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GLOBAL SMOOTH SOLUTIONS OF THE THREE-DIMENSIONAL MODIFIED PHASE FIELD CRYSTAL EQUATION*

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Abstract. The Modified Phase Field Crystal (MPFC) equation, a generalized damped wave equation for which the usual Phase Field Crystal (PFC) equation is a special case, is analyzed in detail in three dimensions. A time-discrete numerical scheme, based on a convex splitting for the functional energy, is utilized to construct an approximate solution, which is then shown to converge to a solution of the MPFC equation as the time step approaches zero. In detail, a uniform-in-time bound of the pseudo energy for the numerical solution is obtained owing to the structure of the convex-splitting scheme. As an immediate result, we obtain a bound of the $L_s^\infty(0,T;H_{per}^2)$ norm of the numerical solution. More detailed energy estimates, which are obtained by taking the inner product of the numerical scheme with $(-\Delta)^m(\phi^{k+1}-\phi^k)$, give bounds for the numerical solution and it first and second temporal backward differences in the $L_s^\infty(0,T;H_{per}^{m+3})$, $L_s^\infty(0,T;H_{per}^{m})$ and $L_s^\infty(0,T;H_{per}^{m-3})$ norms, respectively. These estimates of the numerical solutions in turn result in a global weak solution (with $m=0$) and a unique global strong solution ($m=3$) upon passage to the limit as the time step size approaches zero. A global smooth solution can also be established by taking arbitrarily large values of m.

Key words. phase field crystal, modified phase field crystal, pseudo energy, nonlinear partial differential equations, global weak solution, global strong solution, global smooth solution

AMS subject classifications. 35G25, 35L75, 65M12

1. Introduction. The Phase Field Crystal (PFC) model, which is a sixth-order, parabolic-type PDE, was recently proposed in [3] as a new approach to simulating the morphological evolution of crystalline solids at the atomic length scale in space but on a coarse-grained diffusive time-scale. See, for example, the recent review [12] that describes the variety of applications for the PFC approach. Recently, Stefanovic *et al.* [11] introduced a small but 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, which the PFC fails to do, 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 MPFC approach introduces a separation of time scales that allows for the elastic relaxation of the crystal lattice on a rapid time scale while other processes evolve on a slower diffusion time scale [12, 11].

In the papers [9, 16] we described unconditionally stable, unconditionally solvable and convergent schemes for the PFC equation based on convex-splitting methods. Extending the work from [9, 16], in [15] we devised a convex splitting scheme for the 2-D MPFC equation, proving unconditional energy stability and convergence of the numerical solutions. Here our goal is to prove the unique existence of global smooth solutions to the 3-D MPFC equation. Our approach will be to show that numerical

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solutions of a time-discrete, spatially-continuous convex-splitting scheme, inspired by that in [15], converges to solutions of the 3-D MPFC equation. This analysis will be facilitated, primarily, by the establishment of *a priori* energy estimates of the numerical solutions. To our knowledge, no work has undertaken an investigation of the existence of solutions to either the PFC or MPFC equations. However, some work on closely related problems should and will be mentioned later.

2. The MPFC Equation and a Convex-Splitting Scheme.

2.1. Notation and Conventions. We use the standard notation for the $W^{\ell,p}$ semi-norm:

$$|\phi|_{W^{\ell,p}} := \left(\sum_{|\alpha|=\ell} \|\partial^\alpha \phi\|_{L^p}^p \right)^{1/p} , \tag{2.1}$$

where α is a multi-index. The $W^{k,p}$ norm is then $\|\phi\|_{W^{k,p}} = \left(\sum_{\ell=0}^k |\phi|_{W^{\ell,p}}^p\right)^{1/p}$. We use $H^k = W^{k,2}$. For vector functions $\mathbf{u} : \Omega \to \mathbf{R}^m$, with components $u_i \in L^p(\Omega)$, we define $\|\mathbf{u}\|_{L^p} := \| \, |\mathbf{u}| \, \|_{L_p}$ for $1 \le p \le \infty$, where $|\mathbf{u}| = \sqrt{\mathbf{u} \cdot \mathbf{u}}$. Then $\|\nabla\phi\|_{L^p} = \| \, |\nabla\phi| \, \|_{L^p}$, but note $\|\nabla\phi\|_{L^p} \ne |\phi|_{W^{1,p}}$ in general. For simplicity we will work in the three-dimensional domain $\Omega = (0, L_x) \times (0, L_y) \times (0, L_z)$. Note that for this domain

$$|\phi|_{W^{1,4}} \le \|\nabla\phi\|_{L^4} \le 3^{1/4} \, |\phi|_{W^{1,4}} . \tag{2.2}$$

For matrix functions $A : \Omega \to \mathbf{R}^{m\times m}$ with components $a_{i,j} \in L^p(\Omega)$ we define $\|A\|_{L^p} := \| \, |A| \, \|_{L_p}$ for $1 \le p \le \infty$, where $|A| = \sqrt{A : A}$.

We will work with time-discrete functions of the form $\phi : \{0, 1, \ldots, \ell\} \to W^{k,p}(\Omega)$. For temporal function evaluations, we use the notation $\phi^k := \phi(k) \in W^{k,p}(\Omega)$. We say such time-discrete functions are in the space $L_s^\infty\left(0, T; W^{k,p}(\Omega)\right)$, where $s \cdot \ell = T$, $s > 0$, provided that the following norm is finite:

$$\|\phi\|_{L_s^\infty(0,T;W^{k,p}(\Omega))} := \max_{1\le k\le \ell} \left\|\phi^k\right\|_{W^{k,p}} . \tag{2.3}$$

Similar definitions are available for the spaces $L_s^p\left(0, T; W^{k,p}(\Omega)\right)$, though we won't need them here.

The natural (spatial) function space for the MPFC equation is the subspace of $H^m(\Omega)$ (with $m \ge 0$) that is periodic:

$$H_{per}^m(\Omega) := \left\{\text{closure of } C_{per}^\infty(\Omega) \text{ in } H^m(\Omega)\right\} , \quad m \ge 1 .$$

Of course $H_{per}^0(\Omega) = L_{per}^2(\Omega) = L^2(\Omega)$. (We drop the (Ω) beyond this point.) We denote by H_{per}^{-m}, $m > 0$, the continuous dual space of H_{per}^m. These spaces are equipped with the operator norms

$$\|T\|_{H_{per}^{-m}} = \sup_{\substack{\|\phi\|_{H^m}=1 \\ \phi\in H_{per}^m}} |T(\phi)| . \tag{2.4}$$

Functions in L^2 induce continuous linear functionals on H_{per}^1 in a natural way. Let $f \in L^2$, and define $T_f(\phi) := (f, \phi)_{L^2}$. Then $T_f \in H_{per}^{-1}$, and, in fact, such functions are dense in H_{per}^{-1}. We denote by $\mathring{H}_{per}^{-1}$ the closure of the set $\left\{T_f \;\middle|\; f \in \mathring{L}^2\right\}$ in the norm (2.4), where the symbol $\circ$ indicates the subspace of mean-zero functions.

We shall need an equivalent and more convenient norm on H_{per}^{-1}. Define $\psi_f \in \mathring{H}_{per}^1$ to be the unique weak solution to the PDE problem

$$-\Delta\psi_f = f - \bar{f} \ , \tag{2.5}$$

where $f \in L^2$, and $\bar{f} = |\Omega|^{-1}\int_\Omega f \, d\mathbf{x}$. In this case we write $\psi_f = -\Delta^{-1}\left(f - \bar{f}\right)$. Suppose that f and g are in L^2, then we define the inner product [6]

$$(f,g)_{H_{per}^{-1}} := |\Omega| \, \bar{f}\bar{g} + \left(\nabla\psi_f, \nabla\psi_g\right)_{L^2} \ . \tag{2.6}$$

Note that, assuming sufficient regularity of the functions and using integration by parts, we have

$$\begin{aligned}(f,g)_{H_{per}^{-1}} &= |\Omega|\bar{f}\bar{g} - \left(\Delta^{-1}\left(f-\bar{f}\right), g-\bar{g}\right)_{L^2} \\ &= |\Omega|\bar{f}\bar{g} - \left(f-\bar{f}, \Delta^{-1}\left(g-\bar{g}\right)\right)_{L^2} \ .\end{aligned} \tag{2.7}$$

For every $f \in L^2$ we may define the induced norm

$$\|f\|_{H_{per}^{-1}} = \sqrt{(f,f)_{H_{per}^{-1}}} \ . \tag{2.8}$$

One can show that (2.8) is equivalent to (2.4) for L^2 functions [6], and therefore definies a *bona fide* norm on H_{per}^{-1}. Note that (2.6), (2.7), and (2.8) simplify greatly if $f, g \in \mathring{L}^2$.

2.2. Mass Conservation and Pseudo-Energy Dissipation. Consider a dimensionless spatial energy of the form

$$E(\phi) = \int_\Omega \left\{\frac{1}{4}\phi^4 + \frac{\alpha}{2}\phi^2 - |\nabla\phi|^2 + \frac{1}{2}\left(\Delta\phi\right)^2\right\} d\mathbf{x} \ , \tag{2.9}$$

where $\phi : \Omega \subset \mathbf{R}^3 \to \mathbf{R}$ is the "atom" density field, $\alpha > 0$ is a constant. Suppose that $\Omega = (0, L_x) \times (0, L_y) \times (0, L_z)$ and ϕ is periodic on Ω. Define μ to be the chemical potential with respect to E:

$$\mu := \delta_\phi E = \phi^3 + \alpha\phi + 2\Delta\phi + \Delta^2\phi \ , \tag{2.10}$$

where $\delta_\phi E$ denotes the variational derivative with respect to ϕ. The MPFC equation may then be written as

$$\partial_t\phi = \Delta\mu - \beta\partial_{tt}\phi \ , \tag{2.11}$$

where $\beta \geq 0$. Observe that when $\beta > 0$, Eq. (2.11) is not a gradient equation, and the energy (2.9) is not necessarily non-increasing in time along the solution trajectories. However, (sufficiently regular) solutions of the MPFC equation do dissipate a pseudo energy. To see this, let us recast the MPFC equation as the following system of equations:

$$\beta\partial_t\psi = \Delta\mu - \psi \ , \tag{2.12}$$

$$\partial_t\phi = \psi \ . \tag{2.13}$$

And let us introduce the pseudo energy

$$\mathcal{E}(\phi, \psi) := E(\phi) + \frac{\beta}{2}\|\psi\|_{H_{per}^{-1}}^2 \ . \tag{2.14}$$

In [15] we showed that if ϕ is a solution to (2.12) and (2.13) with $\int_\Omega \partial_t\phi(\mathbf{x},0)\,d\mathbf{x} = 0$, then $\int_\Omega \partial_t\phi(\mathbf{x},t)\,d\mathbf{x} = 0$ for all time $t > 0$. In other words, $\bar{\psi} = 0$. Here, as in [15], we shall assume the initial data satisfy $\partial_t\phi(\mathbf{x},0) \equiv 0$. Furthermore, in [15] we showed that

$$d_t\mathcal{E} = -(\psi,\psi)_{H_{per}^{-1}} \le 0 \ , \tag{2.15}$$

provided ϕ is a sufficiently regular periodic solution of (2.12) and (2.13).

