#### **RESEARCH ARTICLE**

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# A second-order energy stable backward differentiation formula method for the epitaxial thin film equation with slope selection

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#### KEYWORDS

convergence analysis, energy stability, fast Fourier transform, finite differences, nonlinear conjugate gradient, p-Laplacian operator, preconditioners, second-order-in-time, steepest descent, thin film epitaxy

# 1 | INTRODUCTION

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In this article, we will devise and analyze a numerical scheme for the epitaxial thin film model with slope selection, or, for short, just the slope selection (SS) equation. This equation is the gradient flow with respect to the energy

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

where  $\Omega = (0, L_x) \times (0, L_y)$ ,  $\phi : \Omega \to \mathbb{R}$  is the height of the thin film and  $\varepsilon$  is a constant that represents the width of the rounded corners on the otherwise faceted crystalline thin films. As is common, and natural, we will assume that  $\phi$  is  $\Omega$ -periodic. The corresponding chemical potential is defined to be the variational derivative of the energy (1.1), that is,

$$\mu := \delta_{\phi} F = -\nabla \cdot (|\nabla \phi|^2 \nabla \phi) + \Delta \phi + \varepsilon^2 \Delta^2 \phi.$$
(1.2)

The SS equation is the  $L^2$  gradient flow associated with the energy (1.1):

$$\partial_t \phi = -\mu = \nabla \cdot (|\nabla \phi|^2 \nabla \phi) - \Delta \phi - \varepsilon^2 \Delta^2 \phi.$$
(1.3)

Models similar to this were studied by Aviles and Giga as a special case of smectic liquid crystals in [1]. The limiting energy (as  $\varepsilon \rightarrow 0$ ) and the singularities of  $\nabla \phi$  were analyzed therein. As then it has attracted considerable attention in several related fields. In [2], this SS energy functional was used to describe those patterns and shapes formed in buckling-driven thin film blisters. In [3], Gioia and Ortiz reviewed the experimental observations of blister morphologies and the models on delamination of compressed thin films. In [4], this functional was viewed as a singular perturbation problem to study the limiting energy. In [5], the similarity between this model and the magnetization energy was observed and used to study the asymptotic limit of a family of functionals related to micro-magnetism theory.

In the thin film context, the energy of the SS equation can be considered as two distinct parts. The first part is

$$F_{\rm ES}[\phi] := \int_{\Omega} \frac{1}{4} \left( |\nabla \phi|^2 - 1 \right)^2 \mathrm{d}\mathbf{x},\tag{1.4}$$

which describes, in some coarse-grained sense, the Ehrlich-Schwoebel effect–the phenomenon where atoms tend to move from a lower terrace to an upper terrace in the growth of atomic steps, promoting surface instability. Mathematically, the term  $F_{ES}$  gives the energetic preference for epitaxial films with slope satisfying  $|\nabla \phi| = 1$ , as this represents the minima of  $F_{ES}$ . The second part,

$$F_{\rm SD}[\phi] = \int_{\Omega} \frac{\varepsilon^2}{2} (\Delta \phi)^2 d\mathbf{x}, \qquad (1.5)$$

represents surface diffusion, which promotes rounded corners in the film. A smaller value of  $\varepsilon$  corresponds to a sharper, less rounded corner. There are some interesting physical predictions coming from the SS model; for instance, the surface roughness is predicted to grow approximately at a rate proportional to  $t^{1/3}$ ; and the energy decays at a rate approximately proportional to  $t^{-1/3}$  [6]. The saturation time scale (for periodic domains) is expected to be on the order of  $\varepsilon^{-2}$  [7]. Energy stable schemes with

higher order temporal accuracy have always been highly desirable because these processes are realized only in the sense of very large times.

There have been several works focused on second-order-in-time schemes for the SS equation in recent years. In [8], the authors proposed a hybrid scheme, one which combined a second-order backward differentiation for the time derivative term and a second-order extrapolation for the explicit treatment of the nonlinear term. A linear stabilization parameter A has to be sufficiently large to guarantee the energy dissipation law for this scheme. A theoretical justification of the lower bound for A has been derived for the first order scheme in [9] for related gradient flow models. Such an analysis for a similar second-order-in-time scheme for the Cahn-Hilliard equation has been provided in [10]. The extension of such an analysis to the SS equation is expected to be available, with the lower bound of A singularly dependent on  $\varepsilon^{-1}$ . As an alternate approach, a second-order-in-time operator splitting scheme was proposed for the SS equation in [11], in which the nonlinear part is solved using the fourthorder central difference approximation combined with the third-order explicit Runge-Kutta method. The corresponding convergence analysis was provided in [12]. Similar operator splitting ideas can also be found in a recent work [13]. Some other second-order-in-time numerical approaches were reported in recent years, such as a linearized finite difference scheme in [14], an adaptive time-stepping strategy with Crank-Nicolson (CN) formulas in [15], the BDF and the CN formulas with invariant energy quadratization (IEQ) strategy proposed in [16]. However, IEQ methods often suffer from spurious oscillations in the numerical solutions, unless small time step sizes are used, due to the introduction of an intermediate variable that has only weak stability control [17]. This may be expected for other linearized auxiliary variable methods as well [17].

It is expected that significantly more spatiotemporal accuracy is achieved by keeping as much of the PDE operator implicit as possible, even if the difficult terms are nonlinear or nonpositive [18]. Furthermore, it is observed that long-time energy stability could not be theoretically justified for many of these numerical works, due to the explicit treatment for the nonlinear terms. In the existing literature, the only second-order-in-time numerical algorithm for the SS equation (1.3) with a long time energy stability could be found in [19], in which modified Crank-Nicolson approximations are used for the nonlinear four-Laplacian term and the surface diffusion term, while an explicit extrapolation formula is applied to the concave diffusion term, respectively. As a result, an unconditional energy stability is derived via a careful energy estimate. Conversely, due to the complicated form of the nonlinear term involved with the CN approximation, constructing efficient solvers for the scheme remains a challenge.

Any numerical scheme that treats the nonlinear terms implicitly—for the purposes of accuracy or stability, or both—requires one to solve a regularized four-Laplacian-type equation, where the highest-order term is a linear biharmonic operator. Consequently, an efficient solver for a regularized p-Laplacian equation has always been highly desirable. In a recent work [20], a preconditioned steepest descent (PSD) algorithm was proposed for such problems. At each iteration stage, only a purely linear elliptic equation needs to be solved to obtain a search direction, and the numerical efficiency for such an elliptic equation could be greatly improved with the use of FFT-based solvers. In turn, an optimization in the given search direction becomes one-dimensional, with its well-posedness assured by convexity arguments. Moreover, a geometric convergence of such an iteration could be theoretically derived, so that a great improvement of the numerical efficiency is justified, in comparison with an application of the Polak-Ribiére variant of NCG (nonlinear conjugate gradient) method [21], reported in [19, 22].

