text{if} \quad k \in \{0,\ell\}\ . \end{cases} \tag{3.13}$$

Proof. This follows directly from [16, Lem. 2.3]. ∎

The following is similar to Lemma 3.1 in [2], but here we make no assumptions about boundary conditions.

LEMMA 3.4. *Suppose that $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$. Then,*

$$\|\phi\|_4 \le C_1 \|\phi\|_{1,2} \ , \quad C_1 := \left(2\max\left[\max\left\{\frac{1}{L_x}, L_x\right\}, \max\left\{\frac{1}{L_y}, L_y\right\}\right]\right)^{1/4} . \tag{3.14}$$

Proof. Using the previous lemma,

$$\begin{aligned}
\|\phi\|_4^4 &= h^2 \sum_{i=1}^m \sum_{j=1}^n |\phi_{i,j}|^2 |\phi_{i,j}|^2 \le h^2 \sum_{i=1}^m \sum_{j=1}^n R_i Q_j = \left(h\sum_{i=1}^m R_i\right)\left(h\sum_{j=1}^n Q_j\right) \\
&= \left(\frac{2}{L_y} h^2 (\phi\|\phi) + 2L_y h^2 [D_y\phi\|D_y\phi]_{\mathrm{ns}}\right) \\
&\quad \times \left(\frac{2}{L_x} h^2 (\phi\|\phi) + 2L_x h^2 [D_x\phi\|D_x\phi]_{\mathrm{ew}}\right) \\
&\le \left(\frac{2}{L_y} h^2 (\phi\|\phi) + 2L_y h^2 [D_y\phi\|D_y\phi]_{\mathrm{ns}} + 2L_y h^2 [D_x\phi\|D_x\phi]_{\mathrm{ew}}\right) \\
&\quad \times \left(\frac{2}{L_x} h^2 (\phi\|\phi) + 2L_x h^2 [D_x\phi\|D_x\phi]_{\mathrm{ew}} + 2L_x h^2 [D_y\phi\|D_y\phi]_{\mathrm{ns}}\right) \\
&\le C_1^4 \|\phi\|_{1,2}^4 \ . \qquad \square
\end{aligned} \tag{3.15}$$

The following is proven in [16].

LEMMA 3.5. *Suppose that $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is periodic. Then, for any $i \in \{1, 2, \ldots, m\}$ and any $j \in \{1, 2, \ldots, n\}$,*

$$|\phi_{i,j}|^2 \le C_2 \|\phi\|_{2,2}^2 \ , \quad C_2 := 4\max\left\{\frac{1}{L_xL_y}, \frac{L_x}{L_y}, \frac{L_y}{L_x}, \frac{L_xL_y}{2}\right\} . \tag{3.16}$$

Hence $\|\phi\|_\infty^2 \le C_2 \|\phi\|_{2,2}^2$.

We now establish a discrete analogue to the space $H_{per}^{-1}(\Omega)$.

LEMMA 3.6. *Let M be a positive constant. For any $\phi \in \mathcal{C}_{m\times n}$, there exists a unique $\psi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ that solves*

$$\mathcal{L}(\psi) := -M\Delta_h\psi = \phi - \frac{1}{m\cdot n}(\phi\|\mathbf{1}), \tag{3.17}$$

$$\psi \textit{ is periodic and } (\psi\|\mathbf{1}) = 0. \tag{3.18}$$

Proof. This follows directly from [16, Lem. 3.2], where it is shown that $\mathcal{L} = -M\Delta_h$ is a symmetric positive definite operator restricted to H. $\square$

Now consider the space

$$H := \{\phi \in \mathcal{C}_{m\times n} | (\phi\|\mathbf{1}) = 0\}, \tag{3.19}$$

and equip this space with the bilinear form

$$(\phi_1\|\phi_2)_{H,\mathcal{L}} := M[D_x\psi_1\|D_x\psi_2]_{\mathrm{ew}} + M[D_y\psi_1\|D_y\psi_2]_{\mathrm{ns}}, \tag{3.20}$$

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

$$\mathcal{L}(\psi_i) = -M\Delta_h\psi_i = \phi_i, \quad \psi_i \text{ periodic}, \quad (\psi_i\|\mathbf{1}) = 0. \tag{3.21}$$

LEMMA 3.7. *Let $\mathcal{L} = -M\Delta_h$. $(\phi_1\|\phi_2)_{H,\mathcal{L}}$ is an inner product on the space H. Moreover,*

$$(\phi_1\|\phi_2)_{H,\mathcal{L}} = \left(\phi_1\middle\|\mathcal{L}^{-1}(\phi_2)\right) = \left(\mathcal{L}^{-1}(\phi_1)\middle\|\phi_2\right). \tag{3.22}$$

Thus

$$\|\phi\|_{H,\mathcal{L}} := \sqrt{h^2\,(\phi\|\phi)_{H,\mathcal{L}}} \tag{3.23}$$

defines a norm on H.

Proof. The results follow from summation-by-parts and from the fact that $\mathcal{L}^{-1} = -M\Delta_h^{-1}$ is a symmetric positive definite operator restricted to H. ◻

LEMMA 3.8 (discrete Poincaré inequality). *Suppose that $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is periodic and $\phi \in H$, i.e., ϕ has mean zero. Then*

$$\|\phi\|_2 \le C_3\,\|\nabla_h\phi\|_2\,, \tag{3.24}$$

where $C_3 > 0$ is a constant that depends upon L_x and L_y only.

Proof. The operator $\mathcal{L} = -\Delta_h$, assuming periodic boundary conditions, is positive definite restricted to H. One can use an eigenfunction expansion with respect to $\mathcal{L}$ to establish this result. We suppress the details. ◻

The next lemma follows immediately from Lemmas 3.4 and 3.8.

LEMMA 3.9. *Suppose that $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is periodic and $\phi \in H$. Then*

$$\|\phi\|_4 \le C_4\,\|\nabla_h\phi\|_2\;, \quad C_4 := C_1\sqrt{C_3^2+1}\;. \tag{3.25}$$

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

$$S := h^2\sum_{i'=0}^{m}\sum_{j'=0}^{n} w_{i'}^m w_{j'}^n \left|D_y\left(D_x\phi\right)_{i'+1/2,j'+1/2}\right|^2 \tag{3.26}$$

using (3.13). *Then $S = h^2\,(\Delta_h^x\phi\|\Delta_h^y\phi)$, where $\Delta_h^x := d_x D_x$ and $\Delta_h^y := d_y D_y$ are the 3-point discrete Lapacian operators in the x- and y-directions, respectively* [16]. *And, since $S \ge 0$, we have*

$$h^2\;(\Delta_h^x\phi\|\Delta_h^x\phi) \le h^2\;(\Delta_h\phi\|\Delta_h\phi) \quad \textit{and} \quad h^2\;(\Delta_h^y\phi\|\Delta_h^y\phi) \le h^2\;(\Delta_h\phi\|\Delta_h\phi)\,. \tag{3.27}$$

Proof. This follows from the proof of Lemma 2.9 from [16]. ◻

LEMMA 3.11. *Suppose that $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is periodic. Then*

$$\|\nabla_h\phi\|_4 \le C_4\,\|\Delta_h\phi\|_2\;. \tag{3.28}$$

Proof. Define $s_x : \mathcal{E}_{m\times n}^{\mathrm{ew}} \to \mathcal{C}_{\overline{m}\times\overline{n}}$ and $s_y : \mathcal{E}_{m\times n}^{\mathrm{ns}} \to \mathcal{C}_{\overline{m}\times\overline{n}}$ to be periodic down shift operators defined via

$$s_x f_{i,j} := f_{i+1/2,j}, \quad s_y g_{i,j} := g_{i,j+1/2}, \quad {\scriptstyle i=1,\ldots,m, \atop j=1,\ldots,n,} \tag{3.29}$$

where $f \in \mathcal{E}_{m\times n}^{\mathrm{ew}}$ and $g \in \mathcal{E}_{m\times n}^{\mathrm{ns}}$ and where $s_x f$ and $s_y g$ are periodic. Now if $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is periodic, then $s_x\left(D_x\phi\right)$ and $s_y\left(D_y\phi\right)$ are periodic functions and, more importantly, are mean-zero functions, i.e., $s_x(D_x\phi)$, $s_y(D_y\phi) \in H$. Then

$$\begin{aligned}
\|\nabla_h\phi\|_4^4 &= \|s_x(D_x\phi)\|_4^4 + \|s_y(D_y\phi)\|_4^4 \\
&\le C_4^4 \left\|\nabla_h\big(s_x(D_x\phi)\big)\right\|_2^4 + C_4^4 \left\|\nabla_h\big(s_y(D_y\phi)\big)\right\|_2^4 \\
&= C_4^4\left(h^2\left[\Big(D_x\big(s_x(D_x\phi)\big)\Big)^2\Big\|\mathbf{1}\right]_{\mathrm{ew}} + h^2\left[\Big(D_y\big(s_x(D_x\phi)\big)\Big)^2\Big\|\mathbf{1}\right]_{\mathrm{ns}}\right)^2 \\
&\quad + C_4^4\left(h^2\left[\Big(D_x\big(s_y(D_y\phi)\big)\Big)^2\Big\|\mathbf{1}\right]_{\mathrm{ew}} + h^2\left[\Big(D_y\big(s_y(D_y\phi)\big)\Big)^2\Big\|\mathbf{1}\right]_{\mathrm{ns}}\right)^2 \\
&= C_4^4\left(h^2\left(\Delta_h^x\phi\|\Delta_h^x\phi\right) + S\right)^2 + C_4^4\left(S + h^2\left(\Delta_h^y\phi\|\Delta_h^y\phi\right)\right)^2 \\
&= C_4^4\|\Delta_h\phi\|_2^4\ . \qquad (3.30)
\end{aligned}$$

The S in this calculation is the same as in Lemma 3.10. □

4. The fully discrete scheme and its properties.

4.1. Discrete energy and the convex-splitting scheme. We begin by defining a fully discrete energy that is consistent with the continuous space energy (2.1). In particular, define the discrete energy $F : \mathcal{C}_{\overline{m}\times\overline{n}} \to \mathbb{R}$ to be

$$F(\phi) := \frac{1}{4}\|\phi\|_4^4 + \frac{\alpha}{2}\|\phi\|_2^2 - \|\nabla_h\phi\|_2^2 + \frac{1}{2}\|\Delta_h\phi\|_2^2 . \qquad (4.1)$$

The discrete analogue to (2.9) is

$$\mathcal{F}(\phi,\psi) := F(\phi) + \frac{\beta}{2}\|\psi\|_{H,\mathcal{L}}^2 , \qquad (4.2)$$

defined for any $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ and any $\psi \in H$, where $\mathcal{L} = -\Delta_h$. Clearly it follows that $\mathcal{F}(\phi,\psi) \ge F(\phi)$, a fact that we shall exploit later. The following is justified by our work in [16].