2.3. Related Work. Equation (2.11) is related in structure to the perturbed viscous Cahn-Hilliard (pvCH) equation [5, 10, 17]

$$\beta\partial_{tt}\phi + \partial_t\phi = \Delta\left(\delta_\phi G + \gamma\partial_t\phi\right), \tag{2.16}$$

where $\beta,\gamma \ge 0$, and where $G = \frac{1}{4}\left\|\phi\right\|_{L^4}^4 - \frac{1}{2}\left\|\phi\right\|_{L^2}^2 + \frac{1}{2}\left\|\nabla\phi\right\|_{L^2}^2$, the standard Cahn-Hilliard spatial energy [2]. Ball [1] has studied global attractors of the semi-linear equation $\beta\partial_{tt}\phi + \partial_t\phi = -\delta_\phi G$, which is the "non-conserved" version of Eq. (2.16). As with the MPFC equation (2.11), (2.16) is "mass" conserving with the appropriate initial data, and the pseudo energy $G(\phi) + {}^{\beta}\!/\!{}_2\left\|\partial_t\phi\right\|_{H_{per}^{-1}}^2$ is non-increasing in time. Zheng and Milani [17], Gatti *et al.* [5], and Kania [10] have studied global attractors of (2.16). When $\gamma = 0$ (2.16) is called the perturbed Cahn-Hilliard (pCH) equation and has been proposed as a model for rapid phase separation in [4].

To our knowledge no PDE analysis has been undertaken for the 3-D MPFC equation (2.11), though the techniques in [5, 10, 17] may be applicable. Because of the presence of the second order temporal derivatives, the establishment of a global strong solution and smooth solution for (2.11) is very subtle. The 1-D pvCH model was analyzed in detail in [17] by applying the continuous embedding $H^1(\Omega)$ to $C(\bar{\Omega})$. In 2-D and 3-D, the well-posedness of the pvCH model was established in [5] under the assumptions

$$\beta,\,\gamma \in [0,1] \quad \text{and} \quad \gamma \ge \mu\beta \ , \tag{2.17}$$

for some μ with $0 < \mu \le 1$. See [5, Thm. 2.2]. A global attractor is also proven under this assumption. Yet, the case for which $\beta > 0$ and $\gamma = 0$ (the pCH model) becomes more challenging, as was pointed out in [5], because the standard energy estimates fail to hold and the existence of higher regularity solutions appears nontrivial. A unique quasi-strong solution for the 2-D pCH model was recently established in [8], with solution regularity $\phi \in H^3$, $\partial_t\phi \in H^1$. For the 3-D pCH model, a local-in-time solution is proven for any initial data, and a global-in-time solution is established for small initial data in another recent paper [7].

In this article we are going to analyze the 3-D MPFC equation with $\beta > 0$ and $\gamma = 0$. A unique global strong solution and smooth solution will be established without an assumption like (2.17) and for any initial data with the required regularity.

2.4. A Discrete-Time, Continuous-Space Convex-Splitting Scheme. To establish a solution for the 3-D MPFC equation (2.11), we first consider a solution to a time-discrete space-continuous numerical scheme. Our aim is to construct a sequence of approximate solutions to (2.11) using the numerical solutions. The scheme is based on the fundamental 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

$$E_c = \frac{1}{4}\left\|\phi\right\|_{L^4}^4 + \frac{\alpha}{2}\left\|\phi\right\|_{L^2}^2 + \frac{1}{2}\left\|\Delta\phi\right\|_{L^2}^2 , \quad E_e = \left\|\nabla\phi\right\|_{L^2}^2 . \tag{2.18}$$

We also note that when $\psi \in \mathring{L}^2$, $\frac{\beta}{2}\left\|\psi\right\|^2_{H^{-1}_{per}}$ is clearly convex. These facts together with [16, Thm. 1.1] yield the following result, which we noted in [15]:

THEOREM 2.1. *Suppose that $\Omega = (0, L_x) \times (0, L_y) \times (0, L_z)$ and ϕ_1, $\phi_2 : \Omega \to \mathbf{R}$ are periodic and sufficiently regular. Assume that ψ_1, $\psi_2 : \Omega \to \mathbf{R}$ are L^2 functions of mean zero. Consider the canonical convex splitting of the energy E in (2.9) into $E = E_c - E_e$ given in (2.18). Then*

$$\begin{aligned} \mathcal{E}(\phi_1, \psi_1) - \mathcal{E}(\phi_2, \psi_2) \le{}& \left(\delta_\phi E_c(\phi_1) - \delta_\phi E_e(\phi_2), \phi_1 - \phi_2\right)_{L^2} \\ & + \beta\left(\psi_1, \psi_1 - \psi_2\right)_{H^{-1}_{per}}, \end{aligned} \tag{2.19}$$

where δ_ϕ represents the variational derivative.

The following convex-splitting scheme was proposed in [15]:

$$\beta\left(\psi^{k+1} - \psi^k\right) = s\Delta\mu^{k+1} - s\psi^{k+1}\ , \tag{2.20}$$

$$\mu^{k+1} = \delta_\phi E_c\left(\phi^{k+1}\right) - \delta_\phi E_e\left(\phi^k\right)\ , \tag{2.21}$$

$$\phi^{k+1} - \phi^k = s\psi^{k+1}\ , \tag{2.22}$$

where $\psi^0 \equiv 0$. It is straightforward to see that this first-order scheme is mass conserving, provided $\int_\Omega \psi^0\, d\mathbf{x} = 0$. (The details are found in [15].) It was shown in [15] that (2.20) – (2.22) is unconditionally (pseudo) energy stable. Reproducing the calculation, by Thm. 2.1 with the proper replacements we have immediately that

$$\begin{aligned} \mathcal{E}\left(\phi^{k+1}, \psi^{k+1}\right) - \mathcal{E}\left(\phi^k, \psi^k\right) \le{}& \left(\delta_\phi E_c\left(\phi^{k+1}\right) - \delta_\phi E_e\left(\phi^k\right), \phi^{k+1} - \phi^k\right)_{L^2} \\ & - \beta\left(\Delta^{-1}\psi^{k+1}, \psi^{k+1} - \psi^k\right)_{L^2}\ . \end{aligned} \tag{2.23}$$

Let $C := |\Omega|^{-1}\int_\Omega \mu^{k+1}\, d\mathbf{x}$. Using Eqs. (2.20) – (2.22) in the RHS of inequality (2.23) we find

$$\begin{aligned} \mathcal{E}\left(\phi^{k+1}, \psi^{k+1}\right) - \mathcal{E}\left(\phi^k, \psi^k\right) &\le \left(\mu^{k+1}, s\psi^{k+1}\right)_{L^2} - \beta\left(\psi^{k+1}, \Delta^{-1}\left(\psi^{k+1} - \psi^k\right)\right)_{L^2} \\ &= \left(\psi^{k+1}, s\left(\mu^{k+1} - C\right) - \beta\Delta^{-1}\left(\psi^{k+1} - \psi^k\right)\right)_{L^2} \\ &\quad + \cancelto{0}{\left(\psi^{k+1}, sC\right)_{L^2}} \\ &= \left(\psi^{k+1}, \Delta^{-1}\left\{s\Delta\mu^{k+1} - \cancelto{0}{s\Delta C} - \beta\left(\psi^{k+1} - \psi^k\right)\right\}\right)_{L^2} \\ &= -s\left(\psi^{k+1}, \psi^{k+1}\right)_{H^{-1}_{per}} = -s\left\|\psi^{k+1}\right\|^2_{H^{-1}_{per}} \le 0\ . \end{aligned} \tag{2.24}$$

Therefore, the scheme is energy stable, not with respect to the spatial energy E, but with respect to the modified energy $\mathcal{E}$.

2.5. Brief Outline. In this article we prove that solutions to the MPFC equation (2.11) can be obtained by taking limits of numerical solutions for the scheme (2.20) – (2.22) as $s \to 0$. Our analysis is based on *a priori* energy estimates of these numerical solutions. In particular, we first use the energy stability result (2.24) to establish a uniform $L^\infty_s\left(0, T; H^2_{per}\right)$ estimate of the numerical solutions to (2.20) – (2.22). Then, by testing the numerical scheme with $\phi^{k+1} - \phi^k$, we can derive an $L^\infty_s\left(0, T; H^3_{per}\right)$ bound of the numerical solution (independent of s) and, additionally, $L^\infty_s\left(0, T; L^2\right)$ and $L^\infty_s\left(0, T; H^{-3}_{per}\right)$ bounds of its first and second temporal backward differences. More detailed energy estimates, which are obtained by taking the inner product of the numerical scheme with $(-\Delta)^m(\phi^{k+1}-\phi^k)$, give bounds for the numerical solution and its first and second temporal backward differences in the $L_s^\infty(0,T;H_{per}^{m+3})$, $L_s^\infty(0,T;H_{per}^{m})$, and $L_s^\infty(0,T;H_{per}^{m-3})$ norms, respectively. These estimates of the numerical solutions in turn result in a global weak solution (with $m=0$) and a unique global strong solution ($m=3$) upon passage to the limit $s\to 0$, with the solution regularity satisfying $\phi \in L^\infty\left(0,T;H_{per}^{m+3}\right)$, $\psi=\partial_t\phi\in L^\infty\left(0,T;H_{per}^{m}\right)$, $\partial_t\psi=\partial_{tt}\phi\in L^\infty\left(0,T;H_{per}^{m-3}\right)$. A global smooth solution can also be established by taking arbitrarily large values of m, depending on the regularity of the initial data.

To facilitate the analysis we first establish a couple of basic estimates in Sec. 3. The existence of a weak solution is established in Sec. 4, assuming H^3 initial data. In Sec. 5 we provide existence and uniqueness analyses for the strong solution, assuming H^6 initial data. We give a summary of our results in Sec. 6.

3. Elementary Estimates. In this section we provide some elementary estimates that will be needed in the PDE analysis. The first lemma shows that the PFC energy (2.9) is bounded.

LEMMA 3.1. *Suppose that $\phi\in H_{per}^2$. Then*

$$C_1\left\|\phi\right\|_{H^1}^4 + C_2\left\|\phi\right\|_{H^2}^2 \ge E(\phi) \ge C_3\left\|\phi\right\|_{H^2}^2 - \frac{|\Omega|}{4} \tag{3.1}$$

for some positive constants C_1, C_2, and C_3 that depend upon L_x, L_y, L_z, and α.