The PSD algorithm has been very efficiently applied to the first order energy stable scheme for the SS equation, as reported in [20]. However, its application to the CN version of the second-order energy stable scheme—what we will call the CN-ES scheme, proposed in [19]—faces some theoretical questions. These difficulties come from a subtle fact that the approximation to the four-Laplacian term in the CN-ES does not correspond to a convex energy functional. In this article, we propose a second order BDF scheme for the SS Equation 1.3, so that the unique solvability, energy stability could

be theoretically derived, and the PSD solver could be efficiently applied. In more details, an alternate second order energy stable scheme is proposed, based on the second-order BDF temporal approximation framework. The second-order BDF scheme treats and approximates every term at the time step  $t^{k+1}$  (instead of the time instant  $t^{k+1/2}$ ): a second-order BDF three-point stencil is applied in the temporal derivative approximation, the nonlinear term and the surface diffusion terms are updated implicitly for their strong convexities, and a second-order accurate, explicit extrapolation formula is applied in the approximation of the concave diffusion term. Such a structure makes the numerical scheme uniquely solvable. In addition, to ensure the energy stability of the numerical scheme, we need to add a second order Douglas-Dupont regularization, in the form of  $-A\tau\Delta(\phi^{k+1} - \phi^k)$ . We prove that under a mild requirement  $A \ge \frac{1}{16}$ , rigorous energy stability is guaranteed.

In fact, the second-order accurate, energy stable BDF scheme for the Cahn-Hilliard model was analyzed in a recent article [23] with similar ideas. In particular, the nonlinear solver required for the BDF scheme is reported to require 20 to 25% less computational effort than that for the Crank-Nicolson version, due to the simpler form and stronger convexity properties of the nonlinear term. For the SS equation (1.3), a much greater improvement (in terms of numerical efficiency) is expected for the BDF approach, due to the more complicated form of the four-Laplacian term. This is observed in our testing. Based on the unconditional energy stability, we derive an  $\ell^{\infty}(0, T; H_{per}^2)$  stability for the numerical solution. In turn, with the help of Sobolev embedding from  $H_{per}^2$  into  $W^{1,6}$ , we prove the convergence of the proposed scheme.

The remainder of the article is organized as follows. In Section 2, we present the discrete spatial difference operators, function space, inner products and norms, define the proposed second-order-intime fully discrete finite difference scheme and prove that the scheme is unconditionally stable and uniquely solvable, provide that the stabilized parameter  $A \ge 1/16$ . In Section 3, we provide a rigorous convergence analysis and error estimate for the proposed scheme. The preconditioned steepest descent solver and preconditioned nonlinear conjugate gradient solver is outlined in Sections 4.1 and 4.2, respectively. Finally, numerical experiments are presented Section 5, and some concluding remarks are given in Section 6.

## 2 | THE FULLY DISCRETE SCHEME WITH FINITE DIFFERENCE SPATIAL DISCRETIZATION IN 2D

### 2.1 | Notation

In this section, we define the discrete spatial difference operators, function spaces, inner products and norms, following the notation used in [7, 19, 20, 22, 24, 25]. Let  $\Omega = (0, L_x) \times (0, L_y)$ , where, for simplicity of presentation, we assume  $L_x = L_y =: L > 0$ . We write  $L = m \cdot h$ , where *m* is a positive integer. The parameter  $h = \frac{L}{m}$  is called the mesh or grid spacing. We define the following two uniforms, infinite grids with grid spacing h > 0:

$$E := \left\{ x_{i+\frac{1}{2}} \mid i \in \mathbb{Z} \right\}, \quad C := \left\{ x_i \mid i \in \mathbb{Z} \right\},$$

where  $x_i = x(i) := (i - \frac{1}{2}) \cdot h$ . Consider the following 2D discrete periodic function spaces:

$$\begin{split} \mathcal{V}_{\text{per}} &:= \left\{ \upsilon : E \times E \to \mathbb{R} \mid \upsilon_{i+\frac{1}{2},j+\frac{1}{2}} = \upsilon_{i+\frac{1}{2}+\alpha \cdot m,j+\frac{1}{2}+\beta \cdot m}, \; \forall i,j,\alpha,\beta \in \mathbb{Z} \right\}, \\ \mathcal{C}_{\text{per}} &:= \left\{ \upsilon : C \times C \to \mathbb{R} \mid \upsilon_{i,j} = \upsilon_{i+\alpha \cdot m,j+\beta \cdot m}, \; \forall i,j,\alpha,\beta \in \mathbb{Z} \right\}, \\ \mathcal{E}_{\text{per}}^{\text{ew}} &:= \left\{ \upsilon : E \times C \to \mathbb{R} \mid \upsilon_{i+\frac{1}{2},j} = \upsilon_{i+\frac{1}{2}+\alpha \cdot m,j+\beta \cdot m}, \; \forall i,j,\alpha,\beta \in \mathbb{Z} \right\}, \end{split}$$

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$$\mathcal{E}_{\text{per}}^{\text{ns}} := \left\{ \nu : C \times E \to \mathbb{R} \mid \nu_{ij+\frac{1}{2}} = \nu_{i+\alpha \cdot m j+\frac{1}{2}+\beta \cdot m}, \, \forall i, j, \alpha, \beta \in \mathbb{Z} \right\}.$$

The functions of  $\mathcal{V}_{per}$  are called *vertex centered functions*; those of  $\mathcal{C}_{per}$  are called *cell centered functions*. The functions of  $\mathcal{E}_{per}^{ew}$  are called *east-west edge-centered functions*, and the functions of  $\mathcal{E}_{per}^{ns}$  are called *north-south edge-centered functions*. We also define the mean zero space

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$$\mathring{\mathcal{C}}_{\mathrm{per}} := \left\{ \upsilon \in \mathcal{C}_{\mathrm{per}} \; \middle| \; \frac{h^2}{L^2} \sum_{i,j=1}^m \upsilon_{i,j} =: \overline{\upsilon} = 0 \right\}.$$

We now introduce the important average and difference operators on the spaces:

$$\begin{split} A_{x} v_{i+\frac{1}{2},\Box} &:= \frac{1}{2} \left( v_{i+1,\Box} + v_{i,\Box} \right), \quad D_{x} v_{i+\frac{1}{2},\Box} &:= \frac{1}{h} \left( v_{i+1,\Box} - v_{i,\Box} \right), \\ A_{y} v_{\Box,i+\frac{1}{2}} &:= \frac{1}{2} \left( v_{\Box,i+1} + v_{\Box,i} \right), \quad D_{y} v_{\Box,i+\frac{1}{2}} &:= \frac{1}{h} \left( v_{\Box,i+1} - v_{\Box,i} \right), \end{split}$$

with  $A_x, D_x : \mathcal{C}_{per} \to \mathcal{E}_{per}^{ew}$  if  $\Box$  is an integer, and  $A_x, D_x : \mathcal{E}_{per}^{ns} \to \mathcal{V}_{per}$  if  $\Box$  is a half-integer, with  $A_y, D_y : \mathcal{C}_{per} \to \mathcal{E}_{per}^{ns}$  if  $\Box$  is an integer, and  $A_y, D_y : \mathcal{E}_{per}^{ew} \to \mathcal{V}_{per}$  if  $\Box$  is a half-integer. Likewise,

$$\begin{aligned} a_{x} \mathbf{v}_{i,\Box} &:= \frac{1}{2} \left( \mathbf{v}_{i+\frac{1}{2},\Box} + \mathbf{v}_{i-\frac{1}{2},\Box} \right), \quad d_{x} \mathbf{v}_{i,\Box} &:= \frac{1}{h} \left( \mathbf{v}_{i+\frac{1}{2},\Box} - \mathbf{v}_{i-\frac{1}{2},\Box} \right), \\ a_{y} \mathbf{v}_{\Box,j} &:= \frac{1}{2} \left( \mathbf{v}_{\Box,j+\frac{1}{2}} + \mathbf{v}_{\Box,j-\frac{1}{2}} \right), \quad d_{y} \mathbf{v}_{\Box,j} &:= \frac{1}{h} \left( \mathbf{v}_{\Box,j+\frac{1}{2}} - \mathbf{v}_{\Box,j-\frac{1}{2}} \right), \end{aligned}$$

with  $a_x, d_x : \mathcal{E}_{per}^{ew} \to \mathcal{C}_{per}$  if  $\Box$  is an integer, and  $a_x, d_x : \mathcal{V}_{per} \to \mathcal{E}_{per}^{ns}$  if  $\Box$  is a half-integer; and with  $a_y, d_y : \mathcal{E}_{per}^{ns} \to \mathcal{C}_{per}$  if  $\Box$  is an integer, and  $a_y, d_y : \mathcal{V}_{per} \to \mathcal{E}_{per}^{ew}$  if  $\Box$  is a half-integer.