LEMMA 4.1 (existence of a convex splitting). *Suppose that $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is periodic. The energies*

$$F_c(\phi) = \frac{1}{4}\|\phi\|_4^4 + \frac{\alpha}{2}\|\phi\|_2^2 + \frac{1}{2}\|\Delta_h\phi\|_2^2 \quad \textit{and} \quad F_e(\phi) = \|\nabla_h\phi\|_2^2 \qquad (4.3)$$

are convex. Hence F, as defined in (4.1), admits the convex splitting $F = F_c - F_e$.

We are now prepared to describe the fully discrete scheme in detail. Define the cell-centered chemical potential $\mu^{k+1} \in \mathcal{C}_{\overline{m}\times\overline{n}}$ to be

$$\begin{aligned}
\mu^{k+1} &:= \delta_\phi F_c(\phi^{k+1}) - \delta_\phi F_e(\phi^k) \\
&= \left(\phi^{k+1}\right)^3 + \alpha\phi^{k+1} + 2\Delta_h\phi^k + \Delta_h\kappa^{k+1}, \qquad (4.4)
\end{aligned}$$

where $\kappa^{k+1} := \Delta_h\phi^{k+1}$. The scheme for the MPFC equation is the following: given ϕ^k, $\psi^k \in \mathcal{C}_{\overline{m}\times\overline{n}}$ periodic, find ϕ^{k+1}, ψ^{k+1}, μ^{k+1}, $\kappa^{k+1} \in \mathcal{C}_{\overline{m}\times\overline{n}}$ periodic such that

$$\beta\left(\psi^{k+1} - \psi^k\right) = s\Delta_h\mu^{k+1} - s\psi^{k+1}, \qquad (4.5)$$

$$\phi^{k+1} - \phi^k = s\psi^{k+1}, \qquad (4.6)$$

where $\psi^0 \equiv 0$. An equivalent formulation of the scheme is given as

$$\phi^{k+1} - \phi^k = s\Delta_h\mu^{k+1} - \beta\left(\frac{\phi^{k+1} - \phi^k}{s} - \psi^k\right), \qquad (4.7)$$

$$\phi^{k+1} - \phi^k = s\psi^{k+1}. \qquad (4.8)$$

The utility of this latter formulation is that the equations are decoupled. In particular, we will use (4.7) and (4.8) to demonstrate solvability. If the time step-size s is unchanging from one step to the next, then the scheme is given as

$$\phi^{k+1} - \phi^k = s\Delta_h \mu^{k+1} - \beta\left(\frac{\phi^{k+1} - 2\phi^k + \phi^{k-1}}{s}\right), \tag{4.9}$$

which is explicitly a two-step scheme. In this case we take $\phi^{-1} \equiv \phi^0$, which implies $\psi^0 \equiv 0$ in the two previous versions.

4.2. Mass conservation and unconditional unique solvability. Here we demonstrate that the scheme is discrete mass conserving and uniquely solvable, regardless of the time step-size s.

THEOREM 4.2 (mass conservation). *The MPFC scheme* (4.5) *and* (4.6) *is discretely mass conserving for any time step-size $s > 0$, provided solutions to the scheme exist.*

Proof. Let us assume that the MPFC scheme (4.5) and (4.6) has a solution for some $s > 0$. Summing (4.6) we see that

$$\left(\phi^{k+1} - \phi^k \middle\| \mathbf{1}\right) = 0 \text{ if and only if } \left(\psi^{k+1}\middle\|\mathbf{1}\right) = 0. \tag{4.10}$$

Summing (4.5) we find

$$\begin{aligned}\beta\left(\psi^{k+1} - \psi^k\middle\|\mathbf{1}\right) + s\left(\psi^{k+1}\middle\|\mathbf{1}\right) &= s\left(\Delta_h\mu\|\mathbf{1}\right)\\ &= -s\left[D_x\mu^{k+1}\middle\|D_x\mathbf{1}\right]_{\mathrm{ew}} - s\left[D_y\mu^{k+1}\middle\|D_y\mathbf{1}\right]_{\mathrm{ns}}\\ &= 0.\end{aligned} \tag{4.11}$$

Hence

$$(\beta + s)\left(\psi^{k+1}\middle\|\mathbf{1}\right) = \beta\left(\psi^k\middle\|\mathbf{1}\right). \tag{4.12}$$

But, since $\psi^0 \equiv 0$, $\left(\psi^0\middle\|\mathbf{1}\right) = 0$. It is evident from (4.12) that $\left(\psi^k\middle\|\mathbf{1}\right) = 0$ for $k = 1, 2, 3, \ldots$. Thus, if (4.5) and (4.6) 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 mass. ∎

THEOREM 4.3 (unique solvability). *The MPFC scheme* (4.5) *and* (4.6) *is uniquely solvable for any time step-size $s > 0$.*

Proof. 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 in (3.19). Note that $\psi^k \in H$ naturally. Since the scheme is mass conserving, the appropriate space for solutions of (4.5) and (4.6) must necessarily be H. In other words, ϕ^{k+1}, $\psi^{k+1} \in H$, provided solutions exist. Now consider the following functional on H:

$$\begin{aligned}G(\phi) := \left(1 + \frac{\beta}{s}\right)\frac{h^2}{2}\left(\phi\|\phi\right)_{H,\mathcal{L}} - h^2\left(\phi\middle\|\left(1+\frac{\beta}{s}\right)\phi^k + \beta\psi^k\right)_{H,\mathcal{L}} + F_c(\phi)\\ -h^2\left(\phi\middle\|\delta_\phi F_e(\phi^k)\right),\end{aligned} \tag{4.13}$$

where the H inner product is defined as

$$\left(\phi_1\|\phi_2\right)_{H,\mathcal{L}} := s\left[D_x\psi_1\|D_x\psi_2\right]_{\mathrm{ew}} + s\left[D_y\psi_1\|D_y\psi_2\right]_{\mathrm{ns}}, \tag{4.14}$$

and $\psi_i \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is the unique solution (by Lemma 3.6) to

$$\mathcal{L}(\psi_i) = -s\Delta_h\psi_i = \phi_i, \tag{4.15}$$

such that ψ_i is periodic mean-zero, i.e., $(\psi_i \| \mathbf{1}) = 0$. From here the proof essentially follows that of [16, Thm. 3.4]. One may show that the functional G in (4.13) is coercive and strictly convex and that minimizing G is equivalent to solving (4.7) and (4.8), which in turn is equivalent to solving (4.5) and (4.6). ◻

4.3. Unconditional stability. The following estimate is proven in [16, Thm. 3.5].

THEOREM 4.4 (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* (4.1)*, and take the convex splitting $F = F_c - F_e$ in Lemma* 4.1*. Then*

$$F(\phi^{k+1}) - F(\phi^k) \le h^2 \left(\delta_\phi F_c(\phi^{k+1}) - \delta_\phi F_e(\phi^k) \middle\| \phi^{k+1} - \phi^k\right). \tag{4.16}$$

LEMMA 4.5 (H-norm estimate). *Let $\mathcal{L} = -\Delta_h$, and suppose that ψ^{k+1}, $\psi^k \in H$. Then*

$$\begin{aligned} \frac{1}{2}\left\|\psi^{k+1}\right\|_{H,\mathcal{L}}^2 - \frac{1}{2}\left\|\psi^k\right\|_{H,\mathcal{L}}^2 &\le h^2 \left(\psi^{k+1} \middle\| \psi^{k+1} - \psi^k\right)_{H,\mathcal{L}} \\ &= h^2 \left(\mathcal{L}^{-1}\left(\psi^{k+1}\right) \middle\| \psi^{k+1} - \psi^k\right) . \end{aligned} \tag{4.17}$$

Proof. This follows immediately because $\|\psi^{k+1}\|_{H,\mathcal{L}}^2$ is a strictly convex functional on H. ◻

The energy decay estimate Theorem 4.4 readily yields the energy stability of the scheme.