Proof. The first inequality follows from the Sobolev inequality $\left\|\phi\right\|_{L^4}\le C\left\|\phi\right\|_{H^1}$, for some positive constant C. A finite-difference version of the second inequality in 2-D is proved in [16, Lem. 3.7]. The proof for the present case is similar to that. ∎

LEMMA 3.2. *Suppose that $\phi\in H_{per}^3$. Then*

$$\left\|\Delta\phi\right\|_{L^2}^2 \le \frac{1}{3\epsilon^2}\left\|\phi\right\|_{L^2}^2 + \frac{2\epsilon}{3}\left\|\nabla\left(\Delta\phi\right)\right\|_{L^2}^2 \ , \tag{3.2}$$

valid for arbitrary $\epsilon>0$.

Proof. The proof is similar to that for the 2-D finite-difference version [16, Lem. 3.10] and is omitted. ∎

LEMMA 3.3. *Suppose that $\phi\in H_{per}^2$. Then*

$$\left\|\Delta\phi^3\right\|_{L^2} \le 3\left\|\phi\right\|_{L^\infty}^2\cdot\left\|\Delta\phi\right\|_{L^2} + 6\left\|\phi\right\|_{L^\infty}\cdot\left\|\nabla\phi\right\|_{L^4}^2 \ . \tag{3.3}$$

Proof. Use the expansion

$$\Delta\phi^3 = 3\phi^2\Delta\phi + 6\phi\left|\nabla\phi\right|^2 \tag{3.4}$$

and the triangle inequality. ∎

LEMMA 3.4. *Suppose that $\phi\in H_{per}^3$. Then*

$$\begin{aligned}\left\|\nabla\left(\Delta\phi^3\right)\right\|_{L^2} \le{}& 6\left\|\phi\right\|_{L^\infty}\cdot\left\|\nabla\phi\right\|_{L^\infty}\cdot\left\|\Delta\phi\right\|_{L^2} + 3\left\|\phi\right\|_{L^\infty}^2\cdot\left\|\nabla\left(\Delta\phi\right)\right\|_{L^2}\\ &+6\left\|\nabla\phi\right\|_{L^\infty}\cdot\left\|\nabla\phi\right\|_{L^4}^2 + 36\left\|\phi\right\|_{L^\infty}\cdot\left\|\nabla\phi\right\|_{L^\infty}\cdot\left|\phi\right|_{H^2} \ .\end{aligned} \tag{3.5}$$

Proof. First we use the expansion

$$\nabla\left(\Delta\phi^3\right) = 6\phi\Delta\phi\nabla\phi + 3\phi^2\nabla\left(\Delta\phi\right) + 6\left|\nabla\phi\right|^2\nabla\phi + 12\phi H(\phi)\nabla\phi\ , \tag{3.6}$$

where $H(\phi)$ is the Hessian matrix and $H(\phi)\nabla\phi$ is understood as a matrix vector product. We then use the triangle inequality noting the following estimate for the last term:

$$\left\|\phi\, H(\phi)\nabla\phi\right\|_{L^2} \le 3\left\|\phi\right\|_{L^\infty}\cdot\left\|\nabla\phi\right\|_{L^\infty}\cdot\left\|H(\phi)\right\|_{L^2}\ . \tag{3.7}$$

But, $\left\|H(\phi)\right\|_{L^2} = |\phi|_{H^2}$. ∎

LEMMA 3.5. *Suppose* Φ, $\phi \in H^2_{per}$, *and denote their difference by* $\tilde\phi := \Phi - \phi$. *Then*

$$\begin{aligned}\left\|\Delta\left(\Phi^3-\phi^3\right)\right\|_{L^2} \le 6\Big\{&\left\|\phi\right\|^2_{L^\infty}\cdot\left\|\Delta\tilde\phi\right\|_{L^2} + \Big(\left\|\Phi\right\|_{L^\infty}+\left\|\phi\right\|_{L^\infty}\Big)\cdot\left\|\Delta\Phi\right\|_{L^2}\cdot\left\|\tilde\phi\right\|_{L^\infty}\\ &+\left\|\nabla\Phi\right\|^2_{L^4}\cdot\left\|\tilde\phi\right\|_{L^\infty} + \left\|\phi\right\|_{L^\infty}\cdot\Big(\left\|\nabla\Phi\right\|_{L^4}+\left\|\nabla\phi\right\|_{L^4}\Big)\cdot\left\|\nabla\tilde\phi\right\|_{L^4}\Big\}\ .\end{aligned} \tag{3.8}$$

Proof. Subtracting formula (3.4) from the analogous formula for Φ we find

$$\Delta\Big(\Phi^3-\phi^3\Big) = 3\phi^2\Delta\tilde\phi + 3\tilde\phi\left(\Phi+\phi\right)\Delta\Phi + 6\tilde\phi\left|\nabla\Phi\right|^2 + 6\phi\nabla\tilde\phi\cdot\nabla\big(\Phi+\phi\big)\ . \tag{3.9}$$

Next we use the triangle inequality and estimate the norms of the four terms. The first three estimates are straightforward:

$$\left\|3\phi^2\Delta\tilde\phi\right\|_{L^2} \le 3\left\|\phi\right\|^2_{L^\infty}\cdot\left\|\Delta\tilde\phi\right\|_{L^2}\ , \tag{3.10}$$

$$\left\|3\tilde\phi\left(\Phi+\phi\right)\Delta\Phi\right\|_{L^2} \le 3\Big(\left\|\Phi\right\|_{L^\infty}+\left\|\phi\right\|_{L^\infty}\Big)\left\|\Delta\Phi\right\|_{L^2}\cdot\left\|\tilde\phi\right\|_{L^\infty}\ , \tag{3.11}$$

$$\left\|6\tilde\phi\left|\nabla\Phi\right|^2\right\|_{L^2} \le 6\left\|\nabla\Phi\right\|^2_{L^4}\cdot\left\|\tilde\phi\right\|_{L^\infty}\ . \tag{3.12}$$

The last estimate follows from

$$\begin{aligned}\left\|6\phi\nabla\tilde\phi\cdot\nabla\big(\Phi+\phi\big)\right\|_{L^2} &\le 6\left\|\phi\right\|_{L^\infty}\cdot\left\|\nabla\tilde\phi\cdot\nabla\big(\Phi+\phi\big)\right\|_{L^2}\\ &\le 6\left\|\phi\right\|_{L^\infty}\cdot\left\|\left|\nabla\tilde\phi\right|\cdot\left|\nabla\big(\Phi+\phi\big)\right|\right\|_{L^2}\\ &\le 6\left\|\phi\right\|_{L^\infty}\cdot\left\|\left|\nabla\tilde\phi\right|\right\|_{L^4}\cdot\left\|\left|\nabla\big(\Phi+\phi\big)\right|\right\|_{L^4}\\ &\le 6\left\|\phi\right\|_{L^\infty}\cdot\left\|\left|\nabla\Phi\right|+\left|\nabla\phi\right|\right\|_{L^4}\cdot\left\|\nabla\tilde\phi\right\|_{L^4}\\ &\le 6\left\|\phi\right\|_{L^\infty}\cdot\Big(\left\|\nabla\Phi\right\|_{L^4}+\left\|\nabla\phi\right\|_{L^4}\Big)\cdot\left\|\nabla\tilde\phi\right\|_{L^4}\ .\end{aligned} \tag{3.13}$$

∎

4. Existence of a Weak Solution. We define weak solutions of (2.11) in the following way. For any positive final time $T > 0$, a periodic function ϕ with

$$\begin{aligned}\phi &\in L^\infty\left(0,T;H^3_{per}\right)\ ,\\ \psi = \partial_t\phi &\in L^\infty\left(0,T;L^2\right)\ ,\\ \partial_t\psi = \partial_{tt}\phi &\in L^\infty\left(0,T;H^{-3}_{per}\right)\ ,\end{aligned}$$

is called a weak solution if and only if

$$\int_0^T\int_\Omega \Big\{ \left(\beta\partial_t\psi + \psi\right)\xi - \left(\phi^3 + \alpha\phi + 2\Delta\phi\right)\Delta\xi + \nabla\left(\Delta\phi\right)\cdot\nabla\left(\Delta\xi\right) \Big\} d\mathbf{x}dt = 0 \ , \tag{4.1}$$

for all $\xi \in C^2(0,T;H^3_{per}(\Omega))$, where $\int_\Omega \partial_t\psi\,\xi\,d\mathbf{x}$ is understood as the duality paring between H^{-3}_{per} and H^3_{per}.

Numerical solutions are obtained from the spatially continuous, temporally discrete MPFC scheme (2.20) – (2.22), which can also be formulated in an equivalent way:

$$\begin{aligned}\beta\left(\frac{\phi^{k+1}-2\phi^k+\phi^{k-1}}{s^2}\right) + \frac{\phi^{k+1}-\phi^k}{s} \\ = \Delta\left((\phi^{k+1})^3 + \alpha\phi^{k+1} + 2\Delta\phi^k + \Delta^2\phi^{k+1}\right) \ .\end{aligned} \tag{4.2}$$

Note that we always assume that $\psi^0 \equiv 0$, or, equivalently, that $\phi^{-1} \equiv \phi^0$. The analysis here is based on the following result, which guarantees unique, smooth, and energy-stable solutions for the scheme:

THEOREM 4.1. *For any $s > 0$, given ϕ^k, $\phi^{k-1} \in C^\infty_{per}$, with $\left(\phi^k - \phi^{k-1}, 1\right)_{L^2} = 0$, there exists a unique solution $\phi^{k+1} \in C^\infty_{per}$ to the scheme (2.20) – (2.22), or equivalently (4.2), with $\left(\phi^{k+1} - \phi^k, 1\right)_{L^2} = 0$. Consequently,*

$$\mathcal{E}(\phi^{k+1},\psi^{k+1}) + s\left\|\psi^{k+1}\right\|^2_{H^{-1}_{per}} \le \mathcal{E}(\phi^k,\psi^k) \ , \tag{4.3}$$

where $\mathcal{E}$ is the pseudo-energy defined in (2.14), and $\psi^k := \left(\phi^k - \phi^{k-1}\right)/s$.

Proof. Given ϕ^k, $\phi^{k-1} \in C^\infty_{per}$, it may be shown that (suitably defined) weak solutions to (4.2) are equivalent to minimizers of the strictly convex functional

$$G(\phi) := \frac{1+\frac{\beta}{s}}{2s}\left\|\phi - \phi^k\right\|^2_{H^{-1}_{per}} - \frac{\beta}{s}\left(\phi - \phi^k, \psi^k\right)_{H^{-1}_{per}} + E_c(\phi) - \left(\phi, \delta_\phi E_e(\phi^k)\right)_{L^2} \ , \tag{4.4}$$

over the class of admissible functions

$$\mathcal{A} = \left\{\phi \in H^2_{per} \ \middle|\ \left(\phi - \phi^k, 1\right)_{L^2} = 0\right\} \ . \tag{4.5}$$

Existence of a unique solution is straightforwardly obtained via the direct method in the calculus of variations, and we call this solution, naturally, $\phi = \phi^{k+1}$. One then may use a (nonlinear) regularity result to ultimately establish smoothness of the solution. See the relevant discussions in [13], for example, for more details. The energy stability property (4.3) then follows from the calculation in (2.24) ∎

The energy stability property (4.3) can be easily exploited to obtain a number of *a priori* estimates of the numerical solutions ϕ^k.