Also define the 2D center-to-vertex derivatives  $\mathfrak{D}_x, \mathfrak{D}_y : \mathcal{C}_{per} \to \mathcal{V}_{per}$  component-wise as

$$\begin{split} \mathfrak{D}_{x} \mathfrak{v}_{i+\frac{1}{2}j+\frac{1}{2}} &:= A_{y}(D_{x}\mathfrak{v})_{i+\frac{1}{2}j+\frac{1}{2}} = D_{x}(A_{y}\mathfrak{v})_{i+\frac{1}{2}j+\frac{1}{2}} \\ &= \frac{1}{2h} \left( \mathfrak{v}_{i+1,j+1} - \mathfrak{v}_{i,j+1} + \mathfrak{v}_{i+1,j} - \mathfrak{v}_{i,j} \right), \\ \mathfrak{D}_{y} \mathfrak{v}_{i+\frac{1}{2}j+\frac{1}{2}} &:= A_{x}(D_{y}\mathfrak{v})_{i+\frac{1}{2}j+\frac{1}{2}} = D_{y}(A_{x}\mathfrak{v})_{i+\frac{1}{2}j+\frac{1}{2}} \\ &= \frac{1}{2h} \left( \mathfrak{v}_{i+1,j+1} - \mathfrak{v}_{i+1,j} + \mathfrak{v}_{i,j+1} - \mathfrak{v}_{i,j} \right). \end{split}$$

The utility of these definitions is that the differences  $\mathfrak{D}_x$  and  $\mathfrak{D}_y$  are collocated on the grid, unlike  $D_x, D_y$ . We denote the 2D vertex-to-center derivatives  $\mathfrak{d}_x, \mathfrak{d}_y : \mathcal{V}_{per} \to \mathcal{C}_{per}$  component-wise as

$$\begin{aligned} \mathfrak{d}_{x} \mathfrak{v}_{i,j} &:= a_{y}(d_{x}\mathfrak{v})_{i,j} = d_{x}(a_{y}\mathfrak{v})_{i,j} \\ &= \frac{1}{2h} \left( \mathfrak{v}_{i+\frac{1}{2},j+\frac{1}{2}} - \mathfrak{v}_{i-\frac{1}{2},j+\frac{1}{2}} + \mathfrak{v}_{i+\frac{1}{2},j-\frac{1}{2}} - \mathfrak{v}_{i-\frac{1}{2},j-\frac{1}{2}} \right), \\ \mathfrak{d}_{y} \mathfrak{v}_{i,j} &:= a_{x}(d_{y}\mathfrak{v})_{i,j} = d_{y}(a_{x}\mathfrak{v})_{i,j} \\ &= \frac{1}{2h} \left( \mathfrak{v}_{i+\frac{1}{2},j+\frac{1}{2}} - \mathfrak{v}_{i+\frac{1}{2},j-\frac{1}{2}} + \mathfrak{v}_{i-\frac{1}{2},j+\frac{1}{2}} - \mathfrak{v}_{i-\frac{1}{2},j-\frac{1}{2}} \right). \end{aligned}$$

In turn, the discrete gradient operator,  $\nabla_h^{\mathsf{v}}: \mathcal{C}_{\mathsf{per}} \to \mathcal{V}_{\mathsf{per}} \times \mathcal{V}_{\mathsf{per}}$ , is defined as

$$\nabla_{h}^{\mathsf{v}} \mathfrak{v}_{i+\frac{1}{2},j+\frac{1}{2}} := \left(\mathfrak{D}_{x} \mathfrak{v}_{i+\frac{1}{2},j+\frac{1}{2}}, \mathfrak{D}_{y} \mathfrak{v}_{i+\frac{1}{2},j+\frac{1}{2}}\right).$$

The standard 2D discrete Laplacian,  $\Delta_h : C_{per} \to C_{per}$ , is given by

$$\Delta_h v_{ij} := d_x (D_x v)_{ij} + d_y (D_y v)_{ij} = \frac{1}{h^2} \left( v_{i+1,j} + v_{i-1,j} + v_{i,j+1} + v_{i,j-1} - 4 v_{i,j} \right).$$

The 2D vertex-to-center average,  $\mathcal{A}: \mathcal{V}_{per} \rightarrow \mathcal{C}_{per}$ , is defined to be

$$\mathcal{A}v_{i,j} := \frac{1}{4} \left( v_{i+1,j} + v_{i-1,j} + v_{i,j+1} + v_{i,j-1} \right).$$

The 2D skew Laplacian,  $\Delta_h^{\mathsf{v}} : \mathcal{C}_{\mathsf{per}} \to \mathcal{C}_{\mathsf{per}}$ , is defined as

$$\begin{split} \Delta_h^{\mathsf{v}} \mathfrak{v}_{i,j} &= \mathfrak{d}_x(\mathfrak{D}_x \mathfrak{v})_{i,j} + \mathfrak{d}_y(\mathfrak{D}_y \mathfrak{v})_{i,j} \\ &= \frac{1}{2h^2} \left( \mathfrak{v}_{i+1,j+1} + \mathfrak{v}_{i-1,j+1} + \mathfrak{v}_{i+1,j-1} + \mathfrak{v}_{i-1,j-1} - 4\mathfrak{v}_{i,j} \right). \end{split}$$

For  $p \ge 2$ , the 2D discrete p-Laplacian operator is defined as

$$\nabla_{h}^{\mathsf{v}} \cdot \left( \left| \nabla_{h}^{\mathsf{v}} \upsilon \right|^{p-2} \nabla_{h}^{\mathsf{v}} \upsilon \right)_{ij} := \mathfrak{d}_{x} (r \mathfrak{D}_{x} \upsilon)_{i,j} + \mathfrak{d}_{y} (r \mathfrak{D}_{y} \upsilon)_{i,j},$$

with

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$$r_{i+\frac{1}{2},j+\frac{1}{2}} := \left[ \left(\mathfrak{D}_{x}u\right)_{i+\frac{1}{2},j+\frac{1}{2}}^{2} + \left(\mathfrak{D}_{y}u\right)_{i+\frac{1}{2},j+\frac{1}{2}}^{2} \right]^{\frac{p-2}{2}}.$$

Clearly, for p = 2,  $\Delta_h^{\mathsf{v}} v = \nabla_h^{\mathsf{v}} \cdot (|\nabla_h^{\mathsf{v}} v|^{p-2} \nabla_h^{\mathsf{v}} v)$ .

