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CONVERGENCE ANALYSIS OF A SECOND ORDER CONVEX SPLITTING SCHEME FOR THE MODIFIED PHASE FIELD CRYSTAL EQUATION*

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Abstract. In this paper we provide a detailed convergence analysis for an unconditionally energy stable, second order accurate convex splitting 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 fully discrete, fully second order finite difference scheme in question was derived in a recent work [A. Baskaran et al., *J. Comput. Phys.*, 250 (2013), pp. 270–292]. An introduction of a new variable ψ, corresponding to the temporal derivative of the phase variable ϕ, could bring an accuracy reduction in the formal consistency estimate, because of the hyperbolic nature of the equation. A higher order consistency analysis by an asymptotic expansion is performed to overcome this difficulty. In turn, second order convergence in both time and space is established in a discrete $L^\infty(0,T;H^3)$ norm.

Key words. phase field crystal, modified phase field crystal, pseudoenergy, convex splitting, energy stability, second order convergence

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

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1. Introduction.

The modified phase field crystal (MPFC) equation is given by [16]

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

where $\beta \geq 0$ and $\alpha > 0$. Equation (1.1) is a generalized damped wave equation. The parabolic phase field crystal (PFC) equation is recovered in the degenerate case when $\beta = 0$. See [1, 3, 16, 17, 21, 20] and references therein for the physical motivation for the MPFC equation. The existence and uniqueness of global smooth solutions of the MPFC equation were established in our recent article [20], assuming that the initial data are smooth. Very recently, we devised and implemented a second order convex splitting scheme for the MPFC equation [3]. The solver for the discrete equations was based on a nearly optimally efficient nonlinear multigrid method. While we proved a priori unconditional stability and unconditional solvability results for the scheme, we did not perform a convergence analysis. The goal of this paper is to provide a detailed convergence analysis of the second order convex splitting scheme for MPFC equation (1.1) proposed in [3]. To our knowledge no second order convergence analysis exists for this scheme for either the PFC or the MPFC equation.

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Because of the close relationship between the MPFC and PFC models, methods for the latter equation can be adapted and applied to the former. See, for example, [2, 6, 8, 12, 14, 22] for some recent approximation methods specifically for the PFC model. Methods specifically designed for the MPFC equation can be found in [3, 13, 17, 20, 21]. Stefanovic, Haataja, and Provatas [17] employed a semi-implicit finite difference discretization, with a multigrid algorithm for solving the algebraic equations. They provide no numerical analysis for their scheme, which is significantly different from schemes we propose and analyze. The MPFC scheme in [13] is more or less the same as the first order convex splitting that we devised earlier in [20, 21].

The MPFC equation (1.1) may be viewed as a perturbed gradient flow with respect to an energy. Specifically, consider a dimensionless spatial energy of the form [9, 18]

$$E(\phi) = \int_\Omega \left\{ \frac{1}{4}\phi^4 + \frac{\alpha}{2}\phi^2 - |\nabla\phi|^2 + \frac{1}{2}(\Delta\phi)^2 \right\} d\mathbf{x}, \tag{1.2}$$

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:

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

where $\delta_\phi E$ denotes the variational derivative with respect to ϕ. Clearly, the MPFC equation may be redefined as

$$\beta\partial_{tt}\phi + \partial_t\phi = \Delta\mu, \tag{1.4}$$

where $\beta \geq 0$. As mentioned, when $\beta = 0$ the PFC equation is recovered. Herein we will restrict ourselves to the case that $\beta > 0$ to avoid degeneracy. See the discussion in [20] for some equations in the literature that are closely related to (1.1).

First, note that the energy (1.2) is not necessarily nonincreasing in time along the solution trajectories of (1.4). However, solutions of the MPFC equation do dissipate a pseudoenergy, as we show momentarily. Also observe that (1.4) is not precisely a mass conservation equation due to the term $\beta\partial_{tt}\phi$. However, it is clear that if $\int_\Omega \partial_t\phi(\mathbf{x}, 0)\, d\mathbf{x} = 0$, then $\int_\Omega \partial_t\phi\, d\mathbf{x} = 0$ for all time. Herein we assume $\partial_t\phi(\mathbf{x}, 0) \equiv 0$, for simplicity, which trivially satisfies the condition for mass conservation.

We now recast the MPFC equation (1.4) as the following system of equations,

$$\beta\partial_t\psi = \Delta\mu - \psi, \quad \partial_t\phi = \psi, \tag{1.5}$$

and we introduce the pseudoenergy

$$\mathcal{E}(\phi, \psi) := E(\phi) + \frac{\beta}{2}\|\psi\|^2_{H^{-1}}. \tag{1.6}$$

See [21, 20] for precise definitions of the H^{-1} inner product and norm. For well-definedness of the H^{-1} norm, we require that $\int_\Omega \psi\, d\mathbf{x} = 0$. This is the case since we use the initial data

$$\psi(\,\cdot\,, 0) = \partial_t\phi(\,\cdot\,, 0) \equiv 0 \qquad \text{in } \Omega. \tag{1.7}$$

A simple calculation [21, 20] shows that sufficiently regular solutions dissipate the pseudoenergy at the rate

$$d_t\mathcal{E} = -\left(\psi, \psi\right)_{H^{-1}} \leq 0. \tag{1.8}$$

In other words, the pseudoenergy is nonincreasing in time. The primary motivation in the convex splitting framework is to design fully and semidiscrete schemes that mimic this pseudoenergy dissipation [3, 21, 20].

The first order convex splitting scheme for (1.1) was proposed and analyzed in a recent article [21], as we have mentioned. However, the extension to the second order convergence analysis is highly nontrivial, mainly due to an $O(s^2)$ numerical error between the centered difference of ϕ and the midpoint average of ψ. As observed in [3], the introduction of the variable ψ greatly facilitates the numerical implementation. However, if one is not careful, the abovementioned $O(s^2)$ numerical error might seem to introduce a reduction of temporal accuracy, because of the second order time derivative involved in the equation. To overcome this difficulty in the paper, we have to perform a higher order consistency analysis by an asymptotic expansion; as a result, the constructed approximate solution satisfies the numerical scheme with a higher order truncation error. A projection of the exact solution onto the Fourier space is taken so that an optimal regularity requirement is obtained.

Second order convergence analysis has always been very challenging for the nonlinear hyperbolic equation with a second order temporal derivative involved. The nonlinear error term must be carefully expanded, and a discrete Sobolev inequality is needed to bound the discrete L^∞ and $W^{1,4}$ norms of the numerical error function. In addition, we need to take an inner product with the error equation by the (discrete) time derivative of the numerical error, because of the hyperbolic nature of MPFC equation. In the end, a full second order convergence in a discrete $L^\infty\left(0,T;H^3\right)$ norm is established.

In section 2 we define the second order convex splitting scheme and restate some solvability and stability results from [3]. In section 3 we present the convergence analysis for the second order scheme. We give some concluding remarks in section 4. Moreover, some technical details of the forthcoming analysis are provided in two appendices. In Appendix A we give the finite difference background for the analysis, including our notation, some of the necessary difference operators, and the some useful inequalities. In a second appendix, Appendix B, we give the details of the consistency analyses related to our scheme.

2. The second order scheme and its properties. Here we redefine our second order convex splitting scheme from [3]. We also restate some of the unconditional solvability and stability results for this scheme. We note that we used a different nondimensional scaling of the MPFC equation (1.1) in [3] than we do here, and some of the restated results below will be in a slightly modified form. However, this difference is only superficial. The reader is directed to Appendix A for an introduction to the notation, as well as some of the standard tools from cell-centered finite differences, that is used below.

2.1. Discrete energy and the convex splitting scheme. We first introduce a fully discrete energy that is consistent with the continuous space energy (1.2). In particular, define the discrete energy $F : \mathcal{C}_{\overline{m}\times\overline{n}} \to \mathbb{R}$ to be

$$F(\phi) := \frac{1}{4}\left\|\phi\right\|_4^4 + \frac{\alpha}{2}\left\|\phi\right\|_2^2 - \left\|\nabla_h\phi\right\|_2^2 + \frac{1}{2}\left\|\Delta_h\phi\right\|_2^2. \tag{2.1}$$

The discrete analogue to (1.6) is

$$\mathcal{F}(\phi,\psi) := F(\phi) + \frac{\beta}{2}\|\psi\|_{-1}^2, \tag{2.2}$$

defined for any $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ and any $\psi \in H$. The norms above, including the "-1" norm, are defined in Appendix A.

Note that if $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is periodic, then it is easy to see that the energies

$$F_c(\phi) = \frac{1}{4}\|\phi\|_4^4 + \frac{\alpha}{2}\|\phi\|_2^2 + \frac{1}{2}\|\Delta_h\phi\|_2^2 \quad \text{and} \quad F_e(\phi) = \|\nabla_h\phi\|_2^2 \tag{2.3}$$

are convex [21, 22]. Hence F, as defined in (2.1), admits the convex splitting $F = F_c - F_e$. Our second order scheme will exploit this decomposition of F. Eyre [10] is often credited with popularizing the idea that the numerical scheme should respect the convexity structure of the energy for the purposes of numerical stability and solvability. His original scheme was first order accurate in time and was restricted to nonconserved gradient flows. But this approach has been extended to craft schemes for a number of gradient-flow equations of parabolic type; see, for example, [7, 15, 19, 22, 23]. The convex splitting framework was extended for the hyperbolic MPFC equation (1.1) in [21, 20]. We extended the framework for second order schemes in [3, 12, 15].

The following second order convex splitting scheme for the MPFC equation is from our recent paper [3]: given ϕ^{k-1}, ϕ^k, $\psi^k \in \mathcal{C}_{\overline{m}\times\overline{n}}$ periodic, find ϕ^{k+1}, ψ^{k+1}, $\mu^{k+1/2} \in \mathcal{C}_{\overline{m}\times\overline{n}}$ periodic such that

$$\beta\left(\psi^{k+1} - \psi^k\right) = s\Delta_h\mu^{k+1/2} - s\psi^{k+1/2}, \tag{2.4}$$

$$\mu^{k+1/2} = \chi\left(\phi^{k+1},\phi^k\right) + \alpha\phi^{k+1/2} + 2\Delta_h\hat{\phi}^{k+1/2} + \Delta_h^2\phi^{k+1/2}, \tag{2.5}$$

$$\phi^{k+1} - \phi^k = s\psi^{k+1/2}, \tag{2.6}$$

where

$$\phi^{k+\frac{1}{2}} := \frac{\phi^{k+1}+\phi^k}{2}, \quad \chi(\phi,\psi) := \frac{\phi^2+\psi^2}{2}\cdot\frac{\phi+\psi}{2}, \quad \hat{\phi}^{k+\frac{1}{2}} := \frac{3\phi^k - \phi^{k-1}}{2}.$$

It is obvious that $\chi(\phi,\phi) = \phi^3$. As in [3], we will use the initial data

$$\phi^{-1} \equiv \phi^0, \quad \psi^0 \equiv 0. \tag{2.7}$$

By simple manipulations we obtain the following equivalent formulation [3]:

$$\left(1+\frac{2\beta}{s}\right)\phi^{k+1} - s\Delta_h\mu^{k+1/2} = \left(1+\frac{2\beta}{s}\right)\phi^k + 2\beta\psi^k, \tag{2.8}$$

$$\psi^{k+1} = \psi^k + \frac{2}{s}\left(\phi^{k+1}-\phi^k\right), \tag{2.9}$$

which shows that the equations may be decoupled. In fact, we can obtain ϕ^{k+1} first by solving (2.8) and then update ψ^{k+1} using (2.9). Clearly the solvability of the scheme rests on the solvability of (2.8).

2.2. Mass conservation, unique solvability, and unconditional energy stability. Mass conservation, unconditional unique solvability, and unconditional pseudoenergy stability were established in [3]. We recall these facts here, though the reader is directed to the reference for the details. There are two modifications below from what is in [3]. First, our nondimensional scaling of (1.1) is slightly different, and, second, we use different initializations for our multistep, convex splitting scheme.

THEOREM 2.1. *The second order MPFC scheme* (2.5), (2.8)–(2.9) *is uniquely solvable for any time step size* $s > 0$ *and, moreover, solutions are mass conservative,* i.e, $(\phi^k \| \mathbf{1}) = (\phi^0 \| \mathbf{1})$, *for all* $k = 1, 2, \ldots$.