LEMMA 4.2. *Let $M > 0$ be given. Suppose that $\Phi \in H^2_{per}$, $\phi^0 \in C^\infty_{per}$ such that $\left\|\phi^0 - \Phi\right\|_{H^2} \le M$, and $\psi^0 \equiv 0$. We have the estimates*

$$\left\|\phi^k\right\|_{H^2} \le C_4 \ , \quad \left\|\phi^k\right\|_{L^\infty} \le C_5 \ , \quad \left\|\nabla\phi^k\right\|_{L^4} \le C_6 \ , \tag{4.6}$$

for any $k \ge 0$, where the constants depend on L_x, L_y, L_z, α, $\|\Phi\|_{H^2}$ and M, but are independent of s.

Proof. The non-increasing property of the pseudo energy (4.3) together with the upper and lower bounds of the physical energy in Lem. 3.1 show that

$$
\begin{aligned}
C_3 \left\|\phi^k\right\|_{H^2}^2 - \frac{|\Omega|}{4} \le E\left(\phi^k\right) &\le \mathcal{E}\left(\phi^k, \psi^k\right) \\
&\le \mathcal{E}(\phi^0, \psi^0) = E\left(\phi^0\right) \\
&\le C_1 \left(\|\Phi\|_{H^1} + M\right)^4 + C_2 \left(\|\Phi\|_{H^2} + M\right)^2 =: C_7 \ ,
\end{aligned}
\tag{4.7}
$$

for any $k \ge 0$, where we have used $\psi^0 \equiv 0$. The first result follows with

$$
C_4 := \sqrt{\frac{C_7 + \frac{|\Omega|}{4}}{C_3}} \ . \tag{4.8}
$$

Application of standard Sobolev inequalities lead to the L^∞ and $W^{1,4}$ estimates of the numerical solution and its gradient:

$$
\left\|\phi^k\right\|_{L^\infty} \le C \left\|\phi^k\right\|_{H^2} \le C C_4 := C_5 \ , \tag{4.9}
$$

$$
\|\nabla\phi\|_{L^4} \le 3^{1/4} \left|\phi\right|_{W^{1,4}} \le 3^{1/4} C \left\|\phi^k\right\|_{H^2} \le 3^{1/4} C C_4 := C_6 \ , \tag{4.10}
$$

for any $k \ge 0$. The second and third parts of the lemma are proven. ∎

Thus we obtain an $L_s^\infty\left(0, T; H_{per}^2\right)$ estimate of the approximate solution:

$$
\|\phi\|_{L_s^\infty(0,T;H^2)} \le C_4 \ , \tag{4.11}
$$

where $T = s \cdot \ell$. We now proceed to show an estimate of the approximation in $L_s^\infty\left(0, T; H_{per}^3\right)$.

LEMMA 4.3. *Let $M > 0$ be as in the previous lemma. Suppose that $\Phi \in H_{per}^3$, $\phi^0 \in C_{per}^\infty$ such that $\left\|\phi^0 - \Phi\right\|_{H^3} \le M$, and $\psi^0 \equiv 0$. Solutions to the numerical scheme (2.20) – (2.22) satisfy the following estimates:*

$$
\left\|\phi^k\right\|_{H^3} \le C_8, \quad \left\|\psi^k\right\|_{L^2} \le C_9, \quad \left\|\frac{\psi^k - \psi^{k-1}}{s}\right\|_{H^{-3}} \le C_{10} \ , \tag{4.12}
$$

for any $1 \le k \le \ell$, where $T = s \cdot \ell$. C_8, C_9 and C_{10} are positive constants that may depend on L_x, L_y, L_z, α, $\|\Phi\|_{H^3}$, M, and T but are independent of s.

The proof of this result is rather tedious and is given in App. A. With the boundedness of the numerical solution ϕ in $L_s^\infty\left(0, T; H_{per}^3\right)$ we may now prove the following theorem.

THEOREM 4.4. *Suppose $\Phi \in H_{per}^3$. There exists at least one global weak solution $\phi(\mathbf{x}, t)$ of (2.11), in the sense of (4.1), such that for any $T > 0$*

$$
\phi \in L^\infty\left(0, T; H_{per}^3\right) \ , \quad \partial_t\phi \in L^\infty\left(0, T; L^2\right) \ , \quad \partial_{tt}\phi \in L^\infty\left(0, T; H_{per}^{-3}\right) \ , \tag{4.13}
$$

with the initial conditions $\phi(\,\cdot\,, 0) \equiv \Phi$ and $\partial_t\phi(\,\cdot\,, 0) \equiv 0$.

Proof. The proof is based on a construction using the numerical solution and the corresponding *a priori* estimates provided above. We begin by requiring that $0 < s < M$, where M is as above, and choosing $\phi^0 \in C_{per}^\infty$ such that $\left\|\Phi - \phi^0\right\|_{H^3} < s$.

Define ϕ_ℓ to be an approximate function induced by the numerical scheme (2.20) – (2.22):

$$\phi_\ell\left(\mathbf{x},t\right) := \begin{cases} \sum_{i=-1}^{1} \phi^{k+i}(\mathbf{x}) L_i(t) & \text{for} \quad t_k \le t < t_{k+1}, \ k = 0,\ldots,\ell-1 \\ \phi^\ell(\mathbf{x}) & \text{for} \quad t = t_\ell \end{cases} , \tag{4.14}$$

where $s \cdot \ell = T$, $t_k = s \cdot k$, and

$$L_i(t) = \prod_{\substack{j=-1 \\ j\neq i}}^{1} \frac{t - t_{k+j}}{t_{k+i} - t_{k+j}} \ . \tag{4.15}$$

Here we use $\phi^{-1} := \phi^0$. Next, we define $\psi_\ell\left(\,\cdot\,,t\right) := \partial_t \phi_\ell\left(\,\cdot\,,t\right)$ and $\partial_t \psi_\ell\left(\,\cdot\,,t\right) := \partial_{tt}\phi_\ell\left(\,\cdot\,,t\right)$, where such derivaives make sense. Obviously ϕ_ℓ is smooth in $\mathbf{x}$ and continuous in time, and, in particular, $\phi_\ell\left(\,\cdot\,,t_k\right) \equiv \phi^k$ for $k = 0,\ldots,\ell$. On the other hand, note that $\lim_{t\searrow t_k} \psi_\ell(\,\cdot\,,t) \not\equiv \psi^k(\,\cdot\,) \not\equiv \lim_{t\nearrow t_k} \psi_\ell(\,\cdot\,,t)$, and, specifically, $\lim_{t\searrow 0} \psi_\ell(\,\cdot\,,t) \not\equiv 0$. However, calculations reveal that

$$\psi_\ell(\mathbf{x},t) = q_k(t)\psi^{k+1}(\mathbf{x}) + \left(1 - q_k(t)\right)\psi^k(\mathbf{x}) \ , \quad \text{for} \quad t_k < t < t_{k+1} \ , \tag{4.16}$$

where $q_k(t) := {}^1\!/_2 + {}^{(t-t_k)}\!/_s$, and

$$\partial_t \psi_\ell(\mathbf{x},t) = \frac{\phi^{k+1}(\mathbf{x}) - \phi^k(\mathbf{x}) + \phi^{k-1}(\mathbf{x})}{s^2} \ , \quad \text{for} \quad t_k < t < t_{k+1} \ . \tag{4.17}$$

Uniform bounds are available for ϕ_ℓ in the $L^\infty\left(0,T;H^3_{per}\right)$ norm. To see this, first note that on $[t_k, t_{k+1})$

$$\begin{aligned} \|\phi_\ell\|_{H^3} &\le |L_{-1}(t)| \cdot \left\|\phi^{k-1}(\mathbf{x})\right\|_{H^3} + |L_0(t)| \cdot \left\|\phi^k(\mathbf{x})\right\|_{H^3} + |L_1(t)| \cdot \left\|\phi^{k+1}(\mathbf{x})\right\|_{H^3} \\ &\le \frac{1}{8} \cdot C_8 + 1 \cdot C_8 + 1 \cdot C_8 = \frac{17}{8} C_8 \ . \end{aligned} \tag{4.18}$$

Hence,

$$\|\phi_\ell\|_{L^\infty(0,T;H^3)} \le \frac{17}{8} C_8 \ . \tag{4.19}$$

Regarding the temporal derivative $\psi_s = \partial_t \phi_s$, by similar reasoning

$$\|\psi_\ell\|_{L^\infty(0,T;L^2)} \le 2C_9 \ . \tag{4.20}$$

Finally, a combination of (A.21) with (4.17) leads to

$$\|\partial_t \psi_\ell\|_{L^\infty\left(0,T;H^{-3}_{per}\right)} \le C_{10} \ . \tag{4.21}$$

Since the estimates (4.19), (4.20) and (4.21) are uniform in terms of s, there exist subsequences ϕ_{ℓ_n}, ψ_{ℓ_n}, $\partial_t \psi_{\ell_n}$ and limit functions $\phi \in L^\infty\left(0,T;H^3_{per}\right)$, $\psi \in L^\infty\left(0,T;L^2\right)$, $\partial_t \psi \in L^\infty\left(0,T;H^{-3}_{per}\right)$ such that

$$\phi_{\ell_n} \stackrel{w}{\rightharpoonup} \phi \ \text{ in } \ L^2\left(0,T;H^3_{per}\right), \quad \phi_{\ell_n} \stackrel{w^\star}{\rightharpoonup} \phi \ \text{ in } \ L^\infty\left(0,T;H^3_{per}\right) \ , \tag{4.22}$$

$$\psi_{\ell_n} \stackrel{w^\star}{\rightharpoonup} \psi \ \text{ in } \ L^\infty\left(0,T;L^2\right), \quad \partial_t\psi_{\ell_n} \stackrel{w^\star}{\rightharpoonup} \partial_t \psi \ \text{ in } \ L^\infty\left(0,T;H^{-3}_{per}\right) \ . \tag{4.23}$$

Using (4.22) and (4.23) (note that $\psi_\ell = \partial_t \phi_\ell$) and an improvement of a classical compactness result from [14, Thm. 2.3, Ch. 3], we also have

$$\phi_{\ell_n} \to \phi \ \text{ strongly in } \ L^2\left(0,T;L^2\right) \ . \tag{4.24}$$

Now we may pass to the limit showing that the limit function ϕ is indeed a weak solution in the sense of (4.1). The details are omitted for brevity. $\square$

5. Existence and Uniqueness of a Strong Solution. Next we establish the existence and uniqueness of a global strong solution to the MPFC equation (2.11). Namely, for any positive final time $T > 0$, we seek

$$\begin{aligned} \phi &\in L^\infty\left(0,T;H^6_{per}\right) \ , \\ \psi = \partial_t\phi &\in L^\infty\left(0,T;H^3_{per}\right) \ , \\ \partial_t\psi = \partial_{tt}\phi &\in L^\infty\left(0,T;L^2\right) \ , \end{aligned} \tag{5.1}$$

such that (4.1) holds in the strong sense. The following result gives an $L^\infty_s(0,T;H^4_{per})$ estimate for ϕ. Its proof is given in App. B.