THEOREM 4.6 (energy stability). *The MPFC scheme* (4.5) *and* (4.6) *is unconditionally (strongly) energy stable with respect to* (4.2)*, meaning that for any time step-size $s > 0$,*

$$\mathcal{F}\left(\phi^{k+1}, \psi^{k+1}\right) \le \mathcal{F}\left(\phi^k, \psi^k\right) . \tag{4.18}$$

Proof. Let $C := \left(\mu^{k+1} \middle\| \mathbf{1}\right)/(m\,n)$. Using the energy decay and H-norm estimates, we have

$$\begin{aligned} &\mathcal{F}\left(\phi^{k+1}, \psi^{k+1}\right) - \mathcal{F}\left(\phi^k, \psi^k\right) \\ &\quad \le h^2 \left(\delta_\phi F_c(\phi^{k+1}) - \delta_\phi F_e(\phi^k) \middle\| \phi^{k+1} - \phi^k\right) - \beta h^2 \left(\Delta_h^{-1}\left(\psi^{k+1}\right) \middle\| \psi^{k+1} - \psi^k\right) \\ &\quad = s h^2 \left(\mu^{k+1} \middle\| \psi^{k+1}\right) - \beta h^2 \left(\psi^{k+1} \middle\| \Delta_h^{-1}\left(\psi^{k+1} - \psi^k\right)\right) \\ &\quad = h^2 \left(\psi^{k+1} \middle\| s\left(\mu^{k+1} - C\right) - \beta \Delta_h^{-1}\left(\psi^{k+1} - \psi^k\right)\right) + s\,C\left(\psi^{k+1} \middle\| \mathbf{1}\right) \\ &\quad = h^2 \left(\psi^{k+1} \middle\| s\Delta_h^{-1}\left(\Delta_h\left(\mu^{k+1} - C\right)\right) - \beta \Delta_h^{-1}\left(\psi^{k+1} - \psi^k\right)\right) \\ &\quad = h^2 \left(\psi^{k+1} \middle\| \Delta_h^{-1}\left(s\Delta_h \mu^{k+1} - s\Delta_h C - \beta\left(\psi^{k+1} - \psi^k\right)\right)\right) \\ &\quad = s h^2 \left(\psi^{k+1} \middle\| \Delta_h^{-1} \psi^{k+1}\right) = -s\left\|\psi^{k+1}\right\|_{H,\mathcal{L}}^2 \le 0 , \end{aligned} \tag{4.19}$$

and the proof is complete. ◻

LEMMA 4.7. *Suppose that $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is periodic. Then the following estimates hold:*

$$F(\phi) \ge C_5 \|\phi\|_{2,2}^2 - \frac{L_x L_y}{4} , \tag{4.20}$$

$$F(\phi) \ge C_6 \|\phi\|_\infty^2 - \frac{L_x L_y}{4} , \quad C_6 := \frac{C_5}{C_2} , \tag{4.21}$$

$$F(\phi) \ge C_7 \|\nabla_h \phi\|_4^2 - \frac{L_x L_y}{4} , \quad C_7 := \frac{C_5}{C_4} , \tag{4.22}$$

where $C_5 > 0$ and depends upon α only.

Proof. Equation (4.20) is proven in [16, Lem. 3.7]. Estimate (4.21) follows from (4.20) and Lemma 3.5, and estimate (4.22) follows from (4.20) and Lemma 3.9. $\square$

Finally, we can prove the uniform boundedness of the discrete solution of the MPFC scheme in various norms.

THEOREM 4.8. *Let $\Phi(x, y)$ be a sufficiently regular, periodic function on $\Omega = (0, L_x) \times (0 \times L_y)$ and $\phi^0_{i,j} := \Phi(x_i, y_j)$. Suppose E is the continuous energy* (2.1) *and F is the discrete energy* (4.1). *Let $\phi^k_{i,j} \in \mathcal{C}_{\overline{m}\times\overline{n}}$ be the* kth *periodic solution of* (4.5) *and* (4.6). *Then we have the following estimates:*

$$\left\|\phi^k\right\|_{2,2} \le \sqrt{\frac{1}{C_5}\Big(E(\Phi) + C_8 L_x L_y\Big)} =: C_9 \ , \tag{4.23}$$

$$\left\|\phi^k\right\|_{\infty} \le \sqrt{\frac{1}{C_6}\left(E(\Phi) + C_8 L_x L_y\right)} =: C_{10} \ , \tag{4.24}$$

$$\left\|\nabla_h\phi^k\right\|_{4} \le \sqrt{\frac{1}{C_7}\left(E(\Phi) + C_8 L_x L_y\right)} =: C_{11} \ , \tag{4.25}$$

where $C_8 > 0$ and does not depend on either s or h.

Proof. Recall that $\psi^0 \equiv 0$, from which it follows that $F(\phi^0) = \mathcal{F}(\phi^0, \psi^0)$. From the energy stability theorem, Theorem 4.6, and the previous lemma, we have

$$F\left(\phi^0\right) = \mathcal{F}(\phi^0, \psi^0) \ge \mathcal{F}(\phi^k, \psi^k) \ge F(\phi^k) \ge C_5 \left\|\phi^k\right\|^2_{2,2} - \frac{L_x L_y}{4} \ , \tag{4.26}$$

where $C_5 > 0$ depends upon α only. It is straightforward to show (e.g., [6, Cor. 1]) that

$$F\left(\phi^0\right) = E(\Phi) + \tau, \tag{4.27}$$

where τ is an approximation error satisfying

$$|\tau| \le Mh^2 \le M L_x L_y \tag{4.28}$$

for some $M \ge 0$ that does not depend upon h. Then

$$\left(M + \frac{1}{4}\right) L_x L_y + E(\Phi) \ge C_5 \left\|\phi^k\right\|^2_{2,2} \ , \tag{4.29}$$

and (4.23) follows with $C_8 := \left(M + \frac{1}{4}\right)$. The estimates (4.23) and (4.25) follow similarly. $\square$

We remark that, because of the dissipative nature of the MPFC equation, we can establish the following uniform estimates of the PDE solutions using techniques analogous to those already displayed.

THEOREM 4.9. *Suppose that $\Phi(x, y, t)$ is a periodic solution of the MPFC equation* (2.3)*, with the regularity assumed in Theorem* 4.12*, such that $\partial_t\Phi(x, y, 0) = 0$. Then we have the following estimates:*

$$\|\Phi\|_{L^\infty(0,T;H^2(\Omega))} \le \sqrt{C_{12}\left(E\left(\Phi\left(x, y, 0\right)\right) + \frac{L_x L_y}{4}\right)} =: C_{13} \ , \tag{4.30}$$

$$\|\Phi\|_{L^\infty(0,T;L^\infty(\Omega))} \le \sqrt{C_{14}\left(E\left(\Phi\left(x, y, 0\right)\right) + \frac{L_x L_y}{4}\right)} =: C_{15} \ , \tag{4.31}$$

$$\|\Phi\|_{L^\infty(0,T;W^{1,4}(\Omega))} \le \sqrt{C_{16}\left(E\left(\Phi\left(x, y, 0\right)\right) + \frac{L_x L_y}{4}\right)} =: C_{17} \ , \tag{4.32}$$

for any $T \geq 0$, where C_{12}, C_{14}, $C_{16} > 0$ are constants that are independent of T.

4.4. Error estimate for the MPFC equation. We conclude this section with a local-in-time error estimate for the MPFC equation. We will need the following estimate, proved in [16, Lem. 6.11], showing control of the backward diffusion term.

LEMMA 4.10. *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*

$$\left\| \Delta_h \phi \right\|_2^2 \leq \frac{1}{3\epsilon^2} \left\| \phi \right\|_2^2 + \frac{2\epsilon}{3} \left\| \nabla_h \left(\Delta_h \phi \right) \right\|_2^2 , \tag{4.33}$$

valid for arbitrary $\epsilon > 0$.

We need the following lemma to demonstrate control of the error related to the nonlinear term in our scheme.

LEMMA 4.11. *Suppose Φ, $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ are periodic and denote their difference by $\tilde{\phi} := \Phi - \phi$. Then*

$$\begin{aligned}\left\| \Delta_h \left(\Phi^3 - \phi^3 \right) \right\|_2 \leq C_{18} \Big\{ & \left\| \phi \right\|_\infty^2 \cdot \left\| \Delta_h \tilde{\phi} \right\|_2 + \Big(\left\| \Phi \right\|_\infty + \left\| \phi \right\|_\infty \Big) \\ & \times \Big(\left\| \Delta_h^x \Phi \right\|_\infty + \left\| \Delta_h^y \Phi \right\|_\infty \Big) \left\| \tilde{\phi} \right\|_2 + \left\| \nabla_h \Phi \right\|_\infty^2 \cdot \left\| \tilde{\phi} \right\|_2 \\ & + \left\| \phi \right\|_\infty \left(\left\| \nabla_h \Phi \right\|_4 + \left\| \nabla_h \phi \right\|_4 \right) \left\| \nabla_h \tilde{\phi} \right\|_4 \Big\} ,\end{aligned} \tag{4.34}$$

where C_{18} is a positive constant that is independent of h.