Before we state the next result, which is proved in [3], we introduce a third fully discrete energy: for each time step $k \geq 1$, set

$$\tilde{\mathcal{F}}\left(\phi^k, \phi^{k-1}, \psi^k\right) := \mathcal{F}\left(\phi^k, \psi^k\right) + \frac{1}{2}\left\|\nabla_h\left(\phi^k - \phi^{k-1}\right)\right\|_2^2 . \tag{2.10}$$

THEOREM 2.2. *The second order MPFC scheme* (2.5), (2.8)–(2.9) *(or, equivalently,* (2.4)–(2.6)*) is unconditionally energy stable. In particular, suppose that* ϕ^k, ψ^k, $\phi^{k-1} \in \mathcal{C}_{\overline{m}\times\overline{n}}$ *are periodic, and that* ϕ^{k+1}, $\mu^{k+1/2}$, $\psi^{k+1} \in \mathcal{C}_{\overline{m}\times\overline{n}}$ *is a periodic solution triple to* (2.4)–(2.6)*. Then, for any* $k \geq 0$,

$$\tilde{\mathcal{F}}\left(\phi^{k+1}, \phi^k, \psi^{k+1}\right) + s\left\|\psi^{k+1/2}\right\|_{-1}^2 + \frac{s^4}{2}\left\|\nabla_h\left(D_s^2\phi^k\right)\right\|_2^2 = \tilde{\mathcal{F}}\left(\phi^k, \phi^{k-1}, \psi^k\right), \tag{2.11}$$

where

$$D_s^2\phi^k := \frac{1}{s^2}\left(\phi^{k+1} - 2\phi^k + \phi^{k-1}\right). \tag{2.12}$$

This next result follows by summing equation (2.11) from $k = 0$ to $k = \ell - 1$.

COROLLARY 2.3. *With the same assumptions as in Theorem* 2.2 *we have*

$$\begin{aligned}\tilde{\mathcal{F}}\left(\phi^\ell, \phi^{\ell-1}, \psi^\ell\right) + s\sum_{k=0}^{\ell-1}\left\|\psi^{k+1/2}\right\|_{-1}^2 + \frac{s^4}{2}\sum_{k=0}^{\ell-1}\left\|\nabla_h\left(D_s^2\phi^k\right)\right\|_2^2 &= \tilde{\mathcal{F}}\left(\phi^0, \phi^{-1}, \psi^0\right) \\ &= F\left(\phi^0\right).\end{aligned} \tag{2.13}$$

Using Lemmas A.4 and A.7, and Lemma 3.7 of [22], we find the following lemma.

LEMMA 2.4. *Suppose that* $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ *is periodic. Then the following estimates hold:*

$$F(\phi) \geq C_5\|\phi\|_{2,2}^2 - \frac{L_xL_y}{4}, \tag{2.14}$$

$$F(\phi) \geq C_6\|\phi\|_\infty^2 - \frac{L_xL_y}{4}, \quad C_6 := \frac{C_5}{C_2}, \tag{2.15}$$

$$F(\phi) \geq C_7\|\nabla_h\phi\|_4^2 - \frac{L_xL_y}{4}, \quad C_7 := \frac{C_5}{C_4}, \tag{2.16}$$

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

Using the last two results and the simple estimate

$$F\left(\phi^k\right) \leq \tilde{\mathcal{F}}\left(\phi^k, \phi^{k-1}, \psi^k\right) \tag{2.17}$$

for any $k \geq 1$, we obtain the following theorem.

THEOREM 2.5. *Let* Φ *be a sufficiently regular, periodic solution to* (1.1) *on* $\Omega_T = (0, L_x) \times (0, L_y) \times (0, T)$, *with* $\partial_t\Phi(\,\cdot\,, \cdot\,, 0) \equiv 0$ *and* $\phi_{i,j}^0 = \phi_{i,j}^{-1} := \Phi(p_i, p_j, 0)$,

$\psi^0 \equiv 0$. *Suppose E is the continuous energy* (1.2) *and F is the discrete energy* (2.1). *Let $\phi^k_{i,j} \in \mathcal{C}_{\overline{m}\times\overline{n}}$ be the kth periodic solution of* (2.8) *and* (2.9) *for $1 \le k \le \ell$. There exists a constant $C_8 > 0$, which does not depend on either s or h, such that*

$$F(\phi^0) \le E\big(\Phi(\,\cdot\,,\,\cdot\,,0)\big) + C_8 L_x L_y =: M_0, \tag{2.18}$$

and, consequently, we have the following estimates:

$$\max_{0\le k\le \ell} \left\|\phi^k\right\|_{2,2} \le \sqrt{\frac{M_0}{C_5}} =: C_9, \tag{2.19}$$

$$\max_{0\le k\le \ell} \left\|\phi^k\right\|_{\infty} \le \sqrt{\frac{M_0}{C_6}} =: C_{10}, \tag{2.20}$$

$$\max_{0\le k\le \ell} \left\|\nabla_h\phi^k\right\|_{4} \le \sqrt{\frac{M_0}{C_7}} =: C_{11}. \tag{2.21}$$

The following estimates are excerpted from an earlier work [21]. These uniform estimates of the PDE solutions can be derived using analogous techniques to those already displayed.

THEOREM 2.6. *Suppose that $\Phi(x,y,t)$ is a periodic solution of the MPFC equation* (1.4), *with the regularity assumed in Theorem* 3.3 *below, such that $\partial_t\Phi(x,y,0) = 0$. Then we have the following estimates:*

$$\|\Phi\|_{L^\infty(0,T;H^2(\Omega))} \le \sqrt{C_{12}\left(E\left(\Phi\left(x,y,0\right)\right) + \frac{L_xL_y}{4}\right)} =: C_{13}\ , \tag{2.22}$$

$$\|\Phi\|_{L^\infty(0,T;L^\infty(\Omega))} \le \sqrt{C_{14}\left(E\left(\Phi\left(x,y,0\right)\right) + \frac{L_xL_y}{4}\right)} =: C_{15}\ , \tag{2.23}$$

$$\|\Phi\|_{L^\infty(0,T;W^{1,4}(\Omega))} \le \sqrt{C_{16}\left(E\left(\Phi\left(x,y,0\right)\right) + \frac{L_xL_y}{4}\right)} =: C_{17} \tag{2.24}$$

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

3. Error estimate for the second order scheme.

We now prove an error estimate for the second order scheme (2.8)–(2.9) for the MPFC equation. The following estimate, proved in [22], shows control of the backward diffusion term.

LEMMA 3.1. *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*

$$\|\Delta_h\phi\|_2^2 \le \frac{1}{3\epsilon^2}\|\phi\|_2^2 + \frac{2\epsilon}{3}\|\nabla_h\left(\Delta_h\phi\right)\|_2^2, \tag{3.1}$$

valid for arbitrary $\epsilon > 0$.

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

LEMMA 3.2. *Suppose Φ^k, Φ^{k+1}, ϕ^k, $\phi^{k+1} \in \mathcal{C}_{\overline{m}\times\overline{n}}$ are periodic and denote their differences by $\tilde{\phi}^k := \Phi^k - \phi^k$ and $\tilde{\phi}^{k+1} := \Phi^{k+1} - \phi^{k+1}$. Then we have*

$$\begin{aligned}
&\left\|\Delta_h\left(\chi\left(\Phi^{k+1},\Phi^k\right) - \chi\left(\phi^{k+1},\phi^k\right)\right)\right\|_2 \\
&\quad \le C_{18}\Big\{K_1^2\cdot\left(\left\|\Delta_h\tilde{\phi}^{k+1}\right\|_2 + \left\|\Delta_h\tilde{\phi}^k\right\|_2\right) + K_1K_4\left(\left\|\nabla_h\tilde{\phi}^{k+1}\right\|_4 + \left\|\nabla_h\tilde{\phi}^k\right\|_4\right) \\
&\qquad + \left(K_1K_3 + K_4^2\right)\cdot\left(\left\|\tilde{\phi}^{k+1}\right\|_\infty + \left\|\tilde{\phi}^k\right\|_\infty\right) \\
&\qquad + \left(K_5^2 + K_1K_2\right)\cdot\left(\left\|\tilde{\phi}^{k+1}\right\|_2 + \left\|\tilde{\phi}^k\right\|_2\right)\Big\}
\end{aligned} \tag{3.2}$$

with

$$\begin{aligned}
K_1 &= \left\|\Phi^{k+1}\right\|_\infty + \left\|\Phi^k\right\|_\infty + \left\|\phi^{k+1}\right\|_\infty + \left\|\phi^k\right\|_\infty, \\
K_2 &= \left\|\Delta_h^x\Phi^{k+1}\right\|_\infty + \left\|\Delta_h^x\Phi^k\right\|_\infty + \left\|\Delta_h^y\Phi^{k+1}\right\|_\infty + \left\|\Delta_h^y\Phi^k\right\|_\infty, \\
K_3 &= \left\|\Delta_h^x\phi^{k+1}\right\|_2 + \left\|\Delta_h^x\phi^k\right\|_2 + \left\|\Delta_h^y\phi^{k+1}\right\|_2 + \left\|\Delta_h^y\phi^k\right\|_2, \\
K_4 &= \left\|\nabla_h\Phi^{k+1}\right\|_4 + \left\|\nabla_h\Phi^k\right\|_4 + \left\|\nabla_h\phi^{k+1}\right\|_4 + \left\|\nabla_h\phi^k\right\|_4, \\
K_5 &= \left\|\nabla_h\Phi^{k+1}\right\|_\infty + \left\|\nabla_h\Phi^k\right\|_\infty,
\end{aligned} \tag{3.3}$$

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

Proof. First, careful expansions yield the following nonlinear error decompositions:

$$\left(\Phi^{k+1}\right)^3 - \left(\phi^{k+1}\right)^3 = \left(\left(\Phi^{k+1}\right)^2 + \Phi^{k+1}\phi^{k+1} + \left(\phi^{k+1}\right)^2\right)\tilde{\phi}^{k+1}\ , \tag{3.4}$$

$$\left(\Phi^{k+1}\right)^2\Phi^k - \left(\phi^{k+1}\right)^2\phi^k = \left(\Phi^{k+1} + \phi^{k+1}\right)\Phi^k\tilde{\phi}^{k+1} + \left(\phi^{k+1}\right)^2\tilde{\phi}^k\ , \tag{3.5}$$

$$\Phi^{k+1}\left(\Phi^k\right)^2 - \phi^{k+1}\left(\phi^k\right)^2 = \left(\Phi^k + \phi^k\right)\Phi^{k+1}\tilde{\phi}^k + \left(\phi^k\right)^2\tilde{\phi}^{k+1}\ , \tag{3.6}$$

$$\left(\Phi^k\right)^3 - \left(\phi^k\right)^3 = \left(\left(\Phi^k\right)^2 + \Phi^k\phi^k + \left(\phi^k\right)^2\right)\tilde{\phi}^k\ . \tag{3.7}$$

Meanwhile, a detailed calculation yields the following finite difference expansion:

$$\begin{aligned}
\Delta_h^x\left(fgh\right)_{i,j} = {} & f_{i,j}g_{i,j}(\Delta_h^x)h_{i,j} + f_{i,j}h_{i,j}(\Delta_h^x)g_{i,j} + g_{i,j}h_{i,j}(\Delta_h^x)f_{i,j} \\
& + f_{i,j}\left(D_xg_{i+1/2,j}D_xh_{i+1/2,j} + D_xg_{i-1/2,j}D_xh_{i-1/2,j}\right) \\
& + g_{i,j}\left(D_xf_{i+1/2,j}D_xh_{i+1/2,j} + D_xf_{i-1/2,j}D_xh_{i-1/2,j}\right) \\
& + h_{i+1,j}D_xf_{i+1/2,j}D_xg_{i+1/2,j} + h_{i-1,j}D_xf_{i-1/2,j}D_xg_{i-1/2,j}\ .
\end{aligned} \tag{3.8}$$