Lemma 5.1. *Let $M > 0$ be as previously defined. Suppose that $\Phi \in H^4_{per}$, $\phi^0 \in C^\infty_{per}$ such that $\left\|\phi^0-\Phi\right\|_{H^4} \le M$, and $\psi^0 \equiv 0$. Solutions to the numerical scheme (2.20) – (2.22) satisfy the following estimates:*

$$\left\|\phi^k\right\|_{H^4} \le C_{13} \ , \quad \left\|\psi^k\right\|_{H^1} \le C_{14} \ , \quad \left\|\frac{\psi^k-\psi^{k-1}}{s}\right\|_{H^{-2}} \le C_{15} \ , \tag{5.2}$$

for all $1 \le k \le \ell$, where $s\cdot\ell = T$. C_{13}, C_{14} and C_{15} are positive constants that may depend on L_x, L_y, L_z, α, $\|\Phi\|_{H^4}$, M, and T but are independent of s.

Similarly, by taking the inner product of (4.2) with $\Delta^2\left(\phi^{k+1}-\phi^k\right)$ and then with $-\Delta^3\left(\phi^{k+1}-\phi^k\right)$, respectively, we obtain the following results. The details are skipped for the sake of brevity.

Lemma 5.2. *Let $M > 0$ be as previously defined. Suppose that $\Phi \in H^5_{per}$, $\phi^0 \in C^\infty_{per}$ such that $\left\|\phi^0-\Phi\right\|_{H^5} \le M$, and $\psi^0 \equiv 0$. Solutions to the numerical scheme (2.20) – (2.22) satisfy the following estimates:*

$$\left\|\phi^k\right\|_{H^5} \le C_{18} \ , \quad \left\|\psi^k\right\|_{H^2} \le C_{19} \ , \quad \left\|\frac{\psi^k-\psi^{k-1}}{s}\right\|_{H^{-1}} \le C_{20} \ , \tag{5.3}$$

for any $1 \le k \le \ell$, where $s\cdot\ell = T$. Furthermore, if $\Phi \in H^6_{per}$ and $\phi^0 \in C^\infty_{per}$ such that $\left\|\phi^0-\Phi\right\|_{H^6} \le M$ we have the estimates

$$\left\|\phi^k\right\|_{H^6} \le C_{21} \ , \quad \left\|\psi^k\right\|_{H^3} \le C_{22} \ , \quad \left\|\frac{\psi^k-\psi^{k-1}}{s}\right\|_{L^2} \le C_{23} \ , \tag{5.4}$$

for any $1 \le k \le \ell$. As usual, the constants may depend on L_x, L_y, L_z, α, $\|\Phi\|_{H^5}$, ($\|\Phi\|_{H^6}$ in the second case), M, and T but are independent of s.

Theorem 5.3. *Suppose $\Phi \in H^6_{per}$. For any $T > 0$, there exists a unique global solution $\phi(\mathbf{x},t)$ of (2.11), with*

$$\phi \in L^\infty\left(0,T;H^6_{per}\right) \ , \quad \partial_t\phi \in L^\infty\left(0,T;H^3_{per}\right) \ , \quad \partial_{tt}\phi \in L^\infty\left(0,T;L^2\right) \ , \tag{5.5}$$

and the initial conditions $\phi(\,\cdot\,,0) \equiv \Phi$ and $\partial_t\phi(\,\cdot\,,0) \equiv 0$, such that (4.1) holds in the strong sense.

Proof. We denote by ϕ_ℓ the approximation solution defined in (4.14), where $\phi^0 \in C^\infty_{per}$ and $\left\|\phi^0-\Phi\right\|_{H^6} < s < M$. By Lem. 5.2, a uniform bound is available for ϕ_ℓ in the $L^\infty\left(0,T;H^6_{per}\right)$ norm:

$$\|\phi_\ell\|_{L^\infty(0,T;H^6)} \le \frac{17}{8}C_{21} \ . \tag{5.6}$$

Regarding the temporal derivative, we see again from Lem. 5.2 that

$$\|\partial_t \phi_\ell\|_{L^\infty(0,T;H^3)} \le 2C_{22} \; . \tag{5.7}$$

Similarly, for the second order temporal derivative, it is clear that

$$\|\partial_t \psi_\ell\|_{L^\infty(0,T;L^2)} \le C_{23} \; . \tag{5.8}$$

As a result, we have the existence of a weak limit as $\ell \to \infty$ ($s \to 0$): $\phi_{\ell_n} \overset{w^*}{\rightharpoonup} \phi$ in $L^\infty\left(0,T;H^6_{per}\right)$, $\psi_{\ell_n} \overset{w^*}{\rightharpoonup} \psi$ in $L^\infty\left(0,T;H^3_{per}\right)$, and $\partial_t\psi_{\ell_n} \overset{w^*}{\rightharpoonup} \partial_t\psi$ in $L^\infty\left(0,T;L_2\right)$. We can now pass to the limit to show that the weak limit is actually a global strong solution of the MPFC equation.

Regarding the uniqueness, we note that any strong solution ϕ satisfies

$$\beta\partial_{tt}\phi + \partial_t\phi = \Delta\phi^3 + \alpha\Delta\phi + 2\Delta^2\phi + \Delta^3\phi \; , \tag{5.9}$$

in $L^\infty\left(0,T;L^2\right)$ due to the regularity of the solution. Suppose $\phi^{(1)}$, $\phi^{(2)}$ are two strong solutions with the same initial data Φ. Note also that $\partial_t\phi^{(i)}(\,\cdot\,,0) \equiv 0$, $i = 1,2$, is assumed. We set $\tilde\phi = \phi^{(1)} - \phi^{(2)}$ and arrive at

$$\beta\partial_{tt}\tilde\phi + \partial_t\tilde\phi = \Delta\left(\left(\phi^{(1)}\right)^3 - \left(\phi^{(2)}\right)^3\right) + \alpha\Delta\tilde\phi + 2\Delta^2\tilde\phi + \Delta^3\tilde\phi \; , \tag{5.10}$$

in $L^\infty\left(0,T;L^2\right)$, where $\tilde\phi(\,\cdot\,,0) = 0$. Moreover, let us denote $\tilde\psi = \psi^{(1)} - \psi^{(2)} = \partial_t\tilde\phi$ for simplicity of presentation below. Taking the inner product of (5.10) with $\tilde\psi$ in $L^2\left(0,T;L^2\right)$ gives

$$\begin{aligned}&\frac{\beta}{2}\partial_t\left\|\tilde\psi\right\|^2_{L^2} + \left\|\tilde\psi\right\|^2_{L^2} - \alpha\left(\partial_t\tilde\phi,\Delta\tilde\phi\right)_{L^2} - \left(\partial_t\tilde\phi,\Delta^3\tilde\phi\right)_{L^2}\\ &\qquad = \left(\tilde\psi,\Delta\left(\left(\phi^{(1)}\right)^3 - \left(\phi^{(2)}\right)^3\right)\right)_{L^2} + 2\left(\partial_t\tilde\phi,\Delta^2\tilde\phi\right)_{L^2} \; .\end{aligned} \tag{5.11}$$

Both the convex and concave diffusion terms can be manipulated using integration by parts:

$$-\left(\partial_t\tilde\phi,\Delta\tilde\phi\right)_{L^2} = \left(\partial_t\nabla\tilde\phi,\nabla\tilde\phi\right)_{L^2} = \frac{1}{2}\partial_t\left\|\nabla\tilde\phi\right\|^2_{L^2} \; , \tag{5.12}$$

$$-\left(\partial_t\tilde\phi,\Delta^3\tilde\phi\right)_{L^2} = \left(\partial_t\nabla\left(\Delta\tilde\phi\right),\nabla\left(\Delta\tilde\phi\right)\right)_{L^2} = \frac{1}{2}\partial_t\left\|\nabla\left(\Delta\tilde\phi\right)\right\|^2_{L^2} \; , \tag{5.13}$$

and

$$\left(\partial_t\tilde\phi,\Delta^2\tilde\phi\right)_{L^2} = \left(\partial_t\Delta\tilde\phi,\Delta\tilde\phi\right)_{L^2} = \frac{1}{2}\partial_t\left\|\Delta\tilde\phi\right\|^2_{L^2} \; . \tag{5.14}$$

Regarding the nonlinear term, we have the following estimate. The derivation is based on Lem. 3.5, by setting $\Phi = \phi^{(1)}$, $\phi = \phi^{(2)}$:

$$\begin{aligned}\left\|\Delta\left(\left(\phi^{(1)}\right)^3 - \left(\phi^{(2)}\right)^3\right)\right\|_{L^2} \le 6\Bigg\{&\left\|\phi^{(2)}\right\|^2_{L^\infty}\cdot\left\|\Delta\tilde\phi\right\|_{L^2} + \left(\left\|\phi^{(1)}\right\|_{L^\infty} + \left\|\phi^{(2)}\right\|_{L^\infty}\right)\\ &\cdot\left\|\Delta\phi^{(1)}\right\|_{L^2}\cdot\left\|\tilde\phi\right\|_{L^\infty} + \left\|\nabla\phi^{(1)}\right\|^2_{L^4}\cdot\left\|\tilde\phi\right\|_{L^\infty}\\ &+\left\|\phi^{(2)}\right\|_{L^\infty}\cdot\left(\left\|\nabla\phi^{(1)}\right\|_{L^4} + \left\|\nabla\phi^{(2)}\right\|_{L^4}\right)\cdot\left\|\nabla\tilde\phi\right\|_{L^4}\Bigg\} \; ,\end{aligned} \tag{5.15}$$

at any fixed time $0 \le t \le T$. Since both $\phi^{(1)}$ and $\phi^{(2)}$ are strong solutions of the MPFC model we have

$$\begin{aligned} \left\|\phi^{(1)}\right\|_{H^2} \ , \quad \left\|\phi^{(2)}\right\|_{H^2} &\le C_{24} \ , \\ \left\|\phi^{(1)}\right\|_{L^\infty} \ , \quad \left\|\phi^{(2)}\right\|_{L^\infty} &\le C_{24} \ , \\ \left\|\nabla\phi^{(1)}\right\|_{L^4} \ , \quad \left\|\nabla\phi^{(2)}\right\|_{L^4} &\le C_{24} \ , \end{aligned} \tag{5.16}$$

where $C_{24} > 0$ is a common bound. The substitution of these estimates into (5.15) indicates that

$$\left\|\Delta\left(\left(\phi^{(1)}\right)^3 - \left(\phi^{(2)}\right)^3\right)\right\|_{L^2} \le C_{25}\left(\left\|\tilde{\phi}\right\|_{L^\infty} + \left\|\nabla\tilde{\phi}\right\|_{L^4} + \left\|\Delta\tilde{\phi}\right\|_{L^2}\right) \ , \tag{5.17}$$

where $C_{25} := 12C_{24}^2$, for any time $0 \le t \le T$.