Proof. A detailed calculation yields the following expression:

$$\begin{aligned}\Delta_h^x \left(\phi^3 \right)_{i,j} = {} & Q_x \left(\phi \right)_{i,j} \Delta_h^x \phi_{i,j} + 2\phi_{i,j} \left(D_x \phi_{i-1/2,j} + D_x \phi_{i+1/2,j} \right)^2 \\ & - \left(\phi_{i-1,j} + \phi_{i+1,j} \right) D_x \phi_{i-1/2,j} D_x \phi_{i+1/2,j} \ ,\end{aligned} \tag{4.35}$$

where

$$Q_x \left(\phi \right)_{i,j} := \phi_{i-1,j}^2 + \phi_{i,j}^2 + \phi_{i+1,j}^2 - 2\phi_{i-1,j}\phi_{i+1,j} + \phi_{i,j}(\phi_{i-1,j} + \phi_{i+1,j}). \tag{4.36}$$

An analogous formula for $\Delta_h^y \left(\phi^3 \right)_{i,j}$ holds by symmetry. Another calculation confirms that $\Delta_h^x \left(\Phi^3 \right)_{i,j} - \Delta_h^x \left(\phi^3 \right)_{i,j} = \sum_{\ell=1}^7 N_{i,j}^{(\ell)}$, where

$$\begin{aligned}N_{i,j}^{(1)} &= Q_x \left(\phi \right)_{i,j} \Delta_h^x \tilde{\phi}_{i,j} \ , \\ N_{i,j}^{(2)} &= \Big(Q_x \left(\Phi \right)_{i,j} - Q_x \left(\phi \right)_{i,j} \Big) \Delta_h^x \Phi_{i,j} \ , \\ N_{i,j}^{(3)} &= 2\tilde{\phi}_{i,j} \left(D_x \Phi_{i-1/2,j} + D_x \Phi_{i+1/2,j} \right)^2 \ , \\ N_{i,j}^{(4)} &= 2\phi_{i,j} \left(D_x \phi_{i-1/2,j} + D_x \phi_{i+1/2,j} + D_x \Phi_{i-1/2,j} + D_x \Phi_{i+1/2,j} \right) \\ & \qquad \times \Big(D_x \tilde{\phi}_{i-1/2,j} + D_x \tilde{\phi}_{i+1/2,j} \Big) \ , \\ N_{i,j}^{(5)} &= - \Big(\tilde{\phi}_{i-1,j} + \tilde{\phi}_{i+1,j} \Big) D_x \Phi_{i-1/2,j} D_x \Phi_{i+1/2,j} \ , \\ N_{i,j}^{(6)} &= - \left(\phi_{i-1,j} + \phi_{i+1,j} \right) D_x \tilde{\phi}_{i-1/2,j} D_x \Phi_{i+1/2,j} \ , \\ N_{i,j}^{(7)} &= - \left(\phi_{i-1,j} + \phi_{i+1,j} \right) D_x \phi_{i-1/2,j} D_x \tilde{\phi}_{i+1/2,j} \ .\end{aligned}$$

The first term can be directly controlled by Hölder's inequality and Lemma 3.10:

$$\left\| N^{(1)} \right\|_2 \le \| Q_x(\phi) \|_\infty \left\| \Delta_h^x \tilde{\phi} \right\|_2 \le C \|\phi\|_\infty^2 \left\| \Delta_h^x \tilde{\phi} \right\|_2 \le C \|\phi\|_\infty^2 \left\| \Delta_h \tilde{\phi} \right\|_2 \ . \tag{4.37}$$

For the second term, we see the following estimate:

$$\| Q_x(\Phi) - Q_x(\phi) \|_2 \le C \left(\|\Phi\|_\infty + \|\phi\|_\infty \right) \left\| \tilde{\phi} \right\|_2 \ , \tag{4.38}$$

from which we obtain

$$\left\| N^{(2)} \right\|_2 \le C \left(\|\Phi\|_\infty + \|\phi\|_\infty \right) \| \Delta_h^x \Phi \|_\infty \cdot \left\| \tilde{\phi} \right\|_2 \ . \tag{4.39}$$

The other terms can be handled in a similar way (the details are skipped):

$$\left\| N^{(3)} \right\|_2 + \left\| N^{(5)} \right\|_2 \le C \| \nabla_h \Phi \|_\infty^2 \cdot \left\| \tilde{\phi} \right\|_2 \ , \tag{4.40}$$

$$\left\| N^{(4)} \right\|_2 + \left\| N^{(6)} \right\|_2 + \left\| N^{(7)} \right\|_2 \le C \|\phi\|_\infty \left(\|\nabla_h \Phi\|_4 + \|\nabla_h \phi\|_4 \right) \left\| \nabla_h \tilde{\phi} \right\|_4 . \tag{4.41}$$

The nonlinear error term $\Delta_h^y \left((\Phi)^3 - (\phi)^3 \right)$ can be analyzed in exactly the same way. Combining the estimates using the triangle inequality gives the result (4.34) and the lemma is proven. ∎

We now establish an error estimate for the fully discrete approximation to MPFC equation.

Theorem 4.12 (error estimate). *Let $\Omega = (0, L_x) \times (0 \times L_y)$. Suppose the unique periodic solution for the MPFC equation* (2.3) *is given by*

$$\Phi \in L^\infty \left(\Omega; H^3 (0, T) \right) \cap L^\infty \left(0, T; H_{per}^{8+\eta} (\Omega) \right) \cap H^1 \left(0, T; H_{per}^{5+\eta} (\Omega) \right) \tag{4.42}$$

for $\eta > 0$ and $T < \infty$. Define $\Phi_{i,j}^k := \Phi\big((i - 1/2)h, (j - 1/2)h, ks \big)$, and $\tilde{\phi}_{i,j}^k := \Phi_{i,j}^k - \phi_{i,j}^k$, where $\phi_{i,j}^k \in \mathcal{C}_{\overline{m} \times \overline{n}}$ is kth periodic solution of (4.9) *with $\phi_{i,j}^{-1} := \Phi_{i,j}^0$ and $\phi_{i,j}^0 := \Phi_{i,j}^0$. Then*

$$\left\| \tilde{\phi}^k \right\|_2 + \left\| \nabla_h \left(\Delta_h \tilde{\phi}^k \right) \right\|_2 \le C \left(h^2 + s \right) \ , \tag{4.43}$$

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

Proof. We assume that $s > 0$ is unchanging from one time step to the next. A detailed analysis shows that the exact solution Φ solves the fully discrete equation with a local truncation error:

$$\beta \frac{\Phi^{k+1} - 2\Phi^k + \Phi^{k-1}}{s^2} + \frac{\Phi^{k+1} - \Phi^k}{s} = \Delta_h \Bigg(\left(\Phi^{k+1} \right)^3 + \alpha \Phi^{k+1} + 2 \Delta_h \Phi^k + \Delta_h^2 \Phi^{k+1} \Bigg) + \tau^{k+1} \ , \tag{4.44}$$

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

$$\|\tau\|_{L_s^2 \left(0, T; L_h^2(\Omega) \right)} := \sqrt{ s \sum_{k=0}^{T/s} \| \tau^{k+1} \|_2^2 } \le M \left(h^2 + s \right) \ . \tag{4.45}$$

The positive constant M depends only on the exact solution Φ and the final time T. In more detail, we have

$$M \le C\Big(\|\Phi\|_{L^\infty(\Omega;H^3(0,T))} + \|\Phi\|^{3-3\eta}_{L^\infty(0,T;H^4(\Omega))} \cdot \|\Phi\|^{3\eta}_{L^\infty(0,T;H^5(\Omega))} + \|\Phi\|_{H^1(0,T;H^{5+\eta}(\Omega))} + \|\Phi\|_{L^\infty(0,T;H^{8+\eta}(\Omega))}\Big) . \tag{4.46}$$

The proof of this last claim is technical and is given in the appendix.

Subtracting (4.9) from (4.44) yields

$$\beta\frac{\tilde\phi^{k+1} - 2\tilde\phi^k + \tilde\phi^{k-1}}{s^2} + \frac{\tilde\phi^{k+1} - \tilde\phi^k}{s} = \Delta_h\Big(\left(\Phi^{k+1}\right)^3 - \left(\phi^{k+1}\right)^3 + \alpha\tilde\phi^{k+1} + 2\Delta_h\tilde\phi^k + \Delta_h^2\tilde\phi^{k+1}\Big) + \tau^{k+1}. \tag{4.47}$$

Taking the inner product with the error difference function $h^2(\tilde\phi^{k+1} - \tilde\phi^k)$ gives

$$\begin{aligned} h^2 & \left(\tilde\phi^{k+1} - \tilde\phi^k \middle\| \tau^{k+1}\right) + h^2 \left(\tilde\phi^{k+1} - \tilde\phi^k \middle\| \Delta_h\left(\left(\Phi^{k+1}\right)^3 - \left(\phi^{k+1}\right)^3\right)\right) \\ &= \frac{\beta h^2}{s^2}\left(\tilde\phi^{k+1} - 2\tilde\phi^k + \tilde\phi^{k-1} \middle\| \tilde\phi^{k+1} - \tilde\phi^k\right) + \frac{h^2}{s}\left(\tilde\phi^{k+1} - \tilde\phi^k \middle\| \tilde\phi^{k+1} - \tilde\phi^k\right) \\ &\quad -\alpha h^2 \left(\tilde\phi^{k+1} - \tilde\phi^k \middle\| \Delta_h\tilde\phi^{k+1}\right) - 2h^2\left(\tilde\phi^{k+1} - \tilde\phi^k \middle\| \Delta_h^2\tilde\phi^k\right) \\ &\quad -h^2\left(\tilde\phi^{k+1} - \tilde\phi^k \middle\| \Delta_h^3\tilde\phi^{k+1}\right) . \end{aligned} \tag{4.48}$$

With the introduction of the variable $\tilde\psi^k := (\tilde\phi^k - \tilde\phi^{k-1})/s$, the first two terms on the right-hand side can be rewritten and estimated as follows:

$$\begin{aligned} \frac{h^2}{s^2}\left(\tilde\phi^{k+1} - \tilde\phi^k \middle\| \tilde\phi^{k+1} - 2\tilde\phi^k + \tilde\phi^{k-1}\right) &= h^2\left(\tilde\psi^{k+1} \middle\| \tilde\psi^{k+1} - \tilde\psi^k\right) \\ &= \frac{1}{2}\left(\left\|\tilde\psi^{k+1}\right\|_2^2 - \left\|\tilde\psi^k\right\|_2^2\right) + \frac{1}{2}\left\|\tilde\psi^{k+1} - \tilde\psi^k\right\|_2^2 \\ &\ge \frac{1}{2}\left(\left\|\tilde\psi^{k+1}\right\|_2^2 - \left\|\tilde\psi^k\right\|_2^2\right) , \end{aligned} \tag{4.49}$$

and

$$\frac{h^2}{s}\left(\tilde\phi^{k+1} - \tilde\phi^k \middle\| \tilde\phi^{k+1} - \tilde\phi^k\right) = s\left\|\tilde\psi^{k+1}\right\|_2^2 \ge 0 . \tag{4.50}$$