An analogous formula for $\Delta_h^y\left(fgh\right)_{i,j}$ holds by symmetry. First, we bound all of the terms in the expansion of $\Delta_h^x((\Phi^k)^3 - (\phi^k)^3)$. For brevity, we only show how this is done for one term, namely, $\Delta_h^x((\phi^k)^2\tilde{\phi}^k)$. The expansion is given by

$$\Delta_h^x\left(\left(\phi^k\right)^2\tilde{\phi}^k\right)_{i,j} = N_{i,j}^{(1)} + 2N_{i,j}^{(2)} + 2N_{i,j}^{(3)} + N_{i,j}^{(4)} \tag{3.9}$$

with

$$N_{i,j}^{(1)} = \left(\phi_{i,j}^k\right)^2\Delta_h^x\tilde{\phi}_{i,j}^k, \quad N_{i,j}^{(2)} = \phi_{i,j}^k\tilde{\phi}_{i,j}^k\Delta_h^x\phi_{i,j}^k\ , \tag{3.10}$$

$$N_{i,j}^{(3)} = \phi_{i,j}^k\left(D_x\phi_{i+1/2,j}^kD_x\tilde{\phi}_{i+1/2,j}^k + D_x\phi_{i-1/2,j}^kD_x\tilde{\phi}_{i-1/2,j}^k\right)\ , \tag{3.11}$$

$$N_{i,j}^{(4)} = \tilde{\phi}_{i+1,j}^k\left(D_x\phi_{i+1/2,j}^k\right)^2 + \tilde{\phi}_{i-1,j}^k\left(D_x\phi_{i-1/2,j}^k\right)^2\ . \tag{3.12}$$

Discrete Hölder's inequalities can be applied to bound all of the above terms as follows:

$$\left\|N^{(1)}\right\|_2 \le \left\|\phi^k\right\|_\infty^2 \cdot \left\|\Delta_h^x \tilde{\phi}^k\right\|_2 \le \left\|\phi^k\right\|_\infty^2 \cdot \left\|\Delta_h \tilde{\phi}^k\right\|_2 , \tag{3.13}$$

$$\left\|N^{(2)}\right\|_2 \le \left\|\phi^k\right\|_\infty \cdot \left\|\Delta_h \phi^k\right\|_2 \cdot \left\|\tilde{\phi}^k\right\|_\infty , \tag{3.14}$$

$$\left\|N^{(3)}\right\|_2 \le 2\left\|\phi^k\right\|_\infty \cdot \left\|\nabla_h \phi^k\right\|_4 \cdot \left\|\nabla_h \tilde{\phi}^k\right\|_4 , \tag{3.15}$$

$$\left\|N^{(4)}\right\|_2 \le 2\left\|\nabla_h \phi^k\right\|_4^2 \cdot \left\|\tilde{\phi}^k\right\|_\infty \tag{3.16}$$

with repeated application of Lemma A.5. The nonlinear error term $\Delta_h^y((\Phi^k)^3-(\phi^k)^3)$ can be analyzed in exactly the same way. Combining the estimates using the triangle inequality gives the result (3.2) and the lemma is proven. $\square$

We now establish an error estimate for the fully discrete second order convex splitting scheme for the MPFC equation. We do this in three steps. First, we derive a local truncation error for a finite Fourier projection of the exact solution to the MPFC equation (1.1). Second, we derive an estimate of the difference between our numerical solution to the scheme (2.4)–(2.6) and this finite Fourier projection. Third, we use the triangle inequality to derive our global error estimate.

In the rest of the paper, for notational simplicity only, we will assume $L_x = L_y = L$, and hence $\Omega = (0, L)^2$. As a consequence we have $m = n = N$, where we may assume N is even. The more general rectangular case can be handled straightforwardly. Now, suppose that Φ has the following Fourier series representation on Ω:

$$\Phi(x, y, t) = \sum_{k,l=-\infty}^{\infty} \widehat{\Phi}_{k,l}(t) \mathrm{e}^{\frac{2\pi \mathrm{i}}{L}(k\,x+l\,y)} \tag{3.17}$$

with

$$\widehat{\Phi}_{k,l}(t) = \frac{1}{|\Omega|}\int_\Omega \Phi(x, y, t)\mathrm{e}^{-\frac{2\pi \mathrm{i}}{L}(k\,x+l\,y)}\,dx\,dy\ . \tag{3.18}$$

The (finite Fourier) projection of Φ onto the space $\mathcal{B}^{N/2}$, consisting of all trigonometric polynomials in x and y of degree up to $N/2$, is defined as

$$\Phi_N(x, y, t) := \mathcal{P}_N \Phi(x, y, t) := \sum_{k,l=-N/2+1}^{N/2} \widehat{\Phi}_{k,l}(t)\mathrm{e}^{\frac{2\pi \mathrm{i}}{L}(k\,x+l\,y)}\ . \tag{3.19}$$

Define

$$\Psi_N(x, y, t) := \partial_t \Phi_N(x, y, t) - \frac{s^2}{12}\partial_t^3 \Phi_N(x, y, t)\ . \tag{3.20}$$

For any function $G = G(x, y, t)$, given $s > 0$ and $k > 0$, we define $G^k(x, y) := G(x, y, s\cdot k)$.

THEOREM 3.3. *Suppose the unique periodic solution for the MPFC equation* (1.4) *is given by*

$$\begin{aligned}\Phi \in\ & H^4\left(0, T; L^2(\Omega)\right) \cap L^\infty\left(0, T; H^8(\Omega)\right)\\ & \cap W^{2,\infty}\left(0, T; H^2(\Omega)\right) \cap H^2\left(0, T; H^6(\Omega)\right)\end{aligned} \tag{3.21}$$

for $T < \infty$. Set $\Psi := \partial_t \Phi$. Then

$$\beta \frac{\Psi_N^{k+1} - \Psi_N^k}{s} = \Delta_h \left(\chi\left(\Phi_N^{k+1}, \Phi_N^k\right) + \frac{\alpha}{2}\left(\Phi_N^{k+1} + \Phi_N^k\right) + \Delta_h\left(3\Phi_N^k - \Phi_N^{k-1}\right)\right)$$

$$+ \frac{1}{2}\Delta_h^3\left(\Phi_N^{k+1} + \Phi_N^k\right) - \frac{\Phi_N^{k+1} - \Phi_N^k}{s} + \tau_1^k \ , \tag{3.22}$$

$$\frac{\Phi_N^{k+1} - \Phi_N^k}{s} = \frac{1}{2}\left(\Psi_N^{k+1} + \Psi_N^k\right) + s\tau_2^k \ , \tag{3.23}$$

where τ_1^k and τ_2^k satisfy

$$\|\tau_i\|_{L_s^2\left(0,T;L_h^2(\Omega)\right)} := \sqrt{s \sum_{k=0}^{[T/s]-1} \left\|\tau_i^k\right\|_2^2} \leq M\left(s^2 + h^2\right) \tag{3.24}$$

for $i = 1, 2$, with

$$M \leq C\Big(\|\Phi\|_{H^4(0,T;L^2(\Omega))} + \|\Phi\|_{W^{2,\infty}(0,T;H^2(\Omega))} + \|\Phi\|_{H^2(0,T;H^6(\Omega))}$$

$$+ \|\Phi\|_{L^\infty(0,T;H^4(\Omega))}^3 \cdot \left(1 + \|\Phi\|_{H^2(0,T;H^2(\Omega))}^2\right) + \|\Phi\|_{L^\infty(0,T;H^8(\Omega))}\Big) \ . \tag{3.25}$$

The details of the proof are technical and are contained in the appendix.

Remark 3.4. The constructed solution (3.19) comes from the Fourier projection of the exact solution Φ. The reason for the choice of Φ_N instead of Φ is the fact that $\Phi_N \in \mathcal{B}^{N/2}$, which in turn gives a local truncation error estimate without involving an aliasing error, as can be seen in the appendix. Meanwhile, an $O(s^2)$ correction term is added in the construction (3.20) for Ψ_N so that a higher order consistency is obtained in (3.23). Such a correction term is based on an asymptotic expansion of the numerical scheme and the resulting higher order consistency is crucial in the stability and convergence analysis. Finally, a convergence of the numerical solution to (Φ_N, Ψ_N) is equivalent to its convergence to the exact solution (Φ, Ψ), since Φ is a spectrally accurate approximation, and Ψ_N is an $O(s^2)$ approximation to Ψ.

THEOREM 3.5. *Suppose Φ, Φ_N, Ψ, and Ψ_N are as in the last theorem. Define $\tilde{\phi}_{i,j}^k := \Phi_N^k(p_i, p_j) - \phi_{i,j}^k$ and $\tilde{\psi}_{i,j}^k := \Psi_N^k(p_i, p_j) - \psi_{i,j}^k$, where $\phi_{i,j}^k$, $\psi_{i,j}^k \in \mathcal{C}_{\overline{m}\times\overline{n}}$ are the kth periodic solutions of* (2.4)–(2.6), *or equivalently,* (2.5), (2.8)–(2.9), *with $\phi_{i,j}^0 := \Phi_{i,j}^0$, $\phi_{i,j}^{-1} = \phi_{i,j}^0$ and $\psi_{i,j}^0 = 0$. Then*

$$\left\|\tilde{\phi}^k\right\|_2 + \left\|\nabla_h\left(\Delta_h \tilde{\phi}^k\right)\right\|_2 \leq C\left(s^2 + h^2\right) \ , \tag{3.26}$$

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

Proof. Subtracting (2.4)–(2.6) from (3.22), (3.23) yields

$$\beta \frac{\tilde{\psi}^{k+1} - \tilde{\psi}^k}{s} = \Delta_h \Big(\chi\left(\Phi_N^{k+1}, \Phi_N^k\right) - \chi\left(\phi^{k+1}, \phi^k\right) + \alpha\tilde{\phi}^{k+1/2}$$

$$+ \Delta_h\left(3\tilde{\phi}^k - \tilde{\phi}^{k-1}\right) + \Delta_h^2 \tilde{\phi}^{k+1/2}\Big) - \frac{\tilde{\phi}^{k+1} - \tilde{\phi}^k}{s} + \tau_1^k \ , \tag{3.27}$$

$$\frac{\tilde{\phi}^{k+1} - \tilde{\phi}^k}{s} = \tilde{\psi}^{k+1/2} + s\tau_2^k \ , \tag{3.28}$$

where $\tilde\phi^{k+1/2} := \frac{1}{2}(\tilde\phi^{k+1}+\tilde\phi^k)$ and $\tilde\psi^{k+1/2} := \frac{1}{2}(\tilde\psi^{k+1}+\tilde\psi^k)$. Taking the inner product with the error difference function $h^2(\tilde\phi^{k+1}-\tilde\phi^k)$ gives

$$\begin{aligned} h^2\left(\tilde\phi^{k+1}-\tilde\phi^k\middle\|\tau_1^k\right) &+ h^2\left(\tilde\phi^{k+1}-\tilde\phi^k\middle\|\Delta_h\left(\chi\left(\Phi_N^{k+1},\Phi_N^k\right)-\chi\left(\phi^{k+1},\phi^k\right)\right)\right) \\ &= \frac{\beta h^2}{s}\left(\tilde\psi^{k+1}-\tilde\psi^k\middle\|\tilde\phi^{k+1}-\tilde\phi^k\right)+\frac{h^2}{s}\left(\tilde\phi^{k+1}-\tilde\phi^k\middle\|\tilde\phi^{k+1}-\tilde\phi^k\right) \\ &\quad -\alpha h^2\left(\tilde\phi^{k+1}-\tilde\phi^k\middle\|\Delta_h\tilde\phi^{k+1/2}\right)-h^2\left(\tilde\phi^{k+1}-\tilde\phi^k\middle\|\Delta_h^3\tilde\phi^{k+1/2}\right) \\ &\quad -h^2\left(\tilde\phi^{k+1}-\tilde\phi^k\middle\|\Delta_h^2\left(3\tilde\phi^k-\tilde\phi^{k-1}\right)\right)\ . \end{aligned} \tag{3.29}$$

The first term on the right-hand side of (3.29) can be rewritten and estimated as follows. With the help of (3.28) and an application of Cauchy's inequality we have

$$\begin{aligned} &\frac{h^2}{s}\left(\tilde\phi^{k+1}-\tilde\phi^k\middle\|\tilde\psi^{k+1}-\tilde\psi^k\right) \\ &\quad = h^2\left(\frac{\tilde\psi^{k+1}+\tilde\psi^k}{2}+s\tau_2^k\middle\|\tilde\psi^{k+1}-\tilde\psi^k\right) \\ &\quad = \frac{1}{2}\left(\left\|\tilde\psi^{k+1}\right\|_2^2-\left\|\tilde\psi^k\right\|_2^2\right)+sh^2\left(\tau_2^k\middle\|\tilde\psi^{k+1}-\tilde\psi^k\right) \\ &\quad \geq \frac{1}{2}\left(\left\|\tilde\psi^{k+1}\right\|_2^2-\left\|\tilde\psi^k\right\|_2^2\right)-\frac{1}{2}s\left\|\tau_2^k\right\|_2^2-s\left(\left\|\tilde\psi^{k+1}\right\|_2^2+\left\|\tilde\psi^k\right\|_2^2\right)\ . \end{aligned} \tag{3.30}$$