Observe that both the strong solutions $\phi^{(1)}$ and $\phi^{(2)}$ are conserved. This implies that the periodic function $\tilde{\phi}$ is of mean zero:

$$\int_\Omega \tilde{\phi}(\mathbf{x}, t)\, d\mathbf{x} = 0 \ , \quad \forall\ 0 \le t \le T, \tag{5.18}$$

and therefore we have the Poincare inequality

$$\left\|\tilde{\phi}\right\|_{L^2} \le C\left\|\nabla\tilde{\phi}\right\|_{L^2} \ . \tag{5.19}$$

Likewise, since derivatives are also periodic and of mean zero,

$$\left\|\nabla\tilde{\phi}\right\|_{L^2} \le C\left\|H\left(\tilde{\phi}\right)\right\|_{L^2} = C\left|\tilde{\phi}\right|_{H^2} \ . \tag{5.20}$$

Combining the estimates (5.19) and (5.20) and applying an elliptic regularity result we finally obtain

$$\left\|\tilde{\phi}\right\|_{H^2} \le C\left\|\Delta\tilde{\phi}\right\|_{L^2} \ , \tag{5.21}$$

for some constant $C > 0$ that depends only upon L_x, L_y, and L_z. Standard Sobolev imbedding results combined with the last estimate then yield

$$\left\|\tilde{\phi}\right\|_{L^\infty} \ , \quad \left\|\nabla\tilde{\phi}\right\|_{L^4} \le C\left\|\Delta\tilde{\phi}\right\|_{L^2} \ . \tag{5.22}$$

Substitution of (5.22) into (5.17) leads to

$$\left\|\Delta\left(\left(\phi^{(1)}\right)^3 - \left(\phi^{(2)}\right)^3\right)\right\|_{L^2} \le C_{26}\left\|\Delta\tilde{\phi}\right\|_{L^2} \ , \tag{5.23}$$

where $C_{26} := CC_{25}$ and C is a constant of elliptic regularity and Sobolev embedding. Subsequently, the nonlinear term can be controlled by

$$\begin{aligned} \left(\tilde{\psi}, \Delta\left(\left(\phi^{(1)}\right)^3 - \left(\phi^{(2)}\right)^3\right)\right)_{L^2} &\le C_{26}\left\|\tilde{\psi}\right\|_{L^2} \cdot \left\|\Delta\tilde{\phi}\right\|_{L^2} \\ &\le C_{27}\left(\left\|\tilde{\psi}\right\|_{L^2}^2 + \left\|\nabla\left(\Delta\tilde{\phi}\right)\right\|_{L^2}^2\right) \ , \end{aligned} \tag{5.24}$$

where $C_{27} = \max\left\{\frac{1}{2}C_{26}^2, \frac{1}{2}C^2C_{26}^2\right\}$ and C is constant from the Poincare-type estimate $\left\|\Delta\tilde{\phi}\right\|_{L^2} \le C\left\|\nabla\left(\Delta\tilde{\phi}\right)\right\|_{L^2}$, which is found arguing as above.

With an introduction of a modified energy for the difference function via

$$F_7 := \frac{\beta}{2}\left\|\tilde{\psi}\right\|_{L^2}^2 + \frac{\alpha}{2}\left\|\nabla\tilde{\phi}\right\|_{L^2}^2 + \frac{1}{2}\left\|\nabla\left(\Delta\tilde{\phi}\right)\right\|_{L^2}^2 - \left\|\Delta\tilde{\phi}\right\|_{L^2}^2, \tag{5.25}$$

we see that combination of (5.12) – (5.14) and (5.24) results in

$$\partial_t F_7(t) \le C_{27}\left\{\left\|\tilde{\psi}\right\|^2 + \left\|\nabla\left(\Delta\tilde{\phi}\right)\right\|_{L^2}^2\right\}(t)\ . \tag{5.26}$$

Integrating and using the fact that $F_7(0) = 0$ yields

$$F_7(t) \le C_{27}\int_0^t \left\{\left\|\tilde{\psi}\right\|_{L^2}^2 + \left\|\nabla\left(\Delta\tilde{\phi}\right)\right\|_{L^2}^2\right\}(s)\,ds\ . \tag{5.27}$$

We now introduce the positive part F_7:

$$F_8 := \frac{\beta}{2}\left\|\tilde{\psi}\right\|_{L^2}^2 + \frac{\alpha}{2}\left\|\nabla\tilde{\phi}\right\|^2 + \frac{1}{2}\left\|\nabla\left(\Delta\tilde{\phi}\right)\right\|_{L^2}^2 = F_7 + \left\|\Delta\tilde{\phi}\right\|_{L^2}^2\ , \tag{5.28}$$

so that (5.27) becomes

$$F_8(t) \le C_{27}\int_0^t \left\{\left\|\tilde{\psi}\right\|_{L^2}^2 + \left\|\nabla\left(\Delta\tilde{\phi}\right)\right\|_{L^2}^2\right\}(s)\,ds + \left\|\Delta\tilde{\phi}\right\|_{L^2}^2(t)\ . \tag{5.29}$$

Using Lem. 3.2 and Cauchy's inequality, the additional term $\left\|\Delta\tilde{\phi}\right\|_{L^2}^2(t)$ can be controlled by

$$\begin{aligned}\left\|\Delta\tilde{\phi}\right\|_{L^2}^2(t) &\le \frac{1}{3\epsilon^2}\left\|\tilde{\phi}\right\|_{L^2}^2(t) + \frac{2\epsilon}{3}\left\|\nabla\left(\Delta\tilde{\phi}\right)\right\|_{L^2}^2(t) \\ &\le \frac{T}{3\epsilon^2}\int_0^t \left\|\tilde{\psi}\right\|_{L^2}^2(s)\,ds + \frac{2\epsilon}{3}\left\|\nabla\left(\Delta\tilde{\phi}\right)\right\|_{L^2}^2(t)\ ,\end{aligned} \tag{5.30}$$

for any $\epsilon > 0$, where we have used the identity $\tilde{\phi}(t) = \int_0^t \tilde{\psi}(s)ds$. Taking $\alpha = \frac{3}{8}$, the substitution of the last estimate into (5.29) shows that

$$F_8(t) - \frac{1}{4}\left\|\nabla\left(\Delta\tilde{\phi}\right)\right\|_{L^2}^2(t) \le C_{28}\int_0^t \left\{\left\|\tilde{\psi}\right\|_{L^2}^2 + \left\|\nabla\left(\Delta\tilde{\phi}\right)\right\|_{L^2}^2\right\}(s)\,ds\ , \tag{5.31}$$

where $C_{28} := C_{27} + \frac{64}{3}T$. Introducing the more refined energy

$$F_9 := \frac{\beta}{2}\left\|\tilde{\psi}\right\|_{L^2}^2 + \frac{\alpha}{2}\left\|\nabla\tilde{\phi}\right\|_{L^2}^2 + \frac{1}{4}\left\|\nabla\left(\Delta\tilde{\phi}\right)\right\|_{L^2}^2 = F_8 - \frac{1}{4}\left\|\nabla\left(\Delta\tilde{\phi}\right)\right\|_{L^2}^2, \tag{5.32}$$

we arrive at

$$F_9(t) \le CC_{28}\int_0^t F_9(s)\,ds\ , \tag{5.33}$$

where $C = \max\left\{\frac{2}{\beta}, 4\right\}$. Applying Gronwall's inequality and using the fact that $F_9(0) = 0$, we conclude that $F_9(t) = 0$ for any $t > 0$. This in turn shows that

$\left\|\tilde{\phi}\right\|_{L^2}(t) = 0$ for any t, $0 \le t \le T$. Therefore, the uniqueness of the strong solution is proven. ∎

REMARK 5.4. *Similar energy estimate techniques can be applied to analyze the higher order derivatives of the solutions to our scheme (2.20) – (2.22). As a result, a bound for ϕ, $\psi = \partial_t \phi$, $\partial_t \psi = \partial_{tt}\phi$, in the norms of $L^\infty\left(0,T;H^{m+6}_{per}\right)$, $L^\infty\left(0,T;H^{m+3}_{per}\right)$ and $L^\infty\left(0,T;H^{m}_{per}\right)$, respectively, could be obtained, for any integer $m \ge 0$. Passing to the limit as $s \to 0$ does not cause any difficulty. As a result, a unique global smooth solution exists for any smooth initial data.*

6. Summary. The 3-D Modified Phase Field Crystal (MPFC) equation, a generalized damped wave equation for which the parabolic Phase Field Crystal (PFC) equation is a special case, was analyzed in detail. A time-discrete numerical scheme (2.20) – (2.22) (equivalent form in (4.2)) based on a convex splitting for the functional energy (2.9), was utilized to construct an approximate solution (4.14), which was then shown to ultimately converge to a solution of the MPFC equation as the time step size approaches zero.

Specifically, we showed that the pseudo energy (2.14) of the numerical solution ϕ^k was non-increasing from one time step to the next thanks to the structure of the convex-splitting scheme (2.20) – (2.22). Consequently, we obtained a uniform bound of the energy (2.9) of the numerical solution ϕ^k, and as an immediate result, in Lem. 4.2 we obtained a bound of the $L^\infty(0,T;H^2_{per})$ norm of the numerical solution. In Lems. 4.3, 5.1, and 5.2, we obtained more refined energy estimates for ϕ^k and it first and second temporal backward differences in the $L^\infty(0,T;H^{m+3}_{per})$, $L^\infty(0,T;H^{m}_{per})$ and $L^\infty(0,T;H^{m-3}_{per})$ norms, respectively, for $m = 0,1,2,3$. In particular, these estimates were obtained by taking the inner product of the numerical scheme with $(-\Delta)^m(\phi^{k+1}-\phi^k)$. The uniform bounds of the numerical solutions in turn resulted in a global weak solution ($m = 0$, Thm. 4.4) and a unique global strong solution ($m = 3$, Thm. 5.3) when we passed to the limit as the time step size approaches zero. We argued that a global smooth solution could be established by obtaining estimates for arbitrarily large values of m.