Now, we are ready to introduce the following grid inner products:

$$\begin{split} (\mathfrak{v},\xi)_2 &:= h^2 \sum_{i,j=1}^m \mathfrak{v}_{i,j} \psi_{i,j}, \quad \mathfrak{v}, \xi \in \mathcal{C}_{\text{per}}, \\ \langle \mathfrak{v}, \xi \rangle &:= (\mathcal{A}(\mathfrak{v}\xi), 1)_2, \quad \mathfrak{v}, \xi \in \mathcal{V}_{\text{per}}, \\ [\mathfrak{v},\xi]_{\text{ew}} &:= (A_x(\mathfrak{v}\xi), 1)_2, \quad \mathfrak{v}, \xi \in \mathcal{E}_{\text{per}}^{\text{ew}}, \\ [\mathfrak{v},\xi]_{\text{ns}} &:= \left(A_y(\mathfrak{v}\xi), 1\right)_2, \quad \mathfrak{v}, \xi \in \mathcal{E}_{\text{per}}^{\text{ns}}. \end{split}$$

We now define the following norms for cell-centered functions. If  $v \in C_{per}$ , then  $||v||_2^2 := (v, v)_2$ ;  $||v||_p^p := (|v|^p, 1)_2 (1 \le p < \infty)$ , and  $||v||_{\infty} := \max_{1 \le i,j \le m} |v_{i,j}|$ . Similarly, we define the gradient norms: for  $v \in C_{per}$ ,

$$\|\nabla_{h}^{\mathsf{v}}\upsilon\|_{p}^{p} := \langle |\nabla_{h}^{\mathsf{v}}\upsilon|^{p}, 1\rangle, \quad |\nabla_{h}^{\mathsf{v}}\upsilon|^{p} := [(\mathfrak{D}_{x}\upsilon)^{2} + (\mathfrak{D}_{y}\upsilon)^{2}]^{\frac{p}{2}} = [\nabla_{h}^{\mathsf{v}}\upsilon \cdot \nabla_{h}^{\mathsf{v}}\upsilon]^{\frac{p}{2}} \in \mathcal{V}_{\text{per}}, \quad 2 \le p < \infty,$$

and

$$\|\nabla_h v\|_2^2 := [D_x v, D_x v]_{\text{ew}} + [D_y v, D_y v]_{\text{ns}}.$$

The discrete  $\|\cdot\|_{H_h^1}$  and  $\|\cdot\|_{H_h^2}$  norms on periodic boundary domain defined as

$$\|\phi\|_{H_h^1}^2 := \|\phi\|_2^2 + \|\nabla_h \phi\|_2^2, \tag{2.1}$$

$$\|\phi\|_{H_h^2}^2 := \|\phi\|_{H_h^1}^2 + \|\Delta_h \phi\|_2^2.$$
(2.2)

**Lemma 2.1** For any  $\phi \in C_{per}$ , we have

$$\|\nabla_h \varphi\|_2^2 \ge \|\nabla_h^{\mathsf{v}} \varphi\|_2^2. \tag{2.3}$$

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*Proof* By the definition of  $\mathfrak{D}_x \phi$ , we get

$$\mathfrak{D}_x \phi_{i+\frac{1}{2}j+\frac{1}{2}} = \frac{1}{2} \left( (D_x \phi)_{i+\frac{1}{2}j} + (D_x \phi)_{i+\frac{1}{2}j+1} \right), \tag{2.4}$$

which in turn implies that

$$\|\mathfrak{D}_{x}\phi\|_{2}^{2} := h^{2} \sum_{i,j=0}^{m-1} \left(\mathfrak{D}_{x}\phi_{i+\frac{1}{2},j+\frac{1}{2}}\right)^{2} \le h^{2} \sum_{i,j=0}^{m-1} \left(D_{x}\phi_{i+\frac{1}{2},j}\right)^{2},$$
(2.5)

that is

$$\|\mathfrak{D}_x\phi\|_2 \le \|D_x\phi\|_2. \tag{2.6}$$

Likewise, we can also obtain  $\|\mathfrak{D}_y\phi\|_2 \leq \|D_y\phi\|_2$ . These two inequalities lead to the desired estimate; the proof of Lemma. 2.1 is complete.

The following preliminary estimates are needed in the convergence analysis presented in later sections; the detailed proof is left to Appendix A.

**Proposition 2.2** For any  $\phi \in C_{per}$  with  $\overline{\phi} = 0$ , we have

$$\|\Delta_h \phi\|_2^2 \ge C_1 \|\phi\|_{H^2_{\mu}}^2, \tag{2.7}$$

$$\|\phi\|_{\infty} \le C \|\phi\|_{H^2_h},\tag{2.8}$$

$$\|\phi\|_{W_{h}^{1,6}} := \|\phi\|_{6} + \|\nabla_{h}^{\mathsf{v}}\phi\|_{6} \le C \|\phi\|_{H_{h}^{2}}, \tag{2.9}$$

with *C* and  $C_1$  only dependent on  $\Omega$ .

### 2.2 | The fully discrete scheme

Let  $M \in \mathbb{Z}^+$ , and set s := T/M, where T is the final time. We define the mass-conservative grid projection operator  $\mathsf{P}_h: C^0_{\mathsf{per}}(\Omega) \to \mathcal{C}_{\mathsf{per}}$  via

$$[\mathsf{P}_h v]_{i,j} = v(\xi_i, \xi_j) + \alpha_v,$$

where  $\alpha_{\nu}$  is chosen so that

$$\int_{\Omega} v(\mathbf{x}) d\mathbf{x} = (1, \mathsf{P}_h v)_2.$$

We denote by  $\phi_e$  the exact solution to the SS equation (1.3) and take  $\Phi^{\ell} = \mathsf{P}_h \phi_e(\cdot, t_{\ell})$ . With the machinery in last subsection, our second-order-in-time BDF (BDF2-ES) type scheme can be formulated as follows: for  $k \ge 1$ , given  $\phi^{k-1}, \phi^k \in \mathcal{C}_{per}$ , find  $\phi^{k+1} \in \mathcal{C}_{per}$  such that

$$\frac{3\phi^{k+1} - 4\phi^k + \phi^{k-1}}{2s} = \nabla_h^{\mathsf{v}} \cdot (|\nabla_h^{\mathsf{v}}\phi^{k+1}|^2 \nabla_h^{\mathsf{v}}\phi^{k+1}) - \Delta_h^{\mathsf{v}}(2\phi^k - \phi^{k-1}) - As\Delta_h^2(\phi^{k+1} - \phi^k) - \varepsilon^2 \Delta_h^2 \phi^{k+1}, \qquad (2.10)$$

where  $\phi^0 := \Phi^0$ ,  $\phi^1 := \Phi^1$  and *A* is the constant stability coefficient. The SS equation (1.3) is mass conservative, and it is easy see that the numerical Scheme 2.10 is mass conservative at a discrete level. For simplicity of presentation, we assume that  $\overline{\phi^0} = \overline{\phi^1} = 0$ , so that  $\overline{\phi^k} = 0$ , for any  $k \ge 2$ , where, for spatially discrete functions,  $\overline{\phi} := \frac{1}{m^2} \sum_{i,j=1}^m \phi_{i,j}$ .