The left-hand side of (4.48) can be controlled using the Cauchy inequality:

$$h^2\left(\tilde\phi^{k+1} - \tilde\phi^k \middle\| \tau^{k+1}\right) \le \frac{1}{2}s\left\|\tilde\psi^{k+1}\right\|_2^2 + \frac{1}{2}s(s+h^2)^2M^2 . \tag{4.51}$$

The analysis of the convex diffusion terms can be carried out with the help of the discrete Green's identities, (3.3) and (3.4):

$$\begin{aligned} -h^2\left(\tilde\phi^{k+1} - \tilde\phi^k \middle\| \Delta_h\tilde\phi^{k+1}\right) &= \frac{1}{2}\left(\left\|\nabla_h\tilde\phi^{k+1}\right\|_2^2 - \left\|\nabla_h\tilde\phi^k\right\|_2^2\right) + \frac{1}{2}\left\|\nabla_h\left(\tilde\phi^{k+1} - \tilde\phi^k\right)\right\|_2^2 \\ &\ge \frac{1}{2}\left(\left\|\nabla_h\tilde\phi^{k+1}\right\|_2^2 - \left\|\nabla_h\tilde\phi^k\right\|_2^2\right) \end{aligned} \tag{4.52}$$

and

$$-h^2\left(\tilde{\phi}^{k+1}-\tilde{\phi}^k\middle\|\Delta_h^3\tilde{\phi}^{k+1}\right)=\frac{1}{2}\left(\left\|\nabla_h\left(\Delta_h\tilde{\phi}^{k+1}\right)\right\|_2^2-\left\|\nabla_h\left(\Delta_h\tilde{\phi}^{k}\right)\right\|_2^2\right)$$
$$+\frac{1}{2}\left\|\nabla_h\left(\Delta_h\left(\tilde{\phi}^{k+1}-\tilde{\phi}^k\right)\right)\right\|_2^2$$
$$\geq\frac{1}{2}\left(\left\|\nabla_h\left(\Delta_h\tilde{\phi}^{k+1}\right)\right\|_2^2-\left\|\nabla_h\left(\Delta_h\tilde{\phi}^{k}\right)\right\|_2^2\right). \tag{4.53}$$

The concave diffusion term can be handled in a similar way:

$$-h^2\left(\tilde{\phi}^{k+1}-\tilde{\phi}^k\middle\|\Delta_h^2\tilde{\phi}^{k}\right)=-h^2\left(\Delta_h(\tilde{\phi}^{k+1}-\tilde{\phi}^k)\middle\|\Delta_h\tilde{\phi}^{k}\right)$$
$$=-\frac{1}{2}\left(\left\|\Delta_h\tilde{\phi}^{k+1}\right\|_2^2-\left\|\Delta_h\tilde{\phi}^{k}\right\|_2^2\right)+\frac{1}{2}\left\|\Delta_h\left(\tilde{\phi}^{k+1}-\tilde{\phi}^k\right)\right\|_2^2$$
$$\geq-\frac{1}{2}\left(\left\|\Delta_h\tilde{\phi}^{k+1}\right\|_2^2-\left\|\Delta_h\tilde{\phi}^{k}\right\|_2^2\right)\ . \tag{4.54}$$

For the nonlinear term, we start with an application of Cauchy's inequality:

$$h^2\left(\tilde{\phi}^{k+1}-\tilde{\phi}^k\middle\|\Delta_h\left(\left(\Phi^{k+1}\right)^3-\left(\phi^{k+1}\right)^3\right)\right)$$
$$\leq\frac{s}{2}\left\|\tilde{\psi}^{k+1}\right\|_2^2+\frac{s}{2}\left\|\Delta_h\left(\left(\Phi^{k+1}\right)^3-\left(\phi^{k+1}\right)^3\right)\right\|_2^2\ . \tag{4.55}$$

Using Lemma 4.11 we have the estimate

$$\left\|\Delta_h\left(\left(\Phi^{k+1}\right)^3-\left(\phi^{k+1}\right)^3\right)\right\|_2$$
$$\leq C_{18}\Big\{\left\|\phi^{k+1}\right\|_\infty^2\cdot\left\|\Delta_h\tilde{\phi}^{k+1}\right\|_2+\left(\left\|\Phi^{k+1}\right\|_\infty+\left\|\phi^{k+1}\right\|_\infty\right)$$
$$\times\left(\left\|\Delta_h^x\Phi^{k+1}\right\|_\infty+\left\|\Delta_h^y\Phi^{k+1}\right\|_\infty\right)\left\|\tilde{\phi}^{k+1}\right\|_2+\left\|\nabla_h\Phi^{k+1}\right\|_\infty^2\cdot\left\|\tilde{\phi}^{k+1}\right\|_2$$
$$+\left\|\phi^{k+1}\right\|_\infty\left(\left\|\nabla_h\Phi^{k+1}\right\|_4+\left\|\nabla_h\phi^{k+1}\right\|_4\right)\left\|\nabla_h\tilde{\phi}^{k+1}\right\|_4\Big\}\ , \tag{4.56}$$

where C_{18} is a positive constant that is independent of s and h. We have the following uniform estimates from our previous lemmas:

$$\left\|\Phi^{k+1}\right\|_\infty\leq\left\|\Phi^{k+1}\right\|_{L^\infty}\leq C_{15}\ , \tag{4.57}$$
$$\left\|\nabla_h\Phi^{k+1}\right\|_4\leq C\left\|\nabla\Phi^{k+1}\right\|_{L^\infty}+C\leq C\ , \tag{4.58}$$
$$\left\|\phi^{k+1}\right\|_\infty\leq C_{10}\ , \tag{4.59}$$
$$\left\|\nabla_h\phi^{k+1}\right\|_4\leq C_{11}\ , \tag{4.60}$$

where C denotes a generic positive constant that is independent of h. The following estimates are also valid, but on the finite time interval $[0,T]$ only:

$$\left\|\nabla_h\Phi^{k+1}\right\|_\infty\leq\left\|\nabla\Phi^{k+1}\right\|_{L^\infty}+C\leq C\ , \tag{4.61}$$
$$\left\|\Delta_h^x\Phi^{k+1}\right\|_\infty+\left\|\Delta_h^y\Phi^{k+1}\right\|_\infty\leq\left\|\partial_{xx}\Phi^{k+1}\right\|_{L^\infty}+\left\|\partial_{yy}\Phi^{k+1}\right\|_{L^\infty}+C\leq C\,, \tag{4.62}$$

where again C is an h-independent generic positive constant. Applying Lemma 3.11 and estimates (4.56)–(4.62) yields

$$\left\|\Delta_h\left((\Phi^{k+1})^3-(\phi^{k+1})^3\right)\right\|_2\leq C_{19}\left(\left\|\tilde{\phi}^{k+1}\right\|_2+\left\|\Delta_h\tilde{\phi}^{k+1}\right\|_2\right)\ , \tag{4.63}$$

where $C_{19} > 0$ is independent of h and s, but is dependent upon T and also the exact solution Φ. Going back to (4.55) and using the last estimate and Lemma 4.10 (with $\epsilon = 1$), we obtain an estimate for the nonlinear term

$$\begin{aligned} h^2 \left(\tilde{\phi}^{k+1} - \tilde{\phi}^k \middle\| \Delta_h \left((\Phi^{k+1})^3 - (\phi^{k+1})^3 \right) \right) \\ &\le \frac{s}{2} \left\| \tilde{\psi}^{k+1} \right\|_2^2 + s\, C_{19}^2 \left(\left\| \tilde{\phi}^{k+1} \right\|_2^2 + \left\| \Delta_h \tilde{\phi}^{k+1} \right\|_2^2 \right) \\ &\le \frac{s}{2} \left\| \tilde{\psi}^{k+1} \right\|_2^2 + \frac{4s\, C_{19}^2}{3} \left(\left\| \tilde{\phi}^{k+1} \right\|_2^2 + \left\| \nabla_h \left(\Delta_h \tilde{\phi}^{k+1} \right) \right\|_2^2 \right) . \end{aligned} \tag{4.64}$$

Define a modified energy for the error function via

$$F_1\left(\tilde{\phi}^k\right) := \frac{\beta}{2} \left\| \tilde{\psi}^k \right\|_2^2 + \frac{\alpha}{2} \left\| \nabla_h \tilde{\phi}^k \right\|_2^2 + \frac{1}{2} \left\| \nabla_h \left(\Delta_h \tilde{\phi}^k \right) \right\|_2^2 - \left\| \Delta_h \tilde{\phi}^k \right\|_2^2 . \tag{4.65}$$