The second term on the right-hand side of (3.29) is obviously nonnegative:

$$\frac{h^2}{s}\left(\tilde\phi^{k+1}-\tilde\phi^k\middle\|\tilde\phi^{k+1}-\tilde\phi^k\right) = s\left\|\frac{\tilde\phi^{k+1}-\tilde\phi^k}{s}\right\|_2^2 \geq 0\ . \tag{3.31}$$

The first term on the left-hand side of (3.29) can be controlled using Cauchy's inequality:

$$\begin{aligned} h^2\left(\tilde\phi^{k+1}-\tilde\phi^k\middle\|\tau_1^k\right) &= sh^2\left(\frac{\tilde\psi^{k+1}+\tilde\psi^k}{2}+s\tau_2^k\middle\|\tau_1^k\right) \\ &\leq \frac{s}{4}\left(\left\|\tilde\psi^{k+1}\right\|_2^2+\left\|\tilde\psi^k\right\|_2^2\right)+s\left(\left\|\tau_1^k\right\|_2^2+\frac{s^2}{2}\left\|\tau_2^k\right\|_2^2\right)\ . \end{aligned} \tag{3.32}$$

The analysis of the convex diffusion terms can be carried out with the help of the discrete Green's identities (A.9) and (A.10):

$$-h^2\left(\tilde\phi^{k+1}-\tilde\phi^k\middle\|\Delta_h\tilde\phi^{k+1/2}\right) = \frac{1}{2}\left(\left\|\nabla_h\tilde\phi^{k+1}\right\|_2^2-\left\|\nabla_h\tilde\phi^k\right\|_2^2\right) \tag{3.33}$$

and

$$-h^2\left(\tilde\phi^{k+1}-\tilde\phi^k\middle\|\Delta_h^3\tilde\phi^{k+1/2}\right) = \frac{1}{2}\left(\left\|\nabla_h\left(\Delta_h\tilde\phi^{k+1}\right)\right\|_2^2-\left\|\nabla_h\left(\Delta_h\tilde\phi^k\right)\right\|_2^2\right)\ . \tag{3.34}$$

The concave diffusion term can be handled with the identity

$$
\begin{aligned}
-h^2 \left(\tilde{\phi}^{k+1} - \tilde{\phi}^k \middle\| \Delta_h^2 \left(3\tilde{\phi}^k - \tilde{\phi}^{k-1}\right)\right) = & - \left\| \Delta_h \tilde{\phi}^{k+1} \right\|_2^2 + \frac{1}{2} \left\| \Delta_h \left(\tilde{\phi}^{k+1} - \tilde{\phi}^k\right) \right\|_2^2 \\
& + \left\| \Delta_h \tilde{\phi}^k \right\|_2^2 - \frac{1}{2} \left\| \Delta_h \left(\tilde{\phi}^k - \tilde{\phi}^{k-1}\right) \right\|_2^2 \\
& + \frac{1}{2} \left\| \Delta_h \left(\tilde{\phi}^{k+1} - 2\tilde{\phi}^k + \tilde{\phi}^{k-1}\right) \right\|_2^2 . \qquad (3.35)
\end{aligned}
$$

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

$$
\begin{aligned}
& h^2 \left(\tilde{\phi}^{k+1} - \tilde{\phi}^k \middle\| \Delta_h \left\{ \chi\left(\Phi_N^{k+1}, \Phi_N^k\right) - \chi\left(\phi^{k+1}, \phi^k\right) \right\} \right) \\
& \quad = s h^2 \left(\frac{\tilde{\psi}^{k+1} + \tilde{\psi}^k}{2} + s\tau_2^k \middle\| \Delta_h \left\{ \chi\left(\Phi_N^{k+1}, \Phi_N^k\right) - \chi\left(\phi^{k+1}, \phi^k\right) \right\} \right) \\
& \quad \le \frac{s}{2} \left(\left\| \tilde{\psi}^{k+1} \right\|_2^2 + \left\| \tilde{\psi}^k \right\|_2^2 + 2s^2 \left\| \tau_2^k \right\|_2^2 \right) \\
& \quad \quad + \frac{s}{2} \left\| \Delta_h \left\{ \chi\left(\Phi_N^{k+1}, \Phi_N^k\right) - \chi\left(\phi^{k+1}, \phi^k\right) \right\} \right\|_2^2 . \qquad (3.36)
\end{aligned}
$$

Lemma 3.2 can be used to bound the last term appearing above. In more detail, the following uniform (in time) estimates are recalled from (2.19)–(2.21):

$$
\left\| \Phi_N^l \right\|_\infty \le \left\| \Phi_N^l \right\|_{L^\infty} \le C_{15} , \quad \left\| \nabla_h \Phi_N^l \right\|_4 \le C \left\| \nabla \Phi_N^l \right\|_{L^\infty} \le C , \qquad (3.37)
$$

$$
\left\| \Delta_h^x \phi^l \right\|_2 \le C \left\| \phi^l \right\|_{2,2} \le C C_9 , \quad \left\| \Delta_h^y \phi^l \right\|_2 \le C \left\| \phi^l \right\|_{2,2} \le C C_9 , \qquad (3.38)
$$

$$
\left\| \phi^l \right\|_\infty \le C_{10} , \quad \left\| \nabla_h \phi^l \right\|_4 \le C_{11} , \qquad (3.39)
$$

and the following estimates are valid on the finite time interval $[0, T]$, based on Taylor expansion:

$$
\left\| \nabla_h \Phi_N^l \right\|_\infty \le \left\| \nabla \Phi_N^l \right\|_{L^\infty} \le C , \qquad (3.40)
$$

$$
\left\| \Delta_h^x \Phi_N^l \right\|_\infty + \left\| \Delta_h^y \Phi_N^l \right\|_\infty \le \left\| \partial_{xx} \Phi_N^l \right\|_{L^\infty} + \left\| \partial_{yy} \Phi_N^l \right\|_{L^\infty} \le C \qquad (3.41)
$$

for $l = k, k+1$, where C denotes a generic positive constant that is independent of h. Applying Lemmas A.7 and A.4, and substituting estimates (3.37)–(3.41) yield

$$
\begin{aligned}
& \left\| \Delta_h \left\{ \chi\left(\Phi_N^{k+1}, \Phi_N^k\right) - \chi\left(\phi^{k+1}, \phi^k\right) \right\} \right\|_2 \\
& \quad \le C_{19} \left(\left\| \tilde{\phi}^{k+1} \right\|_2 + \left\| \tilde{\phi}^k \right\|_2 + \left\| \Delta_h \tilde{\phi}^{k+1} \right\|_2 + \left\| \Delta_h \tilde{\phi}^k \right\|_2 \right) , \qquad (3.42)
\end{aligned}
$$

where $C_{19} > 0$ is independent of h and s, but is dependent upon T and also the exact solution Φ. Going back to (3.36) and using the last estimate and Lemma 3.1 (with $\epsilon = 1$) we obtain an estimate for the nonlinear term:

$$
\begin{aligned}
& h^2 \left(\tilde{\phi}^{k+1} - \tilde{\phi}^k \middle\| \Delta_h \left\{ \chi\left(\Phi_N^{k+1}, \Phi_N^k\right) - \chi\left(\phi^{k+1}, \phi^k\right) \right\} \right) \\
& \quad \le \frac{s}{2} \left(\left\| \tilde{\psi}^{k+1} \right\|_2^2 + \left\| \tilde{\psi}^k \right\|_2^2 + 2s^2 \left\| \tau_2 \right\|_2^2 \right) \\
& \quad \quad + 2s\, C_{19}^2 \left(\left\| \tilde{\phi}^{k+1} \right\|_2^2 + \left\| \tilde{\phi}^k \right\|_2^2 + \left\| \Delta_h \tilde{\phi}^{k+1} \right\|_2^2 + \left\| \Delta_h \tilde{\phi}^k \right\|_2^2 \right) \\
& \quad \le \frac{s}{2} \left(\left\| \tilde{\psi}^{k+1} \right\|_2^2 + \left\| \tilde{\psi}^k \right\|_2^2 + 2s^2 \left\| \tau_2 \right\|_2^2 \right) \\
& \quad \quad + \frac{8s\, C_{19}^2}{3} \left(\left\| \tilde{\phi}^{k+1} \right\|_2^2 + \left\| \tilde{\phi}^k \right\|_2^2 + \left\| \nabla_h \Delta_h \tilde{\phi}^{k+1} \right\|_2^2 + \left\| \nabla_h \Delta_h \tilde{\phi}^k \right\|_2^2 \right) . \qquad (3.43)
\end{aligned}
$$

Define a modified energy for the error function via

$$F_1^k = F_1\left(\tilde{\phi}^k, \tilde{\phi}^{k-1}, \tilde{\psi}^k\right) := \frac{\beta}{2}\left\|\tilde{\psi}^k\right\|_2^2 + \frac{\alpha}{2}\left\|\nabla_h\tilde{\phi}^k\right\|_2^2 + \frac{1}{2}\left\|\nabla_h\left(\Delta_h\tilde{\phi}^k\right)\right\|_2^2 - \left\|\Delta_h\tilde{\phi}^k\right\|_2^2$$
$$+\frac{1}{2}\left\|\Delta_h\left(\tilde{\phi}^k - \tilde{\phi}^{k-1}\right)\right\|_2^2 . \tag{3.44}$$

A combination of (3.29), (3.31)–(3.35), and (3.43) results in

$$F_1^{k+1} - F_1^k \le s\,C_{20}\Bigg(\left\|\tilde{\phi}^{k+1}\right\|^2 + \left\|\tilde{\phi}^k\right\|^2 + \left\|\tilde{\psi}^{k+1}\right\|_2^2 + \left\|\tilde{\psi}^k\right\|_2^2 + \left\|\nabla_h\left(\Delta_h\tilde{\phi}^{k+1}\right)\right\|_2^2$$
$$+\left\|\nabla_h\left(\Delta_h\tilde{\phi}^k\right)\right\|_2^2\Bigg) + Cs\left(\left\|\tau_1^k\right\|_2^2 + \left\|\tau_2^k\right\|_2^2\right) , \tag{3.45}$$

where $C_{20} > 0$ is independent of h and s. Summing over k and using the fact that $F_1^0 \le C(s^4 + h^4)$ yields

$$F_1^\ell \le 2s\,C_{20}\sum_{k=0}^{\ell}\left(\left\|\tilde{\phi}^k\right\|_2^2 + \left\|\nabla_h\left(\Delta_h\tilde{\phi}^k\right)\right\|_2^2 + \left\|\tilde{\psi}^k\right\|_2^2\right)$$
$$+ C\left(\|\tau_1\|^2_{L_s^2\left(0,T;L_h^2(\Omega)\right)} + \|\tau_2\|^2_{L_s^2\left(0,T;L_h^2(\Omega)\right)}\right)$$
$$\le 2s\,C_{20}\sum_{k=0}^{\ell}\left(\left\|\tilde{\phi}^k\right\|_2^2 + \left\|\nabla_h\left(\Delta_h\tilde{\phi}^k\right)\right\|_2^2 + \left\|\tilde{\psi}^k\right\|_2^2\right) + CM^2T(s^2+h^2)^2. \tag{3.46}$$

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

$$F_2^k := \frac{\beta}{2}\left\|\tilde{\psi}^k\right\|^2 + \frac{\alpha}{2}\left\|\nabla_h\tilde{\phi}^k\right\|^2 + \frac{1}{2}\left\|\nabla_h\left(\Delta_h\tilde{\phi}^k\right)\right\|_2^2$$
$$+\frac{1}{2}\left\|\Delta_h\left(\tilde{\phi}^k - \tilde{\phi}^{k-1}\right)\right\|_2^2 = F_1^k + \left\|\Delta_h\tilde{\phi}^k\right\|_2^2 , \tag{3.47}$$

so that (3.46) becomes

$$F_2^\ell \le 2s\,C_{20}\sum_{k=0}^{\ell}\left(\left\|\tilde{\phi}^k\right\|_2^2 + \left\|\nabla_h\left(\Delta_h\tilde{\phi}^k\right)\right\|_2^2 + \left\|\tilde{\psi}^k\right\|_2^2\right)$$
$$+\left\|\Delta_h\tilde{\phi}^\ell\right\|^2 + CM^2T(s^2+h^2)^2 . \tag{3.48}$$