We now introduce a discrete energy that is consistent with the continuous space energy (1.1) as  $h \to 0$ . In particular, the discrete energy  $F_h : C_{per} \to \mathbb{R}$  is defined as:

$$F_{h}[\phi] = \frac{1}{4} \|\nabla_{h}^{\mathsf{v}}\phi\|_{4}^{4} - \frac{1}{2} \|\nabla_{h}^{\mathsf{v}}\phi\|_{2}^{2} + \frac{1}{2}\varepsilon^{2} \|\Delta_{h}\phi\|_{2}^{2}.$$
(2.11)

*Remark* 2.3 We note that  $\|\nabla_h^{\mathsf{v}}\phi\|_p = 0$  does not imply that  $\phi$  is a constant. (A checkerboard function has norm zero). This defect of the skew stencil is not a concern in the present context as the highest order norm in the energy uses a standard stencil.

We also define a modified numerical energy  $\tilde{F}_h : \mathcal{C}_{per} \to \mathbb{R}$  via

$$\tilde{F}_{h}[\phi,\psi] := F_{h}(\phi) + \frac{1}{4s} \|\phi - \psi\|_{2}^{2} + \frac{1}{2} \|\nabla_{h}(\phi - \psi)\|_{2}^{2}.$$
(2.12)

It is clear that

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$$\tilde{F}_h[\Phi^\ell, \Phi^{\ell-1}] \to F[\phi_e(t)],$$

as  $h, s \to 0$ , for a sufficiently regular spatially  $\Omega$ -periodic solution  $\phi_e$ . Although we cannot guarantee that the energy  $F_h$  is nonincreasing in time, we are able to prove the dissipation of auxiliary energy  $\tilde{F}_h$ . The unique solvability and the unconditional energy stability of Scheme 2.10 is assured by the following theorem.

**Theorem 2.4** Suppose that the exact solution  $\phi_e$  is periodic, mean-zero, and sufficiently regular, and  $\phi^0$ ,  $\phi^1 \in C_{per}$  is obtained via mass-conservative projection, as defined above. Given any  $(\phi^{k-1}, \phi^k) \in C_{per}$ , there is a unique solution  $\phi^{k+1} \in C_{per}$  to the Scheme 2.10. The Scheme 2.10, with starting values  $\phi^0$  and  $\phi^1$ , is unconditionally energy stable, that is, for any s > 0 and h > 0, and any positive integer  $2 \le k \le M - 1$ , The numerical Scheme 2.10 has the following energy-decay property:

$$\tilde{F}_h(\phi^{k+1}, \phi^k) \le \tilde{F}_h(\phi^k, \phi^{k-1}) \le \dots \le \tilde{F}_h(\phi^1, \phi^0) \le C_0,$$
(2.13)

for all  $A \ge \frac{1}{16}$ , where  $C_0 > is$  a constant independent of s, h, and T.

*Proof* The unique solvability follows from a convexity argument, and we omit it for the sake of brevity. For the energy stability, taking an inner product with (2.10) by  $\phi^{k+1} - \phi^k$  yields

$$0 = \left(\frac{3\phi^{k+1} - 4\phi^k + \phi^{k-1}}{2s}, \phi^{k+1} - \phi^k\right) - (\nabla_h^{\mathsf{v}} \cdot (|\nabla_h^{\mathsf{v}}\phi^{k+1}|^2 \nabla_h^{\mathsf{v}}\phi^{k+1}), \phi^{k+1} - \phi^k) + (\Delta_h^{\mathsf{v}}(2\phi^k - \phi^{k-1}), \phi^{k+1} - \phi^k) + As(\Delta_h^2(\phi^{k+1} - \phi^k), \phi^{k+1} - \phi^k) + \varepsilon^2(\Delta_h^2\phi^{k+1}, \phi^{k+1} - \phi^k) := I_1 + I_2 + I_3 + I_4 + I_5.$$
(2.14)

We now establish the estimates for  $I_1, \dots, I_5$ . The temporal difference term could be evaluated as follows

$$\left(\frac{3\phi^{k+1} - 4\phi^k + \phi^{k-1}}{2s}, \phi^{k+1} - \phi^k\right) \ge \frac{1}{s} \left(\frac{5}{4} \|\phi^{k+1} - \phi^k\|_2^2 - \frac{1}{4} \|\phi^k - \phi^{k-1}\|_2^2\right).$$
(2.15)

For the four-Laplacian term, we have

$$\left( -\nabla_{h}^{\mathsf{v}} \cdot (|\nabla_{h}^{\mathsf{v}} \varphi^{k+1}|^{2} \nabla_{h}^{\mathsf{v}} \varphi^{k+1}), \varphi^{k+1} - \varphi^{k} \right) = \left( |\nabla_{h}^{\mathsf{v}} \varphi^{k+1}|^{2} \nabla_{h}^{\mathsf{v}} \varphi^{k+1}, \nabla_{h}^{\mathsf{v}} (\varphi^{k+1} - \varphi^{k}) \right)$$

$$\geq \frac{1}{4} \left( \|\nabla_{h}^{\mathsf{v}} \varphi^{k+1}\|_{4}^{4} - \|\nabla_{h}^{\mathsf{v}} \varphi^{k}\|_{4}^{4} \right).$$

$$(2.16)$$

For the concave diffusive term, the following estimate is valid

$$\begin{split} \left(\Delta_{h}^{\mathsf{v}}(2\varphi^{k}-\varphi^{k-1}),\varphi^{k+1}-\varphi^{k}\right) &= -\left(\nabla_{h}^{\mathsf{v}}(2\varphi^{k}-\varphi^{k-1}),\nabla_{h}^{\mathsf{v}}(\varphi^{k+1}-\varphi^{k})\right) \\ &= -\left(\nabla_{h}^{\mathsf{v}}\varphi^{k},\nabla_{h}^{\mathsf{v}}(\varphi^{k+1}-\varphi^{k})\right) - \left(\nabla_{h}^{\mathsf{v}}(\varphi^{k}-\varphi^{k-1}),\nabla_{h}^{\mathsf{v}}(\varphi^{k+1}-\varphi^{k})\right) \\ &= -\frac{1}{2}\|\nabla_{h}^{\mathsf{v}}\varphi^{k+1}\|_{2}^{2} + \frac{1}{2}\|\nabla_{h}^{\mathsf{v}}\varphi^{k}\|_{2}^{2} + \frac{1}{2}\|\nabla_{h}^{\mathsf{v}}(\varphi^{k+1}-\varphi^{k})\|_{2}^{2} - \left(\nabla_{h}^{\mathsf{v}}(\varphi^{k}-\varphi^{k-1}),\nabla_{h}^{\mathsf{v}}(\varphi^{k+1}-\varphi^{k})\right) \\ &\geq -\frac{1}{2}\left(\|\nabla_{h}^{\mathsf{v}}\varphi^{k+1}\|_{2}^{2} - \|\nabla_{h}^{\mathsf{v}}\varphi^{k}\|_{2}^{2}\right) - \frac{1}{2}\|\nabla_{h}^{\mathsf{v}}(\varphi^{k}-\varphi^{k-1})\|_{2}^{2} \\ &\geq -\frac{1}{2}\left(\|\nabla_{h}^{\mathsf{v}}\varphi^{k+1}\|_{2}^{2} - \|\nabla_{h}^{\mathsf{v}}\varphi^{k}\|_{2}^{2}\right) - \frac{1}{2}\|\nabla_{h}(\varphi^{k}-\varphi^{k-1})\|_{2}^{2}, \end{split}$$
(2.17)

where the last step applied the Lemma 2.1.