A combination of (4.48), (4.50)–(4.54), and (4.64) results in

$$\begin{aligned} F_1\left(\tilde{\phi}^{k+1}\right) - F_1\left(\tilde{\phi}^k\right) \le s\, C_{20} \left(\left\| \tilde{\phi}^{k+1} \right\|^2 + \left\| \nabla_h \left(\Delta_h \tilde{\phi}^{k+1} \right) \right\|_2^2 + \left\| \tilde{\psi}^{k+1} \right\|_2^2 \right) \\ + s \left\| \tau^{k+1} \right\|_2^2 , \end{aligned} \tag{4.66}$$

where $C_{20} > 0$ is independent of h and s. Summing over k and using the fact that $F_1(\tilde{\phi}^0) = 0$ yield

$$\begin{aligned} F_1\left(\tilde{\phi}^\ell\right) &\le s\, C_{20} \sum_{k=1}^{\ell} \left(\left\| \tilde{\phi}^k \right\|_2^2 + \left\| \nabla_h \left(\Delta_h \tilde{\phi}^k \right) \right\|_2^2 + \left\| \tilde{\psi}^k \right\|_2^2 \right) + \left\| \tau^k \right\|_{L_s^2\left(0,T;L_h^2(\Omega)\right)}^2 \\ &\le s\, C_{20} \sum_{k=1}^{\ell} \left(\left\| \tilde{\phi}^k \right\|_2^2 + \left\| \nabla_h \left(\Delta_h \tilde{\phi}^k \right) \right\|_2^2 + \left\| \tilde{\psi}^k \right\|_2^2 \right) + M^2 T (s + h^2)^2 . \end{aligned} \tag{4.67}$$

To carry out further analysis, we introduce the positive part F_1:

$$\begin{aligned} F_2\left(\tilde{\phi}^k\right) &:= \frac{\beta}{2} \left\| \tilde{\psi}^k \right\|^2 + \frac{\alpha}{2} \left\| \nabla_h \tilde{\phi}^k \right\|^2 + \frac{1}{2} \left\| \nabla_h \left(\Delta_h \tilde{\phi}^k \right) \right\|_2^2 \\ &= F_1\left(\tilde{\phi}^k\right) + \left\| \Delta_h \tilde{\phi}^k \right\|_2^2 , \end{aligned} \tag{4.68}$$

so that (4.67) becomes

$$\begin{aligned} F_2\left(\tilde{\phi}^\ell\right) \le s\, C_{20} \sum_{k=1}^{\ell} \left(\left\| \tilde{\phi}^k \right\|_2^2 + \left\| \nabla_h \left(\Delta_h \tilde{\phi}^k \right) \right\|_2^2 + \left\| \tilde{\psi}^k \right\|_2^2 \right) \\ + \left\| \Delta_h \tilde{\phi}^\ell \right\|^2 + M^2 T (s + h^2)^2 . \end{aligned} \tag{4.69}$$

Using Lemma 4.10 and Cauchy's inequality, the additional term $\|\Delta_h \tilde{\phi}^\ell\|_2^2$ can be controlled by

$$\begin{aligned} \left\| \Delta_h \tilde{\phi}^\ell \right\|_2^2 &\le \frac{1}{3\epsilon^2} \left\| \tilde{\phi}^\ell \right\|_2^2 + \frac{2\epsilon}{3} \left\| \nabla_h \left(\Delta_h \tilde{\phi}^\ell \right) \right\|_2^2 \\ &\le \frac{s\,T}{3\epsilon^2} \sum_{k=1}^{\ell} \left\| \tilde{\psi}^k \right\|_2^2 + \frac{2\epsilon}{3} \left\| \nabla_h \left(\Delta_h \tilde{\phi}^\ell \right) \right\|_2^2 \end{aligned} \tag{4.70}$$

for any $\epsilon > 0$. In the derivation of (4.70), we have used the identity $\tilde{\phi}^\ell = s\sum_{k=1}^{\ell}\tilde{\psi}^k$, which indicates that

$$\left\|\tilde{\phi}^\ell\right\|_2^2 \le sT\sum_{k=1}^{\ell}\left\|\tilde{\psi}^k\right\|_2^2 \tag{4.71}$$

via an application of Cauchy's inequality. Taking $\epsilon = \frac{3}{8}$, the substitution of the estimate (4.70) into (4.69) shows that

$$\begin{aligned} F_2\left(\tilde{\phi}^\ell\right) - \frac{1}{4}\left\|\nabla_h\left(\Delta_h\tilde{\phi}^\ell\right)\right\|_2^2 \le s\,C_{21}\sum_{k=1}^{\ell}\left(\left\|\tilde{\phi}^k\right\|_2^2 + \left\|\nabla_h\left(\Delta_h\tilde{\phi}^k\right)\right\|_2^2 + \left\|\tilde{\psi}^k\right\|_2^2\right) \\ + M^2T(s+h^2)^2\ , \end{aligned} \tag{4.72}$$

where $C_{21} > 0$ is independent of h and s. Introducing the more refined energy

$$\begin{aligned} F_3\left(\tilde{\phi}^k\right) &:= \frac{\beta}{2}\left\|\tilde{\psi}^k\right\|_2^2 + \frac{\alpha}{2}\left\|\nabla_h\tilde{\phi}^k\right\|_2^2 + \frac{1}{4}\left\|\nabla_h\left(\Delta_h\tilde{\phi}^k\right)\right\|_2^2 \\ &= F_2\left(\tilde{\phi}^k\right) - \frac{1}{4}\left\|\nabla_h\left(\Delta_h\tilde{\phi}^k\right)\right\|_2^2\ , \end{aligned} \tag{4.73}$$

we obtain, with the aid of the estimate (4.71),

$$F_3\left(\tilde{\phi}^\ell\right) \le s\,C_{22}\sum_{k=1}^{\ell}F_3\left(\tilde{\phi}^k\right) + s^2T\,C_{21}\sum_{k=1}^{\ell}\sum_{\ell'=1}^{k}\left\|\tilde{\psi}^{\ell'}\right\|_2^2 + M^2T(s+h^2)^2\ , \tag{4.74}$$

where $C_{22} > 0$ is independent of h and s. Meanwhile, motivated by the estimate

$$s^2T\,C_{21}\sum_{k=1}^{\ell}\sum_{\ell'=1}^{k}\left\|\tilde{\psi}^{\ell'}\right\|_2^2 \le s^2T\,C_{21}\sum_{k=1}^{\ell}\sum_{\ell'=1}^{\ell}\left\|\tilde{\psi}^{\ell'}\right\|_2^2 \le sT^2\,C_{21}\sum_{k=1}^{\ell}\left\|\tilde{\psi}^k\right\|_2^2\ , \tag{4.75}$$

which follows from

$$\sum_{\ell'=1}^{k}\left\|\tilde{\psi}^{\ell'}\right\|_2^2 \le \sum_{\ell'=1}^{\ell}\left\|\tilde{\psi}^{\ell'}\right\|_2^2 \quad \forall\ k \le \ell\ , \tag{4.76}$$

we arrive at

$$F_3\left(\tilde{\phi}^\ell\right) \le s\,C_{23}\sum_{k=1}^{\ell}F_3\left(\tilde{\phi}^k\right) + M^2T(s+h^2)^2\ , \tag{4.77}$$

where $C_{23} > 0$ is independent of h and s. Applying a discrete Gronwall inequality gives

$$F_3\left(\tilde{\phi}^\ell\right) \le C_{24}\left(s+h^2\right)^2\ , \tag{4.78}$$

which holds provided s is sufficiently small. Note that C_{24} is a positive constant that is dependent upon T (exponentially) and Φ, but is independent of h and s. The result is proven. ∎

REMARK 4.13. By virtue of Theorem 4.12 and Lemma 3.5 and 4.10, along with the estimate (4.71), we immediately get an error estimate of the form

$$\left\|\tilde{\phi}^k\right\|_\infty \le C\left(h^2+s\right). \tag{4.79}$$

REMARK 4.14. The convergence analysis techniques for the MPFC model are nonstandard, due to the existence of a second-order temporal derivative. One must test the scheme with $\tilde{\phi}^{k+1} - \tilde{\phi}^k$ to derive a bound of the numerical error function, instead of with $\tilde{\phi}^{k+1}$ as was done in the PFC model (parabolic type PDE) [16]. In particular, the estimate of the nonlinear term involves more technical details, since we have to analyze the Laplacian of the nonlinear error function. As a result, an $L^\infty\left(0,T;H^3_{per}(\Omega)\right)$ numerical convergence can be directly obtained via such an energy estimate, as stated in Theorem 4.12.

5. Conclusions. In this paper, we have developed and proven convergence of an unconditionally energy stable finite difference scheme for the sixth-order Modified Phase Field Crystal (MPFC) equation. This is a sixth-order PDE in the form of a generalized damped wave equation. The parabolic Phase Field Crystal (PFC) equation, which is a mass conserving gradient flow, is obtained as a special case of the MPFC equation. The numerical scheme is based on a convex splitting of a discrete psuedoenergy 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. In a future work, we will demonstrate an efficient nonlinear multigrid method to solve the unconditionally energy stable algorithm presented here.

Appendix. Consistency analysis of the numerical scheme. In this appendix we give a detailed derivation the local truncation error estimate (4.46). For simplicity of presentation, we assume $m = n = N$ and $L_x = L_y = L_0$. The rectangular case can be handled in the same way. We establish the results for vertex-centered grid functions, rather than cell-centered functions, as the indexing becomes simpler. We assume herein that η is any positive real number.

A.1. Proof of estimate (4.46). The following two results will be used to establish (4.46).

PROPOSITION A.1. *For $f \in H^3(0,T)$, we have*

$$\|D_t f - f'(t)\|_{L^2_s(0,T)} \le Cs\,\|f\|_{H^2(0,T)} \ , \quad \left\|D_t^2 f - f''(t)\right\|_{L^2_s(0,T)} \le Cs\,\|f\|_{H^3(0,T)} \ , \tag{A.1}$$

where C depends on T only, $\|\cdot\|_{L^2_s(0,T)}$ is a discrete L^2 norm (in time) given by $\|g\|_{L^2_s(0,T)} = \sqrt{s\sum_{k=0}^{T/s}\left(g^k\right)^2}$, and

$$(D_t f)^{k+1} = \frac{f^{k+1} - f^k}{s} \ , \quad (D_t^2 f)^{k+1} = \frac{f^{k+1} - 2f^k + f^{k-1}}{s^2} \ . \tag{A.2}$$

The proof of Proposition A.1 is based on the integral form of the Taylor expansion in time. The details are skipped for the sake of brevity. Unfortunately, this simple methodology cannot be applied to the case of multiple space dimensions. In two dimensions, the following proposition gives a corresponding $O(h^2)$ truncation error bound. Its proof will be given in Appendix A.2.