To estimate the additional term $\|\Delta_h\tilde{\phi}^\ell\|_2^2$, we need a bound of $\|\tilde{\phi}^\ell\|_2$ in terms of $\tilde{\psi}^k$. The following identity is observed:

$$\tilde{\phi}^\ell = \tilde{\phi}^0 + s\sum_{k=1}^{\ell}\frac{\tilde{\phi}^k - \tilde{\phi}^{k-1}}{s} = \tilde{\phi}^0 + s\sum_{k=1}^{\ell}\left(\frac{\tilde{\psi}^k + \tilde{\psi}^{k-1}}{2} + s\tau_2^k\right) \tag{3.49}$$

with error equation (3.28) used in the last step. In turn, an application of the Cauchy inequality shows that

$$\left\|\tilde{\phi}^\ell\right\|_2^2 \le 2\left\|\tilde{\phi}^0\right\|_2^2 + 4sT\sum_{k=0}^{\ell}\left\|\tilde{\psi}^k\right\|_2^2 + 4s^3T\,\|\tau_2\|^2_{L_s^2\left(0,T;L_h^2(\Omega)\right)}$$
$$\le 4sT\sum_{k=0}^{\ell}\left\|\tilde{\psi}^k\right\|_2^2 + C\left(h^4 + s^2(s^4+h^4)T\right), \tag{3.50}$$

in which we used the fact that $\|\tilde{\phi}^0\|_2 \le Ch^2$ (which comes from the construction (3.19) of the approximate solution and the initial numerical data $\phi^0_{i,j} = \Phi^0_{i,j}$), along with the truncation error analysis (3.24). Therefore, using Lemma 3.1 shows that

$$\begin{aligned}\left\|\Delta_h \tilde{\phi}^\ell\right\|_2^2 &\le \frac{1}{3\epsilon^2}\left\|\tilde{\phi}^\ell\right\|_2^2 + \frac{2\epsilon}{3}\left\|\nabla_h\left(\Delta_h\tilde{\phi}^\ell\right)\right\|_2^2 \\ &\le \frac{2s\,T}{3\epsilon^2}\sum_{k=0}^{\ell}\left\|\tilde{\psi}^k\right\|_2^2 + \frac{2\epsilon}{3}\left\|\nabla_h\left(\Delta_h\tilde{\phi}^\ell\right)\right\|_2^2 + C(s^4+h^4)\end{aligned} \tag{3.51}$$

for any $\epsilon > 0$, with a trivial requirement that $s^2 T \le 1$. Taking $\epsilon = \frac{3}{8}$, the substitution of the estimate (3.51) into (3.48) shows that

$$\begin{aligned}F_2^\ell - \frac{1}{4}\left\|\nabla_h\left(\Delta_h\tilde{\phi}^\ell\right)\right\|_2^2 &\le s\,C_{21}\sum_{k=0}^{\ell}\left(\left\|\tilde{\phi}^k\right\|_2^2 + \left\|\nabla_h\left(\Delta_h\tilde{\phi}^k\right)\right\|_2^2 + \left\|\tilde{\psi}^k\right\|_2^2\right) \\ &\quad + CM^2T(s^2+h^2)^2\ ,\end{aligned} \tag{3.52}$$

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

$$\begin{aligned}F_3^k :=& \frac{\beta}{2}\left\|\tilde{\psi}^k\right\|_2^2 + \frac{\alpha}{2}\left\|\nabla_h\tilde{\phi}^k\right\|_2^2 + \frac{1}{4}\left\|\nabla_h\left(\Delta_h\tilde{\phi}^k\right)\right\|_2^2 \\ &+ \frac{1}{2}\left\|\Delta_h\left(\tilde{\phi}^k - \tilde{\phi}^{k-1}\right)\right\|_2^2 = F_2^k - \frac{1}{4}\left\|\nabla_h\left(\Delta_h\tilde{\phi}^k\right)\right\|_2^2\ ,\end{aligned} \tag{3.53}$$

we obtain, with the aid of the estimate (3.50),

$$F_3^\ell \le s\,C_{22}\sum_{k=0}^{\ell}F_3\left(\tilde{\phi}^k\right) + s^2T\,C_{21}\sum_{k=0}^{\ell}\sum_{\ell'=0}^{k}\left\|\tilde{\psi}^{\ell'}\right\|_2^2 + CM^2T(s^2+h^2)^2\ , \tag{3.54}$$

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

$$s^2T\,C_{21}\sum_{k=0}^{\ell}\sum_{\ell'=0}^{k}\left\|\tilde{\psi}^{\ell'}\right\|_2^2 \le s^2T\,C_{21}\sum_{k=0}^{\ell}\sum_{\ell'=0}^{\ell}\left\|\tilde{\psi}^{\ell'}\right\|_2^2 \le sT^2\,C_{21}\sum_{k=0}^{\ell}\left\|\tilde{\psi}^k\right\|_2^2\ , \tag{3.55}$$

we arrive at

$$F_3^\ell \le s\,C_{23}\sum_{k=1}^{\ell}F_3^k + CM^2T(s^2+h^2)^2\ , \tag{3.56}$$

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

$$F_3^\ell \le C_{24}\left(s^2+h^2\right)^2\ , \tag{3.57}$$

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. ∎

COROLLARY 3.6. *Define* $\tilde{\tilde{\phi}}^k_{i,j} := \Phi^k(p_i, p_j, k\,s) - \phi^k_{i,j}$. *Then*

$$\left\|\tilde{\tilde{\phi}}^k\right\|_2 + \left\|\nabla_h\left(\Delta_h\tilde{\tilde{\phi}}^k\right)\right\|_2 \le C\left(s^2+h^2\right)\ , \tag{3.58}$$

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

Proof. Estimate (3.57) gives the discrete H^3 estimate for $\tilde{\phi}$. For the projection Φ_N, we have the following approximation estimate,

$$\|\Phi_N - \Phi\|_{L^\infty(0,T;H^r)} \leq Ch^m \|\Phi\|_{L^\infty(0,T;H^{m+r})} \tag{3.59}$$

for $m, r \geq 0$. See, for example, [4, 5, 11]. Combining estimate (3.57) with the approximation result (3.59), we can obtain the estimate (3.58). ◻

Remark 3.7. By virtue of (3.58) and Lemmas A.4 and 3.1, along with the estimate (3.50), we immediately get an error estimate of the form

$$\left\|\tilde{\tilde{\phi}}^k\right\|_\infty \leq C\left(h^2 + s^2\right). \tag{3.60}$$

4. Conclusions. In this paper, we have established the convergence analysis of an unconditionally energy stable second order accurate finite difference scheme for the sixth order MPFC equation. The parabolic 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 second order convex splitting of a discrete psuedoenergy and is semi-implicit.

Appendix A. Tools for cell-centered finite differences. In this first appendix, we recall the summation-by-parts formulas, discrete norms, and estimates in two space dimensions that are used to define and analyze our finite difference scheme. The framework that we describe has a straightforward extension to three space dimensions. Here we use the notation and results for cell-centered functions from [23, 22]; see also [12, 21]. The reader is directed to those references for more complete details. We begin with definitions of grid functions and difference operators needed for our discretization of two-dimensional (2D) space. Let $\Omega = (0, L_x) \times (0, L_y)$, with $L_x = m \cdot h$ and $L_y = n \cdot h$, where m and n are positive integers and $h > 0$ is the spatial step size. Define $p_r := (r - 1/2) \cdot h$, where r takes on integer and half-integer values. For any positive integer ℓ, define $E_\ell = \{p_r \mid r = \frac{1}{2}, \ldots, \ell + \frac{1}{2}\}$, $C_\ell = \{p_r \mid r = 1, \ldots, \ell\}$, $C_{\overline{\ell}} = \{p_r \cdot h \mid r = 0, \ldots, \ell + 1\}$. Define the function spaces

$$\mathcal{C}_{m\times n} = \{\phi : C_m \times C_n \to \mathbb{R}\}, \ \mathcal{C}_{\overline{m}\times\overline{n}} = \{\phi : C_{\overline{m}} \times C_{\overline{n}} \to \mathbb{R}\}, \tag{A.1}$$

$$\mathcal{C}_{\overline{m}\times n} = \{\phi : C_{\overline{m}} \times C_n \to \mathbb{R}\}, \ \mathcal{C}_{m\times\overline{n}} = \{\phi : C_m \times C_{\overline{n}} \to \mathbb{R}\}, \tag{A.2}$$

$$\mathcal{E}^{\rm ew}_{m\times n} = \{u : E_m \times C_n \to \mathbb{R}\}, \ \mathcal{E}^{\rm ns}_{m\times n} = \{v : C_m \times E_n \to \mathbb{R}\}, \tag{A.3}$$

$$\mathcal{E}^{\rm ew}_{m\times\overline{n}} = \{u : E_m \times C_{\overline{n}} \to \mathbb{R}\}, \ \mathcal{E}^{\rm ns}_{\overline{m}\times n} = \{v : C_{\overline{m}} \times E_n \to \mathbb{R}\}. \tag{A.4}$$

We use the notation $\phi_{i,j} := \phi(p_i, p_j)$ for *cell-centered* functions, those in the spaces $\mathcal{C}_{m\times n}$, $\mathcal{C}_{\overline{m}\times n}$, $\mathcal{C}_{m\times\overline{n}}$, or $\mathcal{C}_{\overline{m}\times\overline{n}}$. In component form *east-west edge-centered* functions, those in the spaces $\mathcal{E}^{\rm ew}_{m\times n}$ or $\mathcal{E}^{\rm ew}_{m\times\overline{n}}$, are identified via $u_{i+1/2,j} := u(p_{i+1/2}, p_j)$. In component form *north-south edge-centered* functions, those in the spaces $\mathcal{E}^{\rm ns}_{m\times n}$, or $\mathcal{E}^{\rm ns}_{\overline{m}\times n}$, are identified via $u_{i,j+1/2} := u(p_i, p_{j+1/2})$.

We need the weighted 2D grid inner products $(\cdot\|\cdot)$, $[\cdot\|\cdot]_{\rm ew}$, $[\cdot\|\cdot]_{\rm ns}$ that are defined in [23, 22]. Furthermore, the reader is referred to [23, 22] for the precise definitions of the edge-to-center difference operators $d_x : \mathcal{E}^{\rm ew}_{m\times n} \to \mathcal{C}_{m\times n}$ and $d_y : \mathcal{E}^{\rm ns}_{m\times n} \to \mathcal{C}_{m\times n}$; the x-dimension center-to-edge average and difference operators, respectively, A_x, $D_x : \mathcal{C}_{\overline{m}\times n} \to \mathcal{E}^{\rm ew}_{m\times n}$; the y-dimension center-to-edge average and difference operators, respectively, A_y, $D_y : \mathcal{C}_{m\times\overline{n}} \to \mathcal{E}^{\rm ns}_{m\times n}$; and the standard 2D discrete Laplacian, $\Delta_h : \mathcal{C}_{\overline{m}\times\overline{n}} \to \mathcal{C}_{m\times n}$. 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

$$\phi_{m+1,j} = \phi_{1,j}, \quad \phi_{0,j} = \phi_{m,j}, \quad j = 1, \ldots, n, \tag{A.5}$$

$$\phi_{i,n+1} = \phi_{i,1}, \quad \phi_{i,0} = \phi_{i,n}, \quad i = 0, \ldots, m+1. \tag{A.6}$$

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 $j = 0, 1, \ldots, n+1$.

The summation-by-parts formulas we need from [22] are the following.

Proposition A.1 (summation by parts). *If $\phi \in \mathcal{C}_{\overline{m}\times n} \cup \mathcal{C}_{\overline{m}\times\overline{n}}$ and $f \in \mathcal{E}^{\rm ew}_{m\times n}$ are periodic, then*

$$h^2 \left[D_x\phi \| f\right]_{\rm ew} = -h^2 \left(\phi \| d_x f\right), \tag{A.7}$$

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

$$h^2 \left[D_y\phi \| f\right]_{\rm ns} = -h^2 \left(\phi \| d_y f\right). \tag{A.8}$$

Proposition A.2 (discrete Green's identities). *Let ϕ, $\psi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ be periodic. Then*

$$h^2 \left[D_x\phi \| D_x\psi\right]_{\rm ew} + h^2 \left[D_y\phi \| D_y\psi\right]_{\rm ns} = -h^2 \left(\phi \| \Delta_h\psi\right) \tag{A.9}$$

and

$$h^2 \left(\phi \| \Delta_h\psi\right) = h^2 \left(\Delta_h\phi \| \psi\right). \tag{A.10}$$

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

$$\|\nabla_h\phi\|_2 := \sqrt{h^2 \left[D_x\phi \| D_x\phi\right]_{\rm ew} + h^2 \left[D_y\phi \| D_y\phi\right]_{\rm ns}}\ . \tag{A.11}$$

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

$$\|\phi\|_{1,2} := \sqrt{\|\phi\|_2^2 + \|\nabla_h\phi\|_2^2}\ , \quad \|\phi\|_{2,2} := \sqrt{\|\phi\|_2^2 + \|\nabla_h\phi\|_2^2 + \|\Delta_h\phi\|_2^2}\ . \tag{A.12}$$

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

$$\|\phi\|_4 := \left(h^2 \left(\phi^4 \| \mathbf{1}\right)\right)^{1/4} \quad \text{and} \quad \|\phi\|_\infty = \max_{\substack{1\le i\le m\\ 1\le j\le n}} |\phi_{i,j}|. \tag{A.13}$$

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

$$\|\nabla_h\phi\|_4 := \left(h^2 \left[(D_x\phi)^4 \Big\| \mathbf{1}\right]_{\rm ew} + h^2 \left[(D_y\phi)^4 \Big\| \mathbf{1}\right]_{\rm ns}\right)^{1/4}. \tag{A.14}$$

Some discrete Sobolev-type inequalities for 2D grid functions are needed in the analysis in later sections. The following results are recalled; the detailed proofs can be found in [21, 22].