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Appendix A. Proof of Lemma 4.3. In this appendix we prove Lem. 4.3. We begin by taking the inner product of (4.2) with $\phi^{k+1}-\phi^k$, which gives

$$\begin{aligned}
&\frac{\beta}{s^2}\left(\phi^{k+1}-2\phi^k+\phi^{k-1},\phi^{k+1}-\phi^k\right)_{L^2} + \frac{1}{s}\left(\phi^{k+1}-\phi^k,\phi^{k+1}-\phi^k\right)_{L^2} \\
&\quad = \left(\Delta\left(\phi^{k+1}\right)^3,\phi^{k+1}-\phi^k\right)_{L^2} + \alpha\left(\Delta\phi^{k+1},\phi^{k+1}-\phi^k\right)_{L^2} \\
&\qquad +2\left(\Delta^2\phi^k,\phi^{k+1}-\phi^k\right)_{L^2} + \left(\Delta^3\phi^{k+1},\phi^{k+1}-\phi^k\right)_{L^2} \; . \qquad \text{(A.1)}
\end{aligned}$$

The first two terms can be handled in the following way:

$$\begin{aligned}
\frac{1}{s^2}\left(\phi^{k+1}-2\phi^k+\phi^{k-1},\phi^{k+1}-\phi^k\right)_{L^2} &= \left(\psi^{k+1}-\psi^k,\psi^{k+1}\right)_{L^2} \\
&= \frac{1}{2}\left(\left\|\psi^{k+1}\right\|^2_{L^2} - \left\|\psi^k\right\|^2_{L^2}\right) + \frac{1}{2}\left\|\psi^{k+1}-\psi^k\right\|^2_{L^2} \\
&\ge \frac{1}{2}\left(\left\|\psi^{k+1}\right\|^2_{L^2} - \left\|\psi^k\right\|^2_{L^2}\right) \; , \qquad \text{(A.2)}
\end{aligned}$$

and

$$\frac{1}{s}\left(\phi^{k+1}-\phi^k,\phi^{k+1}-\phi^k\right)_{L^2} = s\left\|\psi^{k+1}\right\|_{L^2}^2 \geq 0 \ . \tag{A.3}$$

Similarly, integration-by-parts using periodic boundary conditions can be applied to analyze the convex and concave diffusion terms.

$$\begin{aligned}
-\left(\Delta\phi^{k+1},\phi^{k+1}-\phi^k\right)_{L^2} &= \left(\nabla\phi^{k+1},\nabla(\phi^{k+1}-\phi^k)\right)_{L^2} \\
&= \frac{1}{2}\left(\left\|\nabla\phi^{k+1}\right\|_{L^2}^2 - \left\|\nabla\phi^k\right\|_{L^2}^2\right) + \frac{1}{2}\left\|\nabla\left(\phi^{k+1}-\phi^k\right)\right\|_{L^2}^2 \\
&\geq \frac{1}{2}\left(\left\|\nabla\phi^{k+1}\right\|_{L^2}^2 - \left\|\nabla\phi^k\right\|_{L^2}^2\right) \ , \qquad \text{(A.4)}
\end{aligned}$$

$$\begin{aligned}
-\left(\Delta^3\phi^{k+1},\phi^{k+1}-\phi^k\right)_{L^2} &= \left(\nabla\left(\Delta\phi^{k+1}\right),\nabla\left(\Delta\left(\phi^{k+1}-\phi^k\right)\right)\right)_{L^2} \\
&= \frac{1}{2}\left(\left\|\nabla\left(\Delta\phi^{k+1}\right)\right\|_{L^2}^2 - \left\|\nabla\left(\Delta\phi^k\right)\right\|_{L^2}^2\right) \\
&\qquad + \frac{1}{2}\left\|\nabla\left(\Delta\left(\phi^{k+1}-\phi^k\right)\right)\right\|_{L^2}^2 \\
&\geq \frac{1}{2}\left(\left\|\nabla\left(\Delta\phi^{k+1}\right)\right\|_{L^2}^2 - \left\|\nabla\left(\Delta\phi^k\right)\right\|_{L^2}^2\right) \ , \qquad \text{(A.5)}
\end{aligned}$$

and

$$\begin{aligned}
-\left(\Delta^2\phi^k,\phi^{k+1}-\phi^k\right)_{L^2} &= -\left(\Delta\phi^k,\Delta\left(\phi^{k+1}-\phi^k\right)\right)_{L^2} \\
&= -\frac{1}{2}\left(\left\|\Delta\phi^{k+1}\right\|_{L^2}^2 - \left\|\Delta\phi^k\right\|_{L^2}^2\right) + \frac{1}{2}\left\|\Delta\left(\phi^{k+1}-\phi^k\right)\right\|_{L^2}^2 \\
&\geq -\frac{1}{2}\left(\left\|\Delta\phi^{k+1}\right\|_{L^2}^2 - \left\|\Delta\phi^k\right\|_{L^2}^2\right) \ . \qquad \text{(A.6)}
\end{aligned}$$

Regarding the nonlinear term, using Lem. 3.3 we find

$$\left\|\Delta\left(\phi^{k+1}\right)^3\right\|_{L^2} \leq 3C_5^2C_4 + 6C_5C_6^2 := C_{11} \ . \tag{A.7}$$

As a direct consequence, we have

$$\begin{aligned}
\left(\Delta\left(\phi^{k+1}\right)^3,\phi^{k+1}-\phi^k\right)_{L^2} &\leq s\left\|\Delta\left(\phi^{k+1}\right)^3\right\|_{L^2}\cdot\left\|\psi^{k+1}\right\|_{L^2} \\
&\leq \frac{s}{2}C_{11}^2 + \frac{s}{2}\left\|\psi^{k+1}\right\|_{L^2}^2 \ . \qquad \text{(A.8)}
\end{aligned}$$

Let us now define a modified energy via

$$F_1^k := \frac{\beta}{2}\left\|\psi^k\right\|_{L^2}^2 + \frac{\alpha}{2}\left\|\nabla\phi^k\right\|_{L^2}^2 + \frac{1}{2}\left\|\nabla\left(\Delta\phi^k\right)\right\|_{L^2}^2 - \left\|\Delta\phi^k\right\|_{L^2}^2 \ . \tag{A.9}$$

A combination of (A.2) – (A.6), (A.8), and (A.1) results in

$$F_1^{k+1} - F_1^k \leq \frac{s}{2}\left\|\psi^{k+1}\right\|_{L^2}^2 + \frac{s}{2}C_{11}^2 \ . \tag{A.10}$$

Summing over k and using $F_1^0 \leq C\left\|\phi^0\right\|_{H^3}^2$ (since $\psi^0 \equiv 0$) yields

$$F_1^\ell \leq C\left\|\phi^0\right\|_{H^3}^2 + \frac{T}{2}C_{11}^2 + \frac{s}{2}\sum_{k=1}^{\ell}\left\|\psi^k\right\|_{L^2}^2 \ . \tag{A.11}$$

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

$$\begin{aligned} F_2^k &:= \frac{\beta}{2}\left\|\psi^k\right\|_{L^2}^2 + \frac{\alpha}{2}\left\|\nabla\phi^k\right\|_{L^2}^2 + \frac{1}{2}\left\|\nabla\left(\Delta\phi^k\right)\right\|_{L^2}^2 \\ &= F_1^k + \left\|\Delta\phi^k\right\|_{L^2}^2 \ , \end{aligned} \tag{A.12}$$

so that (A.11) becomes

$$F_2^\ell \le C\left\|\phi^0\right\|_{H^3}^2 + \frac{T}{2}C_{11}^2 + \frac{s}{2}\sum_{k=1}^{\ell}\left\|\psi^k\right\|_{L^2}^2 + \left\|\Delta\phi^\ell\right\|_{L^2}^2 \ . \tag{A.13}$$

Using Lem. 3.2, the additional term $\left\|\Delta\phi^\ell\right\|_{L^2}^2$ can be controlled by

$$\left\|\Delta\phi^\ell\right\|_{L^2}^2 \le \frac{1}{3\epsilon^2}\left\|\phi^\ell\right\|_{L^2}^2 + \frac{2\epsilon}{3}\left\|\nabla\left(\Delta\phi^\ell\right)\right\|_{L^2}^2 \le \frac{C_4^2}{3\epsilon^2} + \frac{2\epsilon}{3}\left\|\nabla\left(\Delta\phi^\ell\right)\right\|_{L^2}^2 \ , \tag{A.14}$$

for any $\epsilon > 0$. Taking $\epsilon = \frac{3}{8}$, the substitution of the last estimate into (A.13) shows that

$$F_2^\ell - \frac{1}{4}\left\|\nabla\left(\Delta\phi^\ell\right)\right\|_{L^2}^2 \le C\left\|\phi^0\right\|_{H^3}^2 + \frac{T}{2}C_{11}^2 + \frac{64}{27}C_4^2 + \frac{s}{2}\sum_{k=1}^{\ell}\left\|\psi^k\right\|_{L^2}^2 \ . \tag{A.15}$$

Introducing the more refined energy

$$\begin{aligned} F_3^k &:= \frac{\beta}{2}\left\|\psi^k\right\|_{L^2}^2 + \frac{\alpha}{2}\left\|\nabla\phi^k\right\|_{L^2}^2 + \frac{1}{4}\left\|\nabla\left(\Delta\phi^k\right)\right\|_{L^2}^2 \\ &= F_2^k - \frac{1}{4}\left\|\nabla\left(\Delta\phi^k\right)\right\|_{L^2}^2 \ , \end{aligned} \tag{A.16}$$

we arrive at

$$F_3^\ell \le \frac{s}{2\beta}\sum_{k=1}^{\ell}F_3^k + C\left(\left\|\Phi\right\|_{H^3}^2 + M\right)^2 + \frac{T}{2}C_{11}^2 + \frac{64}{27}C_4^2 \ . \tag{A.17}$$

Applying a discrete Grownwall inequality gives

$$F_3^\ell \le C_{12} \ , \tag{A.18}$$

where C_{12} is a positive constant that is dependent upon T (exponentially), L_x, L_y, L_z, α, $\|\Phi\|_{H^3}$, and M, but is independent of s. Using an elliptic regularity result we have

$$\left\|\phi^\ell\right\|_{H^3}^2 \le C\left(\left\|\phi^\ell\right\|_{H^2}^2 + \left\|\nabla\left(\Delta\phi^\ell\right)\right\|_{L^2}^2\right) \le C(C_4^2 + 4C_{12}) \ , \tag{A.19}$$

and the first part of the lemma is proven by taking $C_8 := \sqrt{C(C_4^2 + 4C_{12})}$.