PROPOSITION A.2. *For $f \in H^{4+\eta}_{per}(\Omega)$, we have*

$$\|\Delta f - \Delta_h f\|_{L^2_h(\Omega)} \le Ch^2\,\|f\|_{H^{4+\eta}(\Omega)} \ , \tag{A.3}$$

where C depends on L_0 and $\|g\|_{L^2_h(\Omega)} = \sqrt{h^2\sum_{i,j}^{N-1} g_{i,j}^2}$ only.

Let us assume that the exact solution of the MPFC equation has the regularity

$$\Phi \in L^\infty\left(\Omega; H^3(0,T)\right) \cap L^\infty\left(0,T; H^{8+\eta}_{per}(\Omega)\right) \cap H^1\left(0,T; H^{5+\eta}_{per}(\Omega)\right) \quad . \tag{A.4}$$

We denote the following quantities:

$$\begin{array}{lllllll} F_1^{k+1} & = \frac{\Phi^{k+1}-2\Phi^k+\Phi^{k-1}}{s^2} \ , & F_{1e}^{k+1} & = \partial_t^2 \Phi(\ \cdot\ , t^{k+1}) \ , & & \\ F_2^{k+1} & = \frac{\Phi^{k+1}-\Phi^k}{s} \ , & F_{2e}^{k+1} & = \partial_t \Phi(\ \cdot\ , t^{k+1}) \ , & & \\ F_3^{k+1} & = \Delta_h\left((\Phi^{k+1})^3\right) \ , & F_{3e}^{k+1} & = \Delta\left((\Phi^{k+1})^3\right) \ , & & \\ F_4^{k+1} & = \Delta_h^2 \Phi^k \ , & F_{4e}^{k+1} & = \Delta^2 \Phi^{k+1} \ , & F_{4en}^{k+1} & = \Delta^2 \Phi^k \ , \\ F_5^{k+1} & = \Delta_h^3 \Phi^{k+1} \ , & F_{5e}^{k+1} & = \Delta^3 \Phi^{k+1} \ . & & \end{array} \tag{A.5}$$

Note that all these quantities are defined on the numerical grid (in space) pointwise.

The following estimates can be derived in a manner similar to that used to derive Proposition A.2:

$$\left\| F_4^{k+1} - F_{4en}^{k+1} \right\|_{L_h^2(\Omega)} \le Ch^2 \left\| \Phi^k \right\|_{H^{6+\eta}(\Omega)} \ , \tag{A.6}$$

$$\left\| F_5^{k+1} - F_{5e}^{k+1} \right\|_{L_h^2(\Omega)} \le Ch^2 \left\| \Phi^{k+1} \right\|_{H^{8+\eta}(\Omega)} \ . \tag{A.7}$$

For the nonlinear term, a direct application of Proposition A.2 indicates that

$$\begin{aligned} \left\| F_3^{k+1} - F_{3e}^{k+1} \right\|_{L_h^2(\Omega)} &= \left\| \Delta_h\left((\Phi^{k+1})^3\right) - \Delta\left((\Phi^{k+1})^3\right) \right\|_{L_h^2(\Omega)} \\ &\le Ch^2 \left\| (\Phi^{k+1})^3 \right\|_{H^{4+\eta}(\Omega)} \ . \end{aligned} \tag{A.8}$$

Meanwhile, a careful application of a product expansion and a Sobolev imbedding leads to

$$\left\| \left(\Phi^{k+1}\right)^3 \right\|_{H^4(\Omega)} \le C \left\| \Phi^{k+1} \right\|_{H^4(\Omega)}^3 , \quad \left\| \left(\Phi^{k+1}\right)^3 \right\|_{H^5(\Omega)} \le C \left\| \Phi^{k+1} \right\|_{H^5(\Omega)}^3 \ , \tag{A.9}$$

which in turn yields the estimate for $\|\cdot\|_{H^{4+\eta}}$,

$$\begin{aligned} \left\| (\Phi^{k+1})^3 \right\|_{H^{4+\eta}(\Omega)} &\le C \left\| (\Phi^{k+1})^3 \right\|_{H^4(\Omega)}^{1-\eta} \cdot \left\| (\Phi^{k+1})^3 \right\|_{H^5(\Omega)}^{\eta} \\ &\le C \left\| \Phi^{k+1} \right\|_{H^4(\Omega)}^{3-3\eta} \cdot \left\| \Phi^{k+1} \right\|_{H^5(\Omega)}^{3\eta} . \end{aligned} \tag{A.10}$$

As a result, its combination with (A.8) gives

$$\left\| F_3^{k+1} - F_{3e}^{k+1} \right\|_{L_h^2(\Omega)} \le Ch^2 \left\| \Phi^{k+1} \right\|_{H^4(\Omega)}^{3-3\eta} \cdot \left\| \Phi^{k+1} \right\|_{H^5(\Omega)}^{3\eta} . \tag{A.11}$$

For the terms in which a temporal discretization is involved, we have the following estimates, using a methodology similar to that in the derivation of Proposition A.2:

$$\left\| F_1 - F_{1e} \right\|_{L_s^2(0,T)} \le Cs \left\| \Phi \right\|_{H^3(0,T)} \quad \text{for each fixed } (i,j) \ , \tag{A.12}$$

$$\left\| F_2 - F_{2e} \right\|_{L_s^2(0,T)} \le Cs \left\| \Phi \right\|_{H^2(0,T)} \quad \text{for each fixed } (i,j) \ , \tag{A.13}$$

$$\left\| F_{4e} - F_{4en} \right\|_{L_s^2(0,T)} \le Cs \left\| \Delta^2 \Phi \right\|_{H^1(0,T)} \quad \text{for each fixed } (i,j) \ . \tag{A.14}$$

Therefore, we arrive at the following estimates:

$$\|F_1 - F_{1e}\|_{L^2_s\left(0,T;L^2_h(\Omega)\right)} \le Cs\,\|\Phi\|_{L^\infty(\Omega;H^3(0,T))} \ , \tag{A.15}$$

$$\|F_2 - F_{2e}\|_{L^2_s\left(0,T;L^2_h(\Omega)\right)} \le Cs\,\|\Phi\|_{L^\infty(\Omega;H^2(0,T))} \ , \tag{A.16}$$

$$\begin{aligned} &\|F_3 - F_{3e}\|_{L^2_s\left(0,T;L^2_h(\Omega)\right)} \\ &\qquad \le Ch^2\,\|\Phi\|^{3-3\eta}_{L^\infty(0,T;H^4(\Omega))} \cdot Ch^2\,\|\Phi\|^{3\eta}_{L^\infty(0,T;H^5(\Omega))} \ , \end{aligned} \tag{A.17}$$

$$\|\Delta_h\Phi - \Delta\Phi\|_{L^2_s\left(0,T;L^2_h(\Omega)\right)} \le Ch^2\,\|\Phi\|_{L^\infty(0,T;H^{4+\eta}(\Omega))} \ , \tag{A.18}$$

$$\begin{aligned} &\|F_4 - F_{4e}\|_{L^2_s\left(0,T;L^2_h(\Omega)\right)} \\ &\qquad \le C(s+h^2)\left(\|\Phi\|_{L^\infty(0,T;H^{6+\eta}(\Omega))} + \|\Phi\|_{H^1(0,T;H^{5+\eta}(\Omega))}\right) \ , \end{aligned} \tag{A.19}$$

$$\|F_5 - F_{5e}\|_{L^2_s\left(0,T;L^2_h(\Omega)\right)} \le Ch^2\,\|\Phi\|_{L^\infty(0,T;H^{8+\eta}(\Omega))} \ . \tag{A.20}$$

Finally, the local truncation error estimate (4.46) is obtained by a detailed comparison between the truncation equation (4.44) and the original PDE:

$$\begin{aligned} &\beta\partial_t^2\Phi + \partial_t\Phi - \Delta\left(\Phi^3\right) - \alpha\Delta\Phi - 2\Delta^2\Phi - \Delta^3\Phi \\ &\qquad = \beta F_{1e} + F_{2e} - F_{3e} - \alpha\Delta\Phi - F_{4e} - F_{5e} = 0 \ . \end{aligned} \tag{A.21}$$

A.2. Proof of Proposition A.2. Assume that $f \in H^{4+\eta}_{per}$ has the Fourier expansion

$$f(x,y) = \sum_{k,l=-\infty}^{\infty} \hat{f}_{k,l}\exp\left(2\pi\mathrm{i}(kx+ly)/L_0\right) \ . \tag{A.22}$$

The Parseval equality shows that

$$\|f\|^2_{L^2} = L_0^2 \sum_{k,l=-\infty}^{\infty} \left|\hat{f}_{k,l}\right|^2 . \tag{A.23}$$

Similarly, for the derivatives, we have

$$(-\Delta)^{m/2} f = \sum_{k,l=-\infty}^{\infty} \left[\left(\frac{2k\pi}{L_0}\right)^2 + \left(\frac{2l\pi}{L_0}\right)^2\right]^{m/2} \hat{f}_{k,l}\exp\left(2\pi\mathrm{i}(kx+ly)/L_0\right) \tag{A.24}$$

for $m \ge 2$, and the corresponding Parseval equality gives

$$\left\|(-\Delta)^{m/2} f\right\|^2_{L^2} = L_0^2 \sum_{k,l=-\infty}^{\infty} \left[\left(\frac{2k\pi}{L_0}\right)^2 + \left(\frac{2l\pi}{L_0}\right)^2\right]^m \left|\hat{f}_{k,l}\right|^2 . \tag{A.25}$$