Lemma A.3. *Suppose that $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$. Then,*

$$\|\phi\|_4 \le C_1 \|\phi\|_{1,2} \ , \quad C_1 := \left(2\max\left[\max\left\{\frac{1}{L_x}, L_x\right\}, \max\left\{\frac{1}{L_y}, L_y\right\}\right]\right)^{1/4} . \tag{A.15}$$

Lemma A.4. *Suppose that $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is periodic. Then, for any $i \in \{1,2,\ldots,m\}$ and any $j \in \{1,2,\ldots,n\}$,*

$$\left|\phi_{i,j}\right|^2 \le C_2 \|\phi\|_{2,2}^2 \ , \quad C_2 := 4\max\left\{\frac{1}{L_xL_y}, \frac{L_x}{L_y}, \frac{L_y}{L_x}, \frac{L_xL_y}{2}\right\} . \tag{A.16}$$

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

Lemma A.5. *Suppose that $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is periodic. Define*

$$S := h^2 \sum_{i'=0}^{m}\sum_{j'=0}^{n} w_{i'}^m w_{j'}^n \left|D_y\left(D_x\phi\right)_{i'+1/2,j'+1/2}\right|^2, \quad w_k^\ell := \begin{cases} 1, & k \in \{1,\ldots,\ell-1\}, \\ 1/2, & k \in \{0,\ell\}. \end{cases} \tag{A.17}$$

Then $S = h^2(\Delta_h^x\phi\|\Delta_h^y\phi)$, where $\Delta_h^x := d_xD_x$ and $\Delta_h^y := d_yD_y$ are the 3-point discrete Lapacian operators in the x- and y-directions, respectively [22]. *And, since $S \ge 0$, we have*

$$h^2\ (\Delta_h^x\phi\|\Delta_h^x\phi) \le h^2\ (\Delta_h\phi\|\Delta_h\phi) \quad \text{and} \quad h^2\ (\Delta_h^y\phi\|\Delta_h^y\phi) \le h^2\ (\Delta_h\phi\|\Delta_h\phi) . \tag{A.18}$$

Consider the space $H := \{\phi \in \mathcal{C}_{m\times n} | (\phi\|\mathbf{1}) = 0\}$, and equip this space with the bilinear form

$$(\phi_1\|\phi_2)_{-1} := [D_x\psi_1\|D_x\psi_2]_{\text{ew}} + [D_y\psi_1\|D_y\psi_2]_{\text{ns}} \tag{A.19}$$

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

$$-\Delta_h\psi_i = \phi_i, \quad \psi_i \text{ periodic}, \quad (\psi_i\|\mathbf{1}) = 0. \tag{A.20}$$

Lemma A.6. *The bilinear form $(\phi_1\|\phi_2)_{-1}$ is an inner product on the space H. Moreover,*

$$(\phi_1\|\phi_2)_{-1} = -\left(\phi_1\middle\|\Delta_h^{-1}(\phi_2)\right) = -\left(\Delta_h^{-1}(\phi_1)\middle\|\phi_2\right) . \tag{A.21}$$

Thus $\|\phi\|_{-1} := \sqrt{h^2(\phi\|\phi)_{-1}}$ defines a norm on H.

Lemma A.7. *Suppose that $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$ is periodic and set $\bar\phi = \frac{1}{m\cdot n}(\phi\|\mathbf{1})$. Then*

$$\left\|\phi - \bar\phi\right\|_2 \le C_3 \|\nabla_h\phi\|_2 , \tag{A.22}$$

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

$$\left\|\phi - \bar\phi\right\|_4 \le C_4 \|\nabla_h\phi\|_2 , \quad \|\nabla_h\phi\|_4 \le C_4 \|\Delta_h\phi\|_2 , \tag{A.23}$$

where $C_4 := C_1\sqrt{C_3^2+1}$.

Appendix B. Proof of estimate (3.25). In this appendix we establish (3.25). The following three results will be needed.

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

$$\left\|\tau^t f\right\|_{L_s^2(0,T)} \le Cs^m \|f\|_{H^{m+1}(0,T)} \quad \text{with} \quad \tau^t f^k = \frac{f^{k+1}-f^k}{s} - f'(t^{k+1/2}) \tag{B.1}$$

for $0 \le m \le 2$, *where* C *only depends on* T. *Here* $\|\cdot\|_{L^2_s(0,T)}$ *is a discrete* L^2 *norm (in time) given by* $\|g\|_{L^2_s(0,T)} = \sqrt{s \sum_{k=0}^{[T/s]-1} (g^k)^2}$.

PROPOSITION B.2. *For* $f \in H^2(0,T)$, *we have*

$$\left\| D^2_{t/2} f \right\|_{L^2_s(0,T)} := \sqrt{s \sum_{k=0}^{[T/s]-1} \left(D^2_{t/2} f^{k+1/2} \right)^2} \le C \|f\|_{H^2(0,T)}, \tag{B.2}$$

$$\left\| D^2_t f \right\|_{L^2_s(0,T)} := v\sqrt{s \sum_{k=0}^{[T/s]-1} \left(D^2_t f^k \right)^2 v} \le C \|f\|_{H^2(0,T)}, \tag{B.3}$$

where C *only depends on* T, *and*

$$D^2_{t/2} f^{k+1/2} := \frac{4\left(f^{k+1} - 2f(t^{k+1/2}) + f^k\right)}{s^2}, \quad D^2_t f^k := \frac{f^{k+1} - 2f^k + f^{k-1}}{s^2}.$$

The proofs of Propositions B.1 and B.2 are based on the integral form of the Taylor expansion in time. The details are skipped for the sake of brevity. In the spatial discretization, the following proposition gives a corresponding $O(h^2)$ truncation error bound.

PROPOSITION B.3. *If* $f \in \mathcal{B}^{N/2}$ *has a regularity* $f \in H^8_{per}(\Omega)$, *we have*

$$\left\| \Delta^k f - \Delta^k_h f \right\|_{L^2_h(\Omega)} \le C h^2 \|f\|_{H^{2+2k}(\Omega)} \quad \text{for} \quad k = 1, 2, 3, \tag{B.4}$$

where C *only depends on* L *and* $\|g\|_{L^2_h(\Omega)} = \sqrt{h^2 \sum_{i,j=0}^{N-1} g^2_{i,j}}$ *for* $g \in \mathcal{C}_{m\times n}$.

The key point of this proposition is that the projection approximation solution $\Phi_N \in \mathcal{B}^{N/2}$ so that an aliasing error is avoided in its centered difference approximation. This consistency analysis can be carried out by a detailed Fourier expansion of both $\Delta^k_h \Phi_N$ and $\Delta \Phi_N$ at the discrete level, and the comparison of the corresponding discrete Fourier coefficients leads to the above estimates, following a similar methodology to [21]. The details are skipped for brevity.

Observe that the $\mathcal{O}(s^2)$ correction in the definition of (3.20) is added so that a higher order consistency between Ψ_N at $t^{k+1/2}$ and $(\Phi^{k+1}_N - \Phi^k_N)/s$ can be derived. Looking at the time derivative of the projection operator, we observe that

$$\frac{\partial^k}{\partial t^k} \Phi_N(\boldsymbol{x}, t) = \frac{\partial^k}{\partial t^k} \mathcal{P}_N \Phi(\boldsymbol{x}, t) = \mathcal{P}_N \frac{\partial^k \Phi(\boldsymbol{x}, t)}{\partial t^k}. \tag{B.5}$$

In other words, $\partial^k_t \Phi_N$ is the truncation of $\partial^k_t \Phi$ for any $k \ge 0$, since projection and differentiation commute. This in turn implies an accurate approximation of the corresponding temporal derivative, at any fixed time:

$$\left\| \partial^k_t (\Phi_N - \Phi) \right\|_{H^r} \le C h^m \left\| \partial^k_t \Phi \right\|_{H^{m+r}} \tag{B.6}$$

for m, $r \ge 0$, and $0 \le k \le 2$. See the related reference [5].

Since the exact solution of the MPFC equation has the regularity (3.21), the approximation estimates (3.59), (B.6) imply the same regularity for the projection solution Φ_N, Ψ_N, by taking $m = 0$:

$$\|\Phi_N\|_{H^r} \le C \|\Phi\|_{H^r}, \quad \left\| \partial^k_t (\Phi_N - \Phi) \right\|_{H^r} \le C \left\| \partial^k_t \Phi \right\|_{H^r} \tag{B.7}$$

at any fixed time. This inequality can also be derived by using the standard projection estimates presented in [5].

We define the following quantities:

$$
\begin{aligned}
&F_1^{k+1/2} := s^{-1}\left(\Psi_N^{k+1}-\Psi_N^k\right), && F_{1e}^{k+1/2} := \left(\partial_t^2\Phi_N\right)(\,\cdot\,,t^{k+1/2}),\\
&F_2^{k+1/2} := s^{-1}\left(\Phi_N^{k+1}-\Phi_N^k\right), && F_{2e}^{k+1/2} := \left(\partial_t\Phi_N\right)(\,\cdot\,,t^{k+1/2}),\\
&F_3^{k+1/2} := \Delta_h\left(\chi(\Phi_N^{k+1},\Phi_N^k)\right), && F_{3e}^{k+1/2} := \Delta\left((\Phi_N)^3\right)(\,\cdot\,,t^{k+1/2}),\\
&F_4^{k+1/2} := \Delta_h\left(\Phi_N^{k+1/2}\right), && F_{4e}^{k+1/2} := \Delta\left(\Phi_N\right)(\,\cdot\,,t^{k+1/2}),\\
&F_5^{k+1/2} := 1/2\,\Delta_h^2\left(3\Phi_N^k-\Phi_N^{k-1}\right), && F_{5e}^{k+1/2} := \left(\Delta^2\Phi_N\right)(\,\cdot\,,t^{k+1/2}),\\
&F_6^{k+1/2} := \Delta_h^3\Phi_N^{k+1/2}, && F_{6e}^{k+1/2} := \left(\Delta^3\Phi_N\right)(\,\cdot\,,t^{k+1/2}),\\
&F_7^{k+1/2} := 1/2\left(\Psi_N^{k+1}+\Psi_N^k\right).
\end{aligned}
\tag{B.8}
$$

The corresponding values for the exact solution are denoted by

$$
\begin{aligned}
&F_{1en}^{k+1/2} := \partial_t^2\Phi(\,\cdot\,,t^{k+1/2}), && F_{2en}^{k+1/2} := \partial_t\Phi(\,\cdot\,,t^{k+1/2}),\\
&F_{3en}^{k+1/2} := \left(\Delta\Phi^3\right)(\,\cdot\,,t^{k+1/2}), && F_{4en}^{k+1/2} := \left(\Delta\Phi\right)(\,\cdot\,,t^{k+1/2}),\\
&F_{5en}^{k+1/2} := \left(\Delta^2\Phi\right)(\,\cdot\,,t^{k+1/2}), && F_{6en}^{k+1/2} := \left(\Delta^3\Phi\right)(\,\cdot\,,t^{k+1/2}).
\end{aligned}
$$