Furthermore, the a-priori bound (A.18) shows that

$$\left\|\psi^k\right\|_{L^2} \le \sqrt{\frac{2C_{12}}{\beta}} := C_9 \ , \tag{A.20}$$

for any k, $1 \le k \le \ell$, and the second part of the lemma is proven. For the third part, using (4.2), we estimate as follows:

$$\begin{aligned}
\left\| \frac{\psi^{k+1}-\psi^k}{s} \right\|_{H^{-3}} &\le \frac{1}{\beta}\Big\{ \left\| \Delta \left(\phi^{k+1}\right)^3 \right\|_{H^{-3}} + \alpha \left\|\Delta\phi^{k+1}\right\|_{H^{-3}} + 2\left\|\Delta^2\phi^k\right\|_{H^{-3}} \\
&\quad + \left\|\Delta^3\phi^{k+1}\right\|_{H^{-3}} + \left\|\psi^{k+1}\right\|_{H^{-3}} \Big\} \\
&\le \frac{1}{\beta}\Big\{ \left\| \Delta (\phi^{k+1})^3 \right\|_{L^2} + \alpha \left\|\Delta\phi^{k+1}\right\|_{L^2} + 2\left\|\Delta^2\phi^k\right\|_{H^{-1}} \\
&\quad + \left\|\Delta^3\phi^{k+1}\right\|_{H^{-3}} + \left\|\psi^{k+1}\right\|_{L^2} \Big\} \\
&\le \frac{1}{\beta}\left(C_{11} + (\alpha+3)C_8 + C_9\right) := C_{10} \ , \qquad \text{(A.21)}
\end{aligned}$$

for any k, $1 \le k \le \ell$. Thus the third part of the lemma is proven, and the proof of Lem. 4.3 is complete.

Appendix B. Proof of Lemma 5.1. In this appendix we prove Lem. 5.1. We begin by testing (4.2) with $-\Delta\left(\phi^{k+1}-\phi^k\right)$, which gives

$$\begin{aligned}
-\frac{\beta}{s^2}\left(\phi^{k+1}-2\phi^k+\phi^{k-1}, \Delta(\phi^{k+1}-\phi^k)\right)_{L^2} - \frac{1}{s}\left(\phi^{k+1}-\phi^k, \Delta\left(\phi^{k+1}-\phi^k\right)\right)_{L^2} \\
= -\left(\Delta\left(\left(\phi^{k+1}\right)^3\right), \Delta\left(\phi^{k+1}-\phi^k\right)\right)_{L^2} - \alpha\left(\Delta\phi^{k+1}, \Delta\left(\phi^{k+1}-\phi^k\right)\right)_{L^2} \\
-2\left(\Delta^2\phi^k, \Delta\left(\phi^{k+1}-\phi^k\right)\right)_{L^2} - \left(\Delta^3\phi^{k+1}, \Delta\left(\phi^{k+1}-\phi^k\right)\right)_{L^2} \ . \qquad \text{(B.1)}
\end{aligned}$$

The first two terms can be handled in the same way as in (A.2) – (A.3), and the details are skipped:

$$\text{(B.2)} \quad -\frac{1}{s^2}\left(\phi^{k+1}-2\phi^k+\phi^{k-1}, \Delta\left(\phi^{k+1}-\phi^k\right)\right)_{L^2} \ge \frac{1}{2}\left(\left\|\nabla\psi^{k+1}\right\|_{L^2}^2 - \left\|\nabla\psi^k\right\|_{L^2}^2\right)$$

and

$$\text{(B.3)} \qquad -\frac{1}{s}\left(\phi^{k+1}-\phi^k, \Delta\left(\phi^{k+1}-\phi^k\right)\right)_{L^2} = s\left\|\nabla\psi^{k+1}\right\|_{L^2}^2 \ge 0 \ .$$

Similarly, integration-by-parts using periodic boundary conditions can be applied to analyze the convex and concave diffusion terms as in (A.4) – (A.6):

$$\text{(B.4)} \qquad \left(\Delta\phi^{k+1}, \Delta\left(\phi^{k+1}-\phi^k\right)\right)_{L^2} \ge \frac{1}{2}\left(\left\|\Delta\phi^{k+1}\right\|_{L^2}^2 - \left\|\Delta\phi^k\right\|_{L^2}^2\right) \ ,$$

$$\text{(B.5)} \qquad \left(\Delta^3\phi^{k+1}, \Delta\left(\phi^{k+1}-\phi^k\right)\right)_{L^2} \ge \frac{1}{2}\left(\left\|\Delta^2\phi^{k+1}\right\|_{L^2}^2 - \left\|\Delta^2\phi^k\right\|_{L^2}^2\right) \ ,$$

and

$$\text{(B.6)} \qquad \left(\Delta^2\phi^k, \Delta\left(\phi^{k+1}-\phi^k\right)\right)_{L^2} \ge -\frac{1}{2}\left(\left\|\nabla\left(\Delta\phi^{k+1}\right)\right\|_{L^2}^2 - \left\|\nabla\left(\Delta\phi^k\right)\right\|_{L^2}^2\right) \ .$$

For the nonlinear term, we start from an integration by parts:

$$\text{(B.7)} \quad -\left(\Delta\left(\phi^{k+1}\right)^3, \Delta\left(\phi^{k+1}-\phi^k\right)\right)_{L^2} = \left(\nabla\left(\Delta\left(\phi^{k+1}\right)^3\right), \nabla\left(\phi^{k+1}-\phi^k\right)\right)_{L^2} \ .$$

Using Lems. 3.4, 4.2, and 4.3 and standard Sobolev imbedding results, we have

$$\begin{aligned}\left\|\nabla\left(\Delta\left(\phi^{k+1}\right)^3\right)\right\|_{L^2} &\le 6CC_5C_8C_4+3CC_5^2C_8 \\ &\quad +6CC_8C_6^2+12CC_5C_8C_4 := C_{16}\ ,\end{aligned}\tag{B.8}$$

where $C>0$ is our generic imbedding constant. Going back to (B.7), we obtain

$$-\left(\Delta\left(\phi^{k+1}\right)^3,\Delta\left(\phi^{k+1}-\phi^k\right)\right)_{L^2}\le\frac{s}{2}\left\|\nabla\psi^{k+1}\right\|_{L^2}^2+\frac{s}{2}C_{16}^2\ .\tag{B.9}$$

To proceed with an $L_s^\infty(0,T;H_{per}^4)$ analysis for the numerical solution, we introduce a modified energy:

$$F_4^k:=\frac{\beta}{2}\left\|\nabla\psi^k\right\|_{L^2}^2+\frac{\alpha}{2}\left\|\Delta\phi^k\right\|_{L^2}^2+\frac{1}{2}\left\|\Delta^2\phi^k\right\|_{L^2}^2-\left\|\nabla\left(\Delta\phi^k\right)\right\|_{L^2}^2\ .\tag{B.10}$$

A combination of (B.1) – (B.6), and (B.9) results in

$$F_4^{k+1}-F_4^k\le\frac{s}{2}\left\|\nabla\psi^{k+1}\right\|_{L^2}^2+\frac{s}{2}C_{16}^2\ .\tag{B.11}$$

Summing over k and using $F_4\left(\phi^0\right)\le C\left\|\phi^0\right\|_{H^4}^2$ (since $\psi^0\equiv 0$) yields

$$F_4^\ell\le C\left\|\phi^0\right\|_{H^4}^2+\frac{T}{2}C_{16}^2+\frac{s}{2}\sum_{k=1}^{\ell}\left\|\nabla\psi^k\right\|_{L^2}^2\ .\tag{B.12}$$

We now introduce the positive part F_4:

$$\begin{aligned}F_5^k &:= \frac{\beta}{2}\left\|\nabla\psi^k\right\|_{L^2}^2+\frac{\alpha}{2}\left\|\Delta\phi^k\right\|_{L^2}^2+\frac{1}{2}\left\|\Delta^2\phi^k\right\|_{L^2}^2 \\ &= F_4^k+\left\|\nabla\left(\Delta\phi^k\right)\right\|_{L^2}^2\ ,\end{aligned}\tag{B.13}$$

so that (B.12) becomes

$$F_5^\ell\le C\left\|\phi^0\right\|_{H^4}^2+\frac{T}{2}C_{16}^2+\frac{s}{2}\sum_{k=1}^{\ell}\left\|\nabla\psi^k\right\|_{L^2}^2+\left\|\nabla\left(\Delta\phi^\ell\right)\right\|_{L^2}^2\ .\tag{B.14}$$

The term $\left\|\nabla\left(\Delta\phi^\ell\right)\right\|_{L^2}^2$ can be controlled by an application of Cauchy's inequality:

$$\begin{aligned}\left\|\nabla\left(\Delta\phi^\ell\right)\right\|_{L^2}^2=-\left(\Delta\phi^\ell,\Delta^2\phi^\ell\right)_{L^2} &\le \frac{1}{4}\left\|\Delta^2\phi^\ell\right\|_{L^2}^2+\left\|\Delta\phi^\ell\right\|_{L^2}^2 \\ &\le \frac{1}{4}\left\|\Delta^2\phi^\ell\right\|_{L^2}^2+C_4^2\ ,\end{aligned}\tag{B.15}$$

in which the a-priori estimate (4.6) was utilized in the last step. Going back to (B.14) yields

$$F_5^\ell-\frac{1}{4}\left\|\Delta^2\phi^\ell\right\|_{L^2}^2\le C\left\|\phi^0\right\|_{H^4}^2+\frac{T}{2}C_{16}^2+C_4^2+\frac{s}{2}\sum_{k=1}^{\ell}\left\|\nabla\psi^k\right\|_{L^2}^2\ .\tag{B.16}$$

Introducing the more refined energy

$$\begin{aligned}F_6^k &:= \frac{\beta}{2}\left\|\nabla\psi^k\right\|_{L^2}^2+\frac{\alpha}{2}\left\|\Delta\phi^k\right\|_{L^2}^2+\frac{1}{4}\left\|\Delta^2\phi^k\right\|_{L^2}^2 \\ &= F_5^k-\frac{1}{4}\left\|\Delta^2\phi^k\right\|_{L^2}^2,\end{aligned}\tag{B.17}$$

we arrive at

$$F_6^\ell \le \frac{s}{2\beta}\sum_{k=1}^{\ell} F_6^k + C\left(\|\Phi\|_{H^4} + M\right)^2 + \frac{T}{2}C_{16}^2 + C_4^2 \ , \tag{B.18}$$

Applying a discrete Grownwall inequality gives

$$F_6^\ell \le C_{17} \ , \tag{B.19}$$

where C_{17} is a positive constant that is dependent upon T (exponentially), L_x, L_y, L_z, α, $\|\Phi\|_{H^3}$, and M, but is independent of s. Using an elliptic regularity result we have

$$\left\|\phi^\ell\right\|_{H^4}^2 \le C\left(\left\|\phi^\ell\right\|_{H^3}^2 + \left\|\Delta^2\phi^\ell\right\|_{L^2}^2\right) \le C(C_8^2 + 4C_{17}) \ , \tag{B.20}$$

and the first part of the lemma is proven by taking $C_{13} := \sqrt{C(C_8^2 + 4C_{17})}$.

The second estimate of (5.2) comes from a simple calculation:

$$\left\|\nabla\psi^k\right\|_{L^2} \le \sqrt{\frac{2F_6^k}{\beta}} \le \sqrt{\frac{2C_{17}}{\beta}} := C_{14} \ . \tag{B.21}$$

The third estimate of (5.2) comes from a calculation like that in (A.21). This concludes the proof of Lem. 5.1.

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