For the surface diffusion term, we have

$$\left(\Delta_{h}^{2}\phi^{k+1},\phi^{k+1}-\phi^{k}\right) = \left(\Delta_{h}\phi^{k+1},\Delta_{h}(\phi^{k+1}-\phi^{k})\right) \geq \frac{1}{2}\left(\|\Delta_{h}\phi^{k+1}\|_{2}^{2}-\|\Delta_{h}\phi^{k}\|_{2}^{2}\right).$$
(2.18)

Similarly, the following identity is valid for the stabilizing term:

$$s\left(\Delta_{h}^{2}(\phi^{k+1} - \phi^{k}), \phi^{k+1} - \phi^{k}\right) = s \|\Delta_{h}(\phi^{k+1} - \phi^{k})\|_{2}^{2}.$$
(2.19)

Meanwhile, an application of Cauchy inequality indicates the following estimate:

$$\frac{1}{s} \|\phi^{k+1} - \phi^k\|_2^2 + As \|\Delta_h(\phi^{k+1} - \phi^k)\|_2^2 \ge 2A^{1/2} \|\nabla_h(\phi^{k+1} - \phi^k)\|_2^2.$$
(2.20)

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Therefore, a combination of (2.15-2.17) and (2.20) yields

$$F_{h}(\phi^{k+1}) - F_{h}(\phi^{k}) + \frac{1}{4s} \left( \|\phi^{k+1} - \phi^{k}\|_{2}^{2} - \|\phi^{k} - \phi^{k-1}\|_{2}^{2} \right) + \frac{1}{2} \left( \|\nabla_{h}(\phi^{k+1} - \phi^{k})\|_{2}^{2} - \|\nabla_{h}(\phi^{k} - \phi^{k-1})\|_{2}^{2} \right) \leq \left( -2A^{1/2} + \frac{1}{2} \right) \|\nabla_{h}(\phi^{k+1} - \phi^{k})\|_{2}^{2} \leq 0,$$
(2.21)

provided that  $A \ge \frac{1}{16}$ . Then the proof follows from the definition of the  $\tilde{F}_h$  in (2.12).

*Remark* 2.5 There is another epitaxial thin film growth model, namely, the no-slope-selection (NSS) equation that has attracted some attention over the years. Consider the following energy functional:

$$E[\phi] := \int_{\Omega} \left( -\frac{1}{2} \ln(1 + |\nabla \phi|^2) + \frac{\varepsilon^2}{2} (\Delta \phi)^2 \right) \mathrm{d}\mathbf{x}.$$
 (2.22)

The NSS dynamical equation is the  $L^2$  gradient flow with respect to this energy:

$$\partial_t \phi = -\mu, \quad \mu := \delta_{\phi} E = \nabla \cdot \left( \frac{\nabla \phi}{1 + |\nabla \phi|^2} \right) + \varepsilon^2 \Delta^2 \phi.$$
 (2.23)

Some previous works have described and analyzed second-order accurate energy stable numerical schemes for the NSS equation (2.23). In particular, it has been demonstrated in two recent works [26, 27] that, as the nonlinear term has automatically  $L^{\infty}$ -bounded higher order derivatives in this model, either a linear scheme or a linear iteration algorithm could be efficiently designed for the NSS equation (2.23), with energy stability theoretically justified. In other words, the logarithmic nature of the energy functional for the NSS model enables one to derive linear schemes to obtain second order temporal accuracy and energy stability, so that a complicated nonlinear solver may be avoided.

*Remark* 2.6 The idea of the proposed Scheme 2.10, the BDF temporal approximation combined with a second-order Douglas-Dupont regularization, may provide a framework for a more general class of gradient flows, specifically, those with *p*-Laplacian nonlinear terms involved. For example, the square phase field crystal (SPFC) equation [28–31] models crystal dynamics at the atomic scale in space but on diffusive scales in time, while keeping "square" symmetry crystal lattice structures. This model is an  $H^{-1}$  gradient flow of an energy functional containing a four-Laplacian energy density. As another example, for the functionalized Cahn-Hilliard model [32–38] a convex–concave decomposition for the corresponding energy functional has been revealed in a recent work [24], in which a four-Laplacian term appears in the convex part. For these related models, the numerical approach of this article could be extended to obtain second order accurate, energy stable numerical schemes, and the preconditioned steepest descent and preconditioned nonlinear conjugate gradient solvers, which will be outlined in Sections 4.1 and 4.2, could be efficiently applied.

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*Remark* 2.7 The stability property established in Theorem 2.4 is in terms of a modified energy functional, as given by (2.12), which contains the original energy functional, combined with two non-negative numerical corrections terms. In turn, the stability estimate for such a modified energy functional indicates a uniform in time bound for the original energy (at a discrete level), and such a bound is uniform in  $\varepsilon$ . Similar estimates could be derived for the second order energy stable scheme [19], based on the Crank-Nicolson approach. These uniform bounds for the original energy functional will play an essential role in the convergence analysis.

In comparison, there has been other work of second order energy stable schemes for the SS equation [16], with the invariant energy quadratization (IEQ) approach applied. Meanwhile, we notice that, an alternate variable, denoted as a second order approximation to  $v = |\nabla \phi|^2 - 1$ , has been introduced in the IEQ approach, and the energy stability is in terms of a pair of numerical variables ( $\phi$ , v). Conversely, an  $\varepsilon$ -independent bound for the original energy functional is not available for this scheme. Furthermore, the authors of [17] have observed spurious oscillation is the numerical solutions of some IEQ schemes. This is due to the fact that the stability of the variable v is only quite weak.

*Remark* 2.8 It is clear that a fully implicit treatment for the four-Laplacian term is needed in (2.10) to pass through the stability analysis, due to its convexity property. Meanwhile, if the coefficient term, namely  $|\nabla_h^v \phi^{k+1}|^2$ , is replaced by an explicit extrapolation one, such as  $|\nabla_h^v (2\phi^k - \phi^{k-1})|^2$ , the unique solvability could still be established, due to its positivity, while a theoretical justification of the energy stability is not directly available. We believe the stability analysis reported in [10] could be similarly applied for this (variable-coefficient) linear scheme, with a different lower bound requirement for A, expected to be singularly dependent on  $\varepsilon^{-1}$ . The technical details are left to interested readers.

## 2.3 + $\ell^{\infty}(0,T;H_h^2)$ stability of the numerical scheme

The  $\ell^{\infty}(0, T; H_h^2)$  bound of the numerical solution could be derived based on the modified energy stability (2.13).

**Theorem 2.9** Let  $\phi \in C_{\Omega}$ , then the  $\ell^{\infty}(0, T; H_h^2)$  bound of the numerical solution is as follows:

$$\|\phi\|_{H_{h}^{2}} \leq \sqrt{2\frac{C_{0} + |\Omega|}{C_{1}\varepsilon^{2}}} := C_{2}, \qquad (2.24)$$

where  $C_2$  is independent of s, h, and T.