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

First we look at the first order time derivative term, F_2, F_{2e}, and F_{2en}. A direct application of Proposition B.1 indicates that (by taking $m=2$)

$$
\|F_2-F_{2e}\|_{L_s^2(0,T)} \le Cs^2\|\Phi_N\|_{H^3(0,T)} \le Cs^2\|\Phi\|_{H^3(0,T)} \tag{B.9}
$$

for each fixed grid point (i,j), in which the second part of (B.7) was used in the second step. Meanwhile, the approximation estimate (B.6) yields (with $k=1$, $m=2$)

$$
\left\|F_{2e}^{k+1/2}-F_{2en}^{k+1/2}\right\| \le Ch^2\|\partial_t\Phi\|_{H^2}. \tag{B.10}
$$

Herein we denote $\|\cdot\|$ as the standard L^2 norm. Therefore, a careful calculation shows that a combination of the above two estimates results in

$$
\|F_2-F_{2en}\|_{L_s^2\left(0,T;L_h^2(\Omega)\right)} \le C(s^2+h^2)\left(\|\Phi\|_{H^3(0,T;L^2)}+\|\Phi\|_{W^{1,\infty}(0,T;H^2)}\right). \tag{B.11}
$$

Similar analysis can be applied to the second order time derivative terms. The construction (3.20) for the approximate solution Ψ_N gives

$$
F_1^{k+1/2} = \frac{\partial_t\Phi_N^{k+1}-\partial_t\Phi_N^k}{s} - \frac{s^2}{12}\cdot\frac{\partial_t^3\Phi_N^{k+1}-\partial_t^3\Phi_N^k}{s} := F_{11}^{k+1/2}-\frac{s^2}{12}F_{12}^{k+1/2}, \tag{B.12}
$$

where F_{11} and F_{12} are a finite difference (in time) approximation to $\partial_t^2\Phi_N$, $\partial_t^4\Phi_N$, respectively. In more detail, if we denote $F_{11e}^{k+1/2} := \partial_t^2\Phi_N(\,\cdot\,,t^{k+1/2})$, $F_{12e}^{k+1/2} := \partial_t^4\Phi_N(\,\cdot\,,t^{k+1/2})$, the following estimates can be derived by using Proposition B.1 (with $m=2$ and $m=0$):

$$
\|F_{11}-F_{11e}\|_{L_s^2(0,T)} \le Cs^2\|\Phi_N\|_{H^4(0,T)} \le Cs^2\|\Phi\|_{H^4(0,T)}, \tag{B.13}
$$

$$
\|F_{12}-F_{12e}\|_{L_s^2(0,T)} \le C\|\Phi_N\|_{H^4(0,T)} \le C\|\Phi\|_{H^4(0,T)} \tag{B.14}
$$

for each fixed grid point (i,j). Note that the discrete L^2 norm is taken at temporal grid points $t^{k+1/2}$, and these estimates can be derived in a similar manner. Again, the approximation estimate (B.6) gives (with $k=2$, $m=2$)

$$\left\| F_{1e}^{k+1/2} - F_{1en}^{k+1/2} \right\| \le Ch^2 \left\| \partial_t^2 \Phi \right\|_{H^2} . \tag{B.15}$$

A combination of (B.12)–(B.15) leads to

$$\|F_1 - F_{1en}\|_{L_s^2\left(0,T;L_h^2(\Omega)\right)} \le C(s^2+h^2) \left(\|\Phi\|_{H^4(0,T;L^2)} + \|\Phi\|_{W^{2,\infty}(0,T;H^2)} \right) . \tag{B.16}$$

For the convex diffusion terms F_4, F_{4e}, and F_{4en}, we start from an application of Proposition B.3 (recall that $\Phi_N^{k+1/2} = \frac{\Phi_N^{k+1}+\Phi_N^k}{2}$):

$$\begin{aligned} \left\| F_4^{k+1/2} - \Delta \left(\Phi_N^{k+1/2} \right) \right\|_{L_h^2(\Omega)} &\le Ch^2 \left\| \Phi_N^{k+1/2} \right\|_{H^4(\Omega)} \\ &\le Ch^2 \left\| \Phi_N \right\|_{L^\infty(0,T;H^4)} . \end{aligned} \tag{B.17}$$

Meanwhile, a comparison between $\Phi_N^{k+1/2}$ and $\Phi_N(\,\cdot\,, t^{k+1/2})$ shows that

$$\Phi_N^{k+1/2} - \Phi_N(\,\cdot\,, t^{k+1/2}) = \frac{1}{8} s^2 D_{t/2}^2 \Phi_N^{k+1/2} . \tag{B.18}$$

On the other hand, an application of Proposition B.2 gives

$$\left\| D_{t/2}^2 \Delta \Phi_N \right\|_{L_s^2(0,T)} \le C \left\| \Delta \Phi_N \right\|_{H^2(0,T)} \tag{B.19}$$

at each fixed grid (i,j). As a result of (B.17)–(B.19), we get

$$\begin{aligned} \|F_4 - F_{4e}\|_{L_s^2\left(0,T;L_h^2(\Omega)\right)} &\le C(s^2+h^2) \left(\|\Phi_N\|_{L^\infty(0,T;H^4)} + \|\Phi_N\|_{H^2(0,T;H^2)} \right) \\ &\le C(s^2+h^2) \left(\|\Phi\|_{L^\infty(0,T;H^4)} + \|\Phi\|_{H^2(0,T;H^2)} \right) . \end{aligned} \tag{B.20}$$

The approximation estimate of F_{4e} to F_{4en} is straightforward, from (3.59) (with $m = 2$):

$$\|F_{4e} - F_{4en}\|_{L_s^2\left(0,T;L_h^2(\Omega)\right)} \le Ch^2 \|\Phi\|_{L^\infty(0,T;H^4)} . \tag{B.21}$$

Consequently, we arrive at

$$\|F_4 - F_{4en}\|_{L_s^2\left(0,T;L_h^2(\Omega)\right)} \le C(s^2+h^2) \left(\|\Phi\|_{L^\infty(0,T;H^4)} + \|\Phi\|_{H^2(0,T;H^2)} \right) . \tag{B.22}$$

The other convex diffusion terms F_6, F_{6e}, and F_{6en} can be analyzed in the same way. The details are skipped for simplicity.

$$\|F_6 - F_{6en}\|_{L_s^2\left(0,T;L_h^2(\Omega)\right)} \le C(s^2+h^2) \left(\|\Phi\|_{L^\infty(0,T;H^8)} + \|\Phi\|_{H^2(0,T;H^6)} \right) . \tag{B.23}$$

The analysis for the concave diffusion terms F_5, F_{5e}, and F_{5en} is similar to that of the convex diffusion terms; yet more details are involved. An application of Proposition B.3 gives

$$\begin{aligned} \left\| F_5^{k+1/2} - \Delta^2 \left(\frac{3}{2}\Phi_N^k - \frac{1}{2}\Phi_N^{k-1} \right) \right\|_{L_h^2(\Omega)} &\le Ch^2 \left\| \left(\frac{3}{2}\Phi_N^k - \frac{1}{2}\Phi_N^{k-1} \right) \right\|_{H^6(\Omega)} \\ &\le Ch^2 \left\| \Phi_N \right\|_{L^\infty(0,T;H^6)} . \end{aligned} \tag{B.24}$$

Meanwhile, a comparison between $\frac{3}{2}\Phi_N^k - \frac{1}{2}\Phi_N^{k-1}$ and $\Phi_N(\,\cdot\,,t^{k+1/2})$ reveals that

$$\left(\frac{3}{2}\Phi_N^k - \frac{1}{2}\Phi_N^{k-1}\right) - \Phi_N(\,\cdot\,,t^{k+1/2}) = \frac{1}{8}s^2 D_{t/2}^2 \Phi_N^{k+1/2} - \frac{1}{2}s^2 D_t^2 \Phi_N^k. \tag{B.25}$$

Similarly, applications of Proposition B.2 imply

$$\left\| D_{t/2}^2 \Delta^2 \Phi_N \right\|_{L_s^2(0,T)} \le C \left\| \Delta^2 \Phi_N \right\|_{H^2(0,T)}, \quad \left\| D_t^2 \Delta^2 \Phi_N \right\|_{L_s^2(0,T)} \le C \left\| \Delta^2 \Phi_N \right\|_{H^2(0,T)}$$

at each fixed grid (i,j). Then we obtain

$$\begin{aligned} \|F_5 - F_{5e}\|_{L_s^2\left(0,T;L_h^2(\Omega)\right)} &\le C(s^2+h^2)\left(\|\Phi_N\|_{L^\infty(0,T;H^6)} + \|\Phi_N\|_{H^2(0,T;H^4)} \right) \\ &\le C(s^2+h^2)\left(\|\Phi\|_{L^\infty(0,T;H^6)} + \|\Phi\|_{H^2(0,T;H^4)} \right). \end{aligned} \tag{B.26}$$

The approximation estimate of F_{5e} to F_{5en} can be derived in the same manner:

$$\|F_{5e} - F_{5en}\|_{L_s^2\left(0,T;L_h^2(\Omega)\right)} \le Ch^2 \|\Phi\|_{L^\infty(0,T;H^6)}. \tag{B.27}$$

That gives the consistency estimate for the concave diffusion

$$\|F_5 - F_{5en}\|_{L_s^2\left(0,T;L_h^2(\Omega)\right)} \le C(s^2+h^2)\left(\|\Phi\|_{L^\infty(0,T;H^6)} + \|\Phi\|_{H^2(0,T;H^4)} \right). \tag{B.28}$$

Next we look at the nonlinear term. A direct application of Proposition B.3 indicates that

$$\begin{aligned} \left\| F_3^{k+1/2} - \Delta\left(\chi(\Phi_N^{k+1},\Phi_N^k)\right) \right\|_{L_h^2(\Omega)} &\le Ch^2 \left\| \chi(\Phi_N^{k+1},\Phi_N^k) \right\|_{H^4(\Omega)} \\ &\le Ch^2 \left(\left\|\Phi_N^{k+1}\right\|_{H^4(\Omega)}^3 + \left\|\Phi_N^k\right\|_{H^4(\Omega)}^3 \right) \end{aligned} \tag{B.29}$$

in which a product expansion and a Sobolev embedding are repeatedly used in the second step. Subsequently, we need to compare $\chi(\Phi_N^{k+1},\Phi_N^k)$ and $\Phi_N^3(t^{k+1/2})$ and derive an estimate. A careful calculation reveals that

$$\begin{aligned} \chi(\Phi_N^{k+1},\Phi_N^k) - \Phi_N^3(t^{k+1/2}) &= \frac{1}{2}\left((\Phi_N^{k+1})^2 + (\Phi_N^k)^2\right) \cdot \frac{1}{8}s^2 \left(D_{t/2}^2 \Phi_N\right)^{k+1/2} \\ &\quad + \frac{1}{8}s^2 \left(D_{t/2}^2 \Phi_N^2\right)^{k+1/2} \cdot \Phi_N(\,\cdot\,,t^{k+1/2}). \end{aligned} \tag{B.30}$$

Meanwhile, using the identity

$$\Delta(fgh) = fg\Delta h + fh\Delta g + gh\Delta f + 2f\nabla g\nabla h + 2g\nabla f\nabla h + 2h\nabla f\nabla g, \tag{B.31}$$

we obtain

$$\begin{aligned} &\left\| \Delta\left(\chi(\Phi_N^{k+1},\Phi_N^k) - \Phi_N^3(t^{k+1/2}) \right) \right\|_{L_h^2(\Omega)} \\ &\quad \le C\tilde{C}\left(\tilde{C}+1\right)s^2 \left(\left\| \left(D_{t/2}^2\Phi_N\right)^{k+1/2} \right\|_{H^2} + \left\| \left(D_{t/2}^2\Phi_N^2\right)^{k+1/2} \right\|_{H^2} \right), \end{aligned} \tag{B.32}$$

where

$$\tilde{C} := \|\Phi_N\|_{L^\infty(0,T;W^{2,\infty}(\Omega))} \le C\|\Phi_N\|_{L^\infty(0,T;H^4(\Omega))}.$$

Subsequently, applications of Proposition B.2 imply

$$\left\| D_{t/2}^2 \Phi_N \right\|_{L_s^2(0,T;H^2)} \le C \left\| \Phi_N \right\|_{H^2(0,T;H^2)}, \tag{B.33}$$

$$\left\| D_{t/2}^2 (\Phi_N^2) \right\|_{L_s^2(0,T;H^2)} \le C \left\| \Phi_N^2 \right\|_{H^2(0,T;H^2)}. \tag{B.34}$$