Meanwhile, any (periodic) discrete grid function g over x_i, y_j, $0 \le i,j \le N-1$, has a discrete Fourier expansion

$$g_{i,j} = \sum_{k,l=-N/2+1}^{N/2} \hat{g}_{k,l}\exp\left(2\pi\mathrm{i}(kx_i+ly_j)/L_0\right) . \tag{A.26}$$

We observe that the discrete Fourier expansion of f over the uniform grid (x_i, y_j), $0 \le i, j \le N-1$, is not the projection of (A.22), due to the aliasing error. A more careful calculation shows that

(A.27)
$$f_{i,j} = \sum_{k,l=-N/2+1}^{N/2} \tilde{\hat{f}}_{k,l} \exp\left(2\pi \mathrm{i}(kx_i + ly_j)/L_0\right), \quad \tilde{\hat{f}}_{k,l} = \sum_{k_1,l_1=-\infty}^{\infty} \hat{f}_{k+k_1N,l+l_1N}.$$

In turn, taking the centered difference D_x^2, D_y^2 on f and making use of the fact that $e^{i2k\pi x/L_0}$ is also an eigenfunction of the discrete operator Δ_h lead to the following formula:

$$\Delta_h f_{i,j} = \sum_{k,l=-N/2+1}^{N/2} \left(\lambda_{kx} + \lambda_{ly}\right) \tilde{\hat{f}}_{k,l} \exp\left(2\pi \mathrm{i}(kx_i + ly_j)/L_0\right) \ , \tag{A.28}$$

with

$$\lambda_{kx} = \frac{-4\sin^2(k\pi h/L_0)}{h^2} \ , \quad \lambda_{ly} = \frac{-4\sin^2(l\pi h/L_0)}{h^2} \ . \tag{A.29}$$

Moreover, differentiating the Fourier expansion (A.22) yields

$$\Delta f(x,y) = \sum_{k,l=-\infty}^{\infty} \left(\frac{-4k^2\pi^2}{L_0^2} + \frac{-4l^2\pi^2}{L_0^2}\right) \hat{f}_{k,l} \exp\left(2\pi \mathrm{i}(kx + ly)/L_0\right), \tag{A.30}$$

and its interpolation at (x_i, y_j) gives

$$(\Delta f)_{i,j} = \sum_{k,l=-N/2+1}^{N/2} \tilde{\hat{f}}_{k,l}^{(2)} \exp\left(2\pi \mathrm{i}(kx_i + ly_j)/L_0\right) \ , \tag{A.31}$$

where

$$\tilde{\hat{f}}_{k,l}^{(2)} = \sum_{k_1,l_1=-\infty}^{\infty} \left(\frac{-4(k+k_1N)^2\pi^2}{L_0^2} + \frac{-4(l+l_1N)^2\pi^2}{L_0^2}\right) \hat{f}_{k,l} \ . \tag{A.32}$$

Therefore, the difference between (A.28) and (A.31) gives

$$(\Delta_h f - \Delta f)_{i,j} = \sum_{k=-N/2+1}^{N/2} \left(\left(\lambda_{kx} + \lambda_{ly}\right) \tilde{\hat{f}}_{k,l} - \tilde{\hat{f}}_{k,l}^{(2)}\right) \exp\left(2\pi \mathrm{i}(kx_i + ly_j)/L_0\right) \ . \tag{A.33}$$

As a result, an application of the discrete Parseval equality yields

$$\|\Delta_h f - \Delta f\|_{l^2(\Omega)}^2 = L_0^2 \sum_{k,l=-N/2+1}^{N/2} \left|\left(\lambda_{kx} + \lambda_{ly}\right) \tilde{\hat{f}}_{k,l} - \tilde{\hat{f}}_{k,l}^{(2)}\right|^2 \ . \tag{A.34}$$

Moreover, a detailed comparison between (A.27) and (A.31) results in

$$\begin{aligned}(\lambda_{kx} + \lambda_{ly})\, \tilde{\hat{f}}_{k,l} - \tilde{\hat{f}}^{(2)}_{k,l} = &\left(\left(\lambda_{kx} + \frac{4k^2\pi^2}{L_0^2}\right) + \left(\lambda_{ly} + \frac{4l^2\pi^2}{L_0^2}\right)\right)\hat{f}_{k,l} \\ &+ \sum_{\substack{k_1,l_1=-\infty \\ (k_1,l_1)\neq(0,0)}}^{\infty} \left\{ \left(\lambda_{kx} + \frac{4(k+k_1N)^2\pi^2}{L_0^2}\right)\right. \\ &\left. + \left(\lambda_{ly} + \frac{4(l+l_1N)^2\pi^2}{L_0^2}\right)\right\}\hat{f}_{k+k_1N,l+l_1N}. \end{aligned} \tag{A.35}$$

The estimates of each term are given by the following lemmas. The proofs are based on a subtle analysis of the Fourier coefficients and the corresponding eigenvalues. The proofs are skipped here for brevity of presentation, though we plan to provide them in a future paper.

LEMMA A.3. *We have*

$$\left|\lambda_{kx} + \frac{4k^2\pi^2}{L_0^2}\right| \le C_1 h^2 \left(\frac{2k\pi}{L_0}\right)^4, \quad \left|\lambda_{ly} + \frac{4l^2\pi^2}{L_0^2}\right| \le C_1 h^2 \left(\frac{2l\pi}{L_0}\right)^4 \tag{A.36}$$

for all $-N/2 \le k, l \le N/2$, where C_1 depends on L_0 only.

LEMMA A.4. *We have*

$$\begin{aligned}\sum_{k,l=-N/2+1}^{N/2} \left| \sum_{\substack{k,l=-\infty \\ (k_1,l_1)\neq(0,0)}}^{\infty} \left(\lambda_{kx} + \frac{4(k+k_1N)^2\pi^2}{L_0^2}\right)\hat{f}_{k+k_1N,l+l_1N}\right|^2 &\le C_2 h^{4+2\eta}\, \|f\|^2_{H^{4+\eta}}, \\ \sum_{k,l=-N/2+1}^{N/2} \left| \sum_{\substack{k,l=-\infty \\ (k_1,l_1)\neq(0,0)}}^{\infty} \left(\lambda_{ly} + \frac{4(l+l_1N)^2\pi^2}{L_0^2}\right)\hat{f}_{k+k_1N,l+l_1N}\right|^2 &\le C_2 h^{4+2\eta}\, \|f\|^2_{H^{4+\eta}}, \end{aligned} \tag{A.37}$$

where C_2 depends on L_0 only.

A direct consequence of Lemma A.3 shows that

$$\begin{aligned}\sum_{k,l=-N/2+1}^{N/2} \left(\lambda_{kx} + \frac{4k^2\pi^2}{L_0^2}\right)^2 \left|\hat{f}_{k,l}\right|^2 &\le \tilde{C}_1 h^4 \|f\|^2_{H^4}, \\ \sum_{k,l=-N/2+1}^{N/2} \left(\lambda_{ly} + \frac{4l^2\pi^2}{L_0^2}\right)^2 \left|\hat{f}_{k,l}\right|^2 &\le \tilde{C}_1 h^4 \|f\|^2_{H^4}, \end{aligned} \tag{A.38}$$

with $\tilde{C}_1 = \frac{C_1^2}{L_0^2}$, where we have used (A.25) with $m = 4$.

A combination of (A.35), (A.38), and Lemma A.4 indicates that

$$\begin{aligned}
&\sum_{k,l=-N/2+1}^{N/2} \left| (\lambda_{kx} + \lambda_{ly}) \,\tilde{\hat{f}}_{k,l} - \tilde{\hat{f}}_{k,l}^{(2)} \right|^2 \\
&\quad \le 4 \sum_{k,l=-N/2+1}^{N/2} \Bigg\{ \left(\left(\lambda_{kx} + \frac{4k^2\pi^2}{L_0^2} \right)^2 + \left(\lambda_{ly} + \frac{4l^2\pi^2}{L_0^2} \right)^2 \right) \left| \hat{f}_{k,l} \right|^2 \\
&\qquad + \Bigg| \sum_{\substack{k,l=-\infty \\ (k_1,l_1)\neq(0,0)}}^{\infty} \left(\lambda_{kx} + \frac{4(k+k_1N)^2\pi^2}{L_0^2} \right) \hat{f}_{k+k_1N,l+l_1N} \Bigg|^2 \\
&\qquad + \Bigg| \sum_{\substack{k,l=-\infty \\ (k_1,l_1)\neq(0,0)}}^{\infty} \left(\lambda_{ly} + \frac{4(l+l_1N)^2\pi^2}{L_0^2} \right) \hat{f}_{k+k_1N,l+l_1N} \Bigg|^2 \Bigg\} \\
&\quad \le \tilde{C}_2 h^4 \, \|f\|_{H^{4+\eta}}^2 \ , \qquad \text{(A.39)}
\end{aligned}$$

where $\tilde{C}_2 = 8\tilde{C}_1 + 8C_2$, and where the Cauchy inequality $|\sum_{i=1}^4 a_i|^2 \le 4\sum_{i=1}^4 |a_i|^2$ was applied in the first step. Finally, a substitution of (A.39) into (A.34) results in (A.3), with the constant C given by

$$C = \sqrt{\tilde{C}_2 L_0^2} \ . \qquad \text{(A.40)}$$

This completes the proof of Proposition A.2.

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