Proof As

$$\frac{1}{8}\psi^4 - \frac{1}{2}\psi^2 \ge -\frac{1}{2},\tag{2.25}$$

then we have

$$\frac{1}{8} \|\nabla_{h}^{\mathsf{v}} \phi\|_{4}^{4} - \frac{1}{2} \|\nabla_{h}^{\mathsf{v}} \phi\|_{2}^{2} \ge -\frac{1}{2} |\Omega|, \qquad (2.26)$$

with the discrete  $H_h^1$  norm introduced in (2.1). Then we arrive at the following bound, for any  $\phi \in C_{\Omega}$ :

$$F_{h}(\phi) \geq \frac{1}{8} \|\nabla_{h}^{\mathsf{v}} \phi\|_{4}^{4} + \frac{\varepsilon^{2}}{2} \|\Delta_{h} \phi\|_{2}^{2} - \frac{1}{2} |\Omega|$$
  

$$\geq \frac{1}{2} \|\nabla_{h}^{\mathsf{v}} \phi\|_{2}^{2} + \frac{\varepsilon^{2}}{2} \|\Delta_{h} \phi\|_{2}^{2} - |\Omega|$$
  

$$\geq \frac{\varepsilon^{2}}{2} \|\Delta_{h} \phi\|_{2}^{2} - |\Omega|$$
  

$$\geq \frac{1}{2} C_{1} \varepsilon^{2} \|\phi\|_{H_{h}^{2}}^{2} - |\Omega|, \qquad (2.27)$$

in which  $C_1$  is a constant associated with the discrete elliptic regularity:  $\|\Delta_h \phi\|_2^2 \ge C_1 \|\phi\|_{H_h^2}^2$ , as stated in (2.7) of Proposition 2.2. Consequently, its combination with (2.12) finishes the proof.

*Remark* 2.10 Note that the constant C<sub>2</sub> is independent of s, h, and T, but does depends on  $\varepsilon$ . In particular,  $C_2 = O(\varepsilon^{-1})$ .

*Remark* 2.11 As a further consequence of the  $H_h^2$  bound (2.24), we are able to obtain an  $\ell^{\infty}$  estimate for the numerical solution

$$\|\phi^m\|_{\infty} \le C \|\phi^m\|_{H^2_r} \le CC_2, \quad \forall m \ge 0,$$
 (2.28)

in which the first inequality comes from a discrete Sobolev inequality,  $||f||_{\infty} \leq C ||f||_{H_h^2}$ , as given by (2.9) in Proposition 2.2.

In addition to the  $\|\cdot\|_{\infty}$  bound for the phase variable, a discrete  $W^{1,\infty}$  estimate could be derived through a more careful analysis. In more details, by taking a discrete inner product with (2.10) by  $-\Delta_h^3 \phi^{k+1}$ , performing a nonlinear estimate, we are able to derive an  $\ell^{\infty}(0, T; H_h^3)$  estimate for the numerical solution, following similar ideas as in [39]. Subsequently, the discrete  $W^{1,\infty}$  bound comes from a similar discrete Sobolev inequality:  $\|f\|_{\infty} + \|\nabla_h f\|_{\infty} \leq C \|f\|_{H_h^3}$ .

## **3 | CONVERGENCE ANALYSIS AND ERROR ESTIMATE**

#### 3.1 | Error equations and consistency analysis

A detailed Taylor expansion implies the following truncation error:

$$\frac{3\Phi^{k+1} - 4\Phi^k + \Phi^{k-1}}{2s} = \nabla_h^{\mathsf{v}} \cdot (|\nabla_h^{\mathsf{v}} \Phi^{k+1}|^2 \nabla_h^{\mathsf{v}} \Phi^{k+1}) - \Delta_h^{\mathsf{v}} (2\Phi^k - \Phi^{k-1}) - As\Delta_h^2 (\Phi^{k+1} - \Phi^k) - \varepsilon^2 \Delta_h^2 \Phi^{k+1} + \tau^k,$$
(3.1)

with  $\|\tau^k\|_2 \le C(h^2 + s^2)$ . Consequently, with an introduction of the error function

$$e^{k} = \Phi^{k} - \phi^{k}, \quad \forall k \ge 0, \tag{3.2}$$

we get the following evolutionary equation, by subtracting (2.10) from (3.1):

$$\frac{3e^{k+1} - 4e^k + e^{k-1}}{2s} = \nabla_h^{\mathsf{v}} \cdot (|\nabla_h^{\mathsf{v}} \Phi^{k+1}|^2 \nabla_h^{\mathsf{v}} \Phi^{k+1} - |\nabla_h^{\mathsf{v}} \phi^{k+1}|^2 \nabla_h^{\mathsf{v}} \phi^{k+1}) - \Delta_h^{\mathsf{v}} (2e^k - e^{k-1}) - As \Delta_h^2 (e^{k+1} - e^k) - \varepsilon^2 \Delta_h^2 e^{k+1} + \tau^k,$$
(3.3)

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In addition, from the PDE analysis for the SS equation in [40, 44] and the global in time  $H_h^2$  stability (2.24) for the numerical solution, we also get the  $\ell^{\infty}$ ,  $W^{1.6}$ , and  $H_h^2$  bounds for both the exact solution and numerical solution, uniform in time:

$$\|\Phi^{k}\|_{\infty}, \|\Phi^{k}\|_{W^{1,6}}, \|\Phi^{k}\|_{H^{2}_{h}} \leq C_{3}, \quad \|\phi^{k}\|_{\infty}, \|\phi^{k}\|_{W^{1,6}}, \|\phi^{k}\|_{H^{2}_{h}} \leq C_{3}, \quad \forall k \geq 0,$$
(3.4)

where the 3D embeddings of  $H_h^2$  into  $\ell^{\infty}$  and into  $W^{1,6}$  have been applied, as well as the discrete Sobolev embedding inequalities (2.8), (2.9) in Proposition 2.2.

#### 3.1.1 | Stability and convergence analysis

The convergence result is stated in the following theorem.

**Theorem 3.1** Let  $\Phi \in \mathcal{R}$  be the projection of the exact periodic solution of the SS equation (1.3) with the initial data  $\phi^0 := \Phi^0 \in H^2_{per}(\Omega)$ ,  $\phi^1 := \Phi^1 \in H^2_{per}(\Omega)$ , and the regularity class

$$\mathcal{R} = H^3(0, T; C^0(\Omega)) \cap H^2(0, T; C^2(\Omega)) \cap H^1(0, T; C^4(\Omega)) \cap L^\infty(0, T; C^6(\Omega)).$$
(3.5)

Suppose  $\phi$  is the fully discrete solution of (2.10). Then, the following convergence result holds as s, h goes to zero:

$$\|e^{k}\|_{2} + \left(\frac{3}{16}\varepsilon^{2}s\sum_{\ell=0}^{k}\|\Delta_{h}e^{\ell}\|^{2}\right)^{1/2} \le C(s^{2}+h^{2}),$$
(3.6)

where the constant C > 0 is independent of s and h.