Note that the second estimate is involved with a nonlinear term Φ_N^2. A detailed expansion in its first and second order time derivatives shows that

$$\partial_t(\Phi_N^2) = 2\Phi_N \partial_t \Phi_N, \quad \partial_t^2(\Phi_N^2) = 2\Phi_N \partial_t^2 \Phi_N + 2(\partial_t \Phi_N)^2, \tag{B.35}$$

which in turn leads to

$$\begin{aligned} \left\| \Phi_N^2 \right\|_{H^2(0,T)} &\le C \left(\left\| \Phi_N \right\|_{L^\infty(0,T)} \cdot \left\| \Phi_N \right\|_{H^2(0,T)} + \left\| \Phi_N \right\|_{W^{1,4}(0,T)}^2 \right) \\ &\le C \left\| \Phi_N \right\|_{H^2(0,T)}^2 \end{aligned} \tag{B.36}$$

at each fixed grid point (i,j), with a one-D Sobolev embedding applied at the last step. Going back to (B.34) gives

$$\left\| D_{t/2}^2 (\Phi_N^2) \right\|_{L_s^2(0,T;H^2)} \le C \left\| \Phi_N \right\|_{H^2(0,T;H^2)}^2. \tag{B.37}$$

Therefore, a substitution of (B.33) and (B.37) into (B.32) yields

$$\begin{aligned} &\left\| \Delta \left((\Phi_N^3)^{k+1/2} - (\Phi_N^3)(\,\cdot\,, t^{k+1/2}) \right) \right\|_{L_s^2(0,T;L_h^2(\Omega))} \\ &\quad \le C \left(\left\| \Phi_N \right\|_{L^\infty(0,T;H^4(\Omega))}^2 \cdot \left\| \Phi_N \right\|_{H^2(0,T;H^2)}^2 + 1 \right) s^2. \end{aligned} \tag{B.38}$$

For the comparison between F_{3e} and F_{3en}, we cannot apply (3.59) directly, since Φ_N^3 is not in $\mathcal{B}^{N/2}$. We observe the difference between Φ_N^3 and Φ^3 is given by

$$\Phi_N^3 - \Phi^3 = (\Phi_N - \Phi) \left(\Phi_N^2 + \Phi_N \Phi + \Phi^2 \right). \tag{B.39}$$

As a result, taking a Laplacian operator to the above terms, applying the nonlinear expansion (B.31), we arrive at

$$\begin{aligned} &\left\| F_{3e}^{k+1/2} - F_{3en}^{k+1/2} \right\|_{L_h^2(\Omega)} \\ &\quad \le C \left(\left\| \Phi_N \right\|_{L^\infty(0,T;W^{2,\infty}(\Omega))}^2 + \left\| \Phi \right\|_{L^\infty(0,T;W^{2,\infty}(\Omega))}^2 \right) \cdot \left\| \Phi_N - \Phi \right\|_{L^\infty(0,T;H^2(\Omega))} \\ &\quad \le C h^2 \left\| \Phi \right\|_{L^\infty(0,T;H^4(\Omega))}^3. \end{aligned} \tag{B.40}$$

Furthermore, a combination of (B.29), (B.38), and (B.40) leads to the consistency estimate of the nonlinear term

$$\begin{aligned} &\left\| F_3 - F_{3en} \right\|_{L_s^2(0,T;L_h^2(\Omega))} \\ &\quad \le C \left(s^2 + h^2 \right) \left(\left\| \Phi \right\|_{L^\infty(0,T;H^4(\Omega))}^3 + \left\| \Phi_N \right\|_{L^\infty(0,T;H^4(\Omega))}^2 \cdot \left\| \Phi_N \right\|_{H^2(0,T;H^2)}^2 \right). \end{aligned} \tag{B.41}$$

Therefore, the local truncation error estimate for τ_1 is obtained by a combination of (B.11), (B.16), (B.22), (B.23), (B.28), (B.41), and a detailed comparison between the truncation equation (3.22), (3.23) and the original PDE:

$$\begin{aligned} &\beta \partial_t^2 \Phi + \partial_t \Phi - \Delta \left(\Phi^3 \right) - (1-\epsilon)\Delta\Phi - 2\Delta^2\Phi - \Delta^3\Phi \\ &\quad = \beta F_{1en} + F_{2en} - F_{3en} - (1-\epsilon) F_{4en} - F_{5en} - F_{6en} = 0. \end{aligned} \tag{B.42}$$

In addition, the constant estimate (3.25) for M is also satisfied, by a careful check.

The estimate for τ_2 is very similar. We denote the following quantity

$$F_{7e}^{k+1/2} = \left(\partial_t \Phi_N + \frac{s^2}{24} \partial_t^3 \Phi_N\right)(\,\cdot\, , t^{k+1/2}). \tag{B.43}$$

A detailed Taylor formula in time gives the following estimate:

$$\|\tau_{21}\|_{L_s^2(0,T)} \le Cs^3 \|\Phi_N\|_{H^4(0,T)} \le Cs^3 \|\Phi\|_{H^4(0,T)} \tag{B.44}$$

at each fixed grid point (i,j), where $\tau_{21}^{k+1/2} := F_2^{k+1/2} - F_{7e}^{k+1/2}$. Its derivation is based on a detailed Taylor expansion (in integral form) of Φ_N^{k+1} and Φ_N^k around the time instant $t^{k+1/2}$ and an estimate in a similar manner following that of Proposition B.1. Meanwhile, it is clear that F_7 has the following decomposition:

$$\begin{aligned} F_7^{k+1/2} = \frac{\Psi_N^{k+1} + \Psi_N^k}{2} &= \frac{\partial_t \Phi_N^{k+1} + \partial_t \Phi_N^k}{2} - \frac{s^2}{12} \cdot \frac{\partial_t^3 \Phi_N^{k+1} + \partial_t^3 \Phi_N^k}{2} \\ &:= F_{7,1}^{k+1/2} + F_{7,2}^{k+1/2}. \end{aligned} \tag{B.45}$$

To facilitate the analysis below, we define two more quantities:

$$\begin{aligned} F_{7e,1}^{k+1/2} &:= \left(\partial_t \Phi_N + \frac{s^2}{8} \partial_t^3 \Phi_N\right)(\,\cdot\, , t^{k+1/2}), \\ F_{7e,2}^{k+1/2} &:= -\frac{s^2}{12} \partial_t^3 \Phi_N(\,\cdot\, , t^{k+1/2}). \end{aligned} \tag{B.46}$$

Similar to the analysis of (B.44), a detailed Taylor expansion (in integral form) of Ψ_N^{k+1} and Ψ_N^k around the time instant $t^{k+1/2}$ gives the following estimates:

$$\|\tau_{22}\|_{L_s^2(0,T)} \le Cs^3 \|\Phi_N\|_{H^4(0,T)} \le Cs^3 \|\Phi\|_{H^4(0,T)}, \tag{B.47}$$

$$\|\tau_{23}\|_{L_s^2(0,T)} \le Cs^3 \|\Phi_N\|_{H^4(0,T)} \le Cs^3 \|\Phi\|_{H^4(0,T)} \tag{B.48}$$

at each fixed grid point (i,j), where $\tau_{22}^{k+1/2} := F_{7,1}^{k+1/2} - F_{7e,1}^{k+1/2}$ and $\tau_{23}^{k+1/2} := F_{7,2}^{k+1/2} - F_{7e,2}^{k+1/2}$. Consequently, a combination of (B.44)–(B.48) shows that

$$F_2^{k+1/2} - F_7^{k+1/2} = \tau_2^{k+1/2} \text{ with } \|\tau_2\|_{L_s^2(0,T)} \le Cs^3 \|\Phi\|_{H^4(0,T)}. \tag{B.49}$$

This in turn implies that

$$\|F_2 - F_7\|_{L_s^2(0,T;L_h^2)} \le Cs^3 \|\Phi\|_{H^4(0,T;L^2)}, \tag{B.50}$$

which is exactly (3.23). Also, the constant M associated with τ_2 satisfies (3.25). The consistency analysis is finished.

REFERENCES

[1] A. Adland, A. Karma, R. Spatschek, D. Buta, and M. Asta, *Phase-field-crystal study of grain boundary premelting and shearing in BCC iron*, Phys. Rev. B (3), 87 (2013), 024110.

[2] R. Backofen, A. Rätz, and A. Voigt, *Nucleation and growth by a phase field crystal (PFC) model*, Phil. Mag. Lett., 87 (2007), pp. 813–820.

[3] A. Baskaran, Z. Hu, J. Lowengrub, C. Wang, S. Wise, and P. Zhou, *Energy stable and efficient finite-difference nonlinear multigrid schemes for the modified phase field crystal equation*, J. Comput. Phys., 250 (2013), pp. 270–292.

[4] J. Boyd, *Chebyshev and Fourier Spectram Methods*, 2nd ed., Dover, New York, 2001.

[5] C. Canuto and A. Quarteroni, *Approximation results for orthogonal polynomials in Sobolev spaces*, Math. Comp., 38 (1982), pp. 257–276.

[6] M. Cheng and J. Warren, *An efficient algorithm for solving the phase field crystal model*, J. Comput. Phys., 227 (2008), pp. 6241–6248.

[7] W. Chen, S. Conde, C. Wang, X. Wang, and S. Wise, *A linear energy stable scheme for a thin film model without slope selection*, J. Sci. Comput., 52 (2012), pp. 546–562.

[8] K. Elder and M. Grant, *Modeling elastic and plastic deformations in nonequilibrium processing using phase filed crystal*, Phys. Rev. E (3), 90 (2004), 051605.

[9] K. Elder, M. Katakowski, M. Haataja, and M. Grant, *Modeling elasticity in crystal growth*, Phys. Rev. Lett., 88 (2002), 245701.

[10] D. Eyre, *Unconditionally gradient stable time marching the Cahn-Hilliard equation*, in Computational and Mathematical Models of Microstructural Evolution Mater. Res. Soc. Sympos. Proc. 529, J. W. Bullard, R. Kalia, M. Stoneham, and L. Chen, eds., Materials Research Society, Warrendale, PA, 1998, pp. 1686–1712.

[11] J. Hesthaven, S. Gottlieb, and D. Gottlieb, *Spectral Methods for Time-dependent Problems*, Cambridge University Press, Cambridge, UK, 2007.

[12] Z. Hu, S. Wise, C. Wang, and J. Lowengrub, *Stable and efficient finite-difference nonlinear-multigrid schemes for the phase-field crystal equation*, J. Comput. Phys., 228 (2009), pp. 5323–5339.

[13] V. Lebedev, A. Sysoeva, and P. Galenko, *Unconditionally gradient-stable computational schemes in problems of fast phase transitions*, Phys. Rev. E (3), 83 (2011), 026705.

[14] J. Mellenthin, A. Karma, and M. Plapp, *Phase-field crystal study of grain-boundary premelting*, Phys. Rev. B (3), 78 (2008), 184110.

[15] J. Shen, C. Wang, X. Wang, and S. M. Wise, *Second-order convex splitting schemes for gradient flows with Ehrlich–Schwoebel type energy: Application to thin film epitaxy*, SIAM J. Numer. Anal., 50 (2012), pp. 105–125.

[16] P. Stefanovic, M. Haataja, and N. Provatas, *Phase-field crystals with elastic interactions*, Phys. Rev. Lett., 96 (2006), 225504.

[17] P. Stefanovic, M. Haataja, and N. Provatas, *Phase field crystal study of deformation and plasticity in nanocrystalline materials*, Phys. Rev. E (3), 80 (2009), 046107.

[18] J. Swift and P. Hohenberg, *Hydrodynamic fluctuations at the convective instability*, Phys. Rev. A (3), 15 (1977), pp. 319–328.

[19] C. Wang, X. Wang, and S. Wise, *Unconditionally stable schemes for equations of thin film epitaxy*, Discrete Contin. Dynam. Systems Ser. A, 28 (2010), pp. 405–423.

[20] C. Wang and S. Wise, *Global smooth solutions of the modified phase field crystal equation*, Methods Appl. Anal., 17 (2010), pp. 191–212.

[21] C. Wang and S. M. Wise, *An energy-stable and convergent finite-difference scheme for the modified phase field crystal equation*, SIAM J. Numer. Anal., 49 (2011), pp. 945–969.

[22] S. M. Wise, C. Wang, and J. S. Lowengrub, *An energy-stable and convergent finite-difference scheme for the phase field crystal equation*, SIAM J. Numer. Anal., 47 (2009), pp. 2269–2288.

[23] S. Wise, *Unconditionally stable finite difference, nonlinear multigrid simulation of the Cahn-Hilliard-Hele-Shaw system of equations*, J. Sci. Comput., 44 (2010), pp. 38–68.