*Proof* Taking an inner product with the numerical error Equation 3.3 by  $e^{k+1}$  gives

$$0 = \left(\frac{3e^{k+1} - 4e^k + e^{k-1}}{2s}, e^{k+1}\right) + \left(|\nabla_h^{\mathsf{v}} \Phi^{k+1}|^2 \nabla_h^{\mathsf{v}} \Phi^{k+1} - |\nabla_h^{\mathsf{v}} \varphi^{k+1}|^2 \nabla_h^{\mathsf{v}} \varphi^{k+1}, \nabla_h^{\mathsf{v}} e^{k+1}\right) - \left(\nabla_h^{\mathsf{v}} (2e^k - e^{k-1}), \nabla_h^{\mathsf{v}} e^{k+1}\right) + As \left(\Delta_h (e^{k+1} - e^k), \Delta_h e^{k+1}\right) + \varepsilon^2 \left(\Delta_h e^{k+1}, \Delta_h e^{k+1}\right) - \left(\tau^k, e^{k+1}\right) =: J_1 + J_2 + J_3 + J_4 + J_5 + J_6.$$
(3.7)

For the time difference error term  $J_1$ ,

$$\left(\frac{3e^{k+1} - 4e^k + e^{k-1}}{2s}, e^{k+1}\right) = \frac{3}{4s} \|e^{k+1}\|_2^2 - \frac{1}{s} \|e^k\|_2^2 + \frac{1}{4s} \|e^{k-1}\|_2^2 + \frac{1}{s} \|e^{k+1} - e^k\|_2^2 - \frac{1}{4s} \|e^{k+1} - e^{k-1}\|_2^2.$$
(3.8)

For the backwards diffusive error term  $J_3$ , we have

$$-\left(\nabla_{h}^{\mathsf{v}}(2e^{k}-e^{k-1}),\nabla_{h}^{\mathsf{v}}e^{k+1}\right) = -\frac{1}{2}\|\nabla_{h}^{\mathsf{v}}e^{k+1}\|_{2}^{2} - \|\nabla_{h}^{\mathsf{v}}e^{k}\|_{2}^{2} + \frac{1}{2}\|\nabla_{h}^{\mathsf{v}}e^{k-1}\|_{2}^{2} + \|\nabla_{h}^{\mathsf{v}}(e^{k+1}-e^{k})\|_{2}^{2} - \frac{1}{2}\|\nabla_{h}^{\mathsf{v}}(e^{k+1}-e^{k-1})\|_{2}^{2}.$$
(3.9)

And for the stabilizing term  $J_4$ ,

$$As\left(\Delta_{h}(e^{k+1}-e^{k}),\Delta_{h}e^{k+1}\right) = \frac{As}{2}\left(\|\Delta_{h}e^{k+1}\|_{2}^{2} - \|\Delta_{h}e^{k}\|_{2}^{2} + \|\Delta_{h}(e^{k+1}-e^{k})\|_{2}^{2}\right).$$
 (3.10)

For the surface diffusion error term  $J_5$  and the local truncation error term  $J_6$ , we have

$$\varepsilon^{2} \left( \Delta_{h} e^{k+1}, \Delta_{h} e^{k+1} \right) = \varepsilon^{2} \| \Delta_{h} e^{k+1} \|_{2}^{2}, \qquad (3.11)$$

and

$$-\left(\tau^{k}, e^{k+1}\right) \leq \|\tau^{k}\|_{2} \cdot \|e^{k+1}\|_{2} \leq \frac{1}{2}\|\tau^{k}\|_{2}^{2} + \frac{1}{2}\|e^{k+1}\|_{2}^{2}.$$
(3.12)

For the nonlinear error term  $J_2$ , we adopt the same trick in [24], and get

$$J_{2} = \left( |\nabla_{h}^{\mathsf{v}} \Phi^{k+1}|^{2} \nabla_{h}^{\mathsf{v}} \Phi^{k+1} - |\nabla_{h}^{\mathsf{v}} \phi^{k+1}|^{2} \nabla_{h}^{\mathsf{v}} \phi^{k+1}, \nabla_{h}^{\mathsf{v}} e^{k+1} \right)$$
  
=  $\left( \nabla_{h}^{\mathsf{v}} (\Phi^{k+1} + \phi^{k+1}) \cdot \nabla_{h}^{\mathsf{v}} e^{k+1} \nabla_{h}^{\mathsf{v}} \Phi^{k+1}, \nabla_{h}^{\mathsf{v}} e^{k+1} \right) + \left( |\nabla_{h}^{\mathsf{v}} \phi^{k+1}|^{2} \nabla_{h}^{\mathsf{v}} e^{k+1}, \nabla_{h}^{\mathsf{v}} e^{k+1} \right)$   
=:  $J_{2,1} + J_{2,2}.$  (3.13)

For the first part  $J_{2,1}$  of (3.13), we have

$$\begin{aligned} -J_{2,1} &\leq C_4 \left( \|\nabla_h^{\mathsf{v}} \Phi^{k+1}\|_6 + \|\nabla_h^{\mathsf{v}} \phi^{k+1}\|_6 \right) \cdot \|\nabla_h^{\mathsf{v}} \Phi^{k+1}\|_6 \cdot \|\nabla_h^{\mathsf{v}} e^{k+1}\|_6 \cdot \|\nabla_h^{\mathsf{v}} e^{k+1}\|_2 \\ &\leq C_5 C_3^2 \|\nabla_h^{\mathsf{v}} e^{k+1}\|_6 \cdot \|\nabla_h^{\mathsf{v}} e^{k+1}\|_2 \\ &\leq C_5 C_3^2 \|\nabla_h^{\mathsf{v}} e^{k+1}\|_6 \cdot \|\nabla_h e^{k+1}\|_2, \end{aligned}$$
(3.14)

in which the  $W^{1,6}$  bound (3.4) for the exact and numerical solutions was recalled in the second step. Moreover, with an application of the discrete Sobolev embedding (2.9) (from  $H_h^2$  into  $W^{1,6}$ ), and the discrete elliptic regularity estimate (2.7), in Proposition 2.2, we get

$$\|\nabla_{h}^{\mathsf{v}} e^{k+1}\|_{6} \le C \|e^{k+1}\|_{H_{h}^{2}} \le C(C_{1})^{-1/2} \|\Delta_{h} e^{k+1}\|_{2}.$$
(3.15)

Meanwhile, the following interpolation inequality is valid:

$$\|\nabla_{h}e^{k+1}\|_{2} \le \|e^{k+1}\|_{2}^{\frac{1}{2}}\|\Delta_{h}e^{k+1}\|_{2}^{\frac{1}{2}}, \text{as}\|\nabla_{h}e^{k+1}\|_{2}^{2} = -(e^{k+1}, \Delta_{h}e^{k+1}) \le \|e^{k+1}\|_{2} \cdot \|\Delta_{h}e^{k+1}\|_{2}.$$
 (3.16)

In turn, a substitution of (3.15) and (3.16) into (3.14) results in

$$-J_{2,1} \leq C_6 \|\Delta_h e^{k+1}\|_2 \cdot \|e^{k+1}\|_2^{\frac{1}{2}} \|\Delta_h e^{k+1}\|_2^{\frac{1}{2}}$$
  
=  $C_6 \|e^{k+1}\|_2^{\frac{1}{2}} \cdot \|\Delta_h e^{k+1}\|_2^{\frac{3}{2}}$   
 $\leq C_7 \|e^{k+1}\|_2^2 + \frac{3}{4} \varepsilon^2 \|\Delta_h e^{k+1}\|_2^2,$  (3.17)

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in which  $C_6 = C(C_1)^{-1/2}C_5C_3^2$ , and the Young's inequality was applied in the last step. The estimate for the second part  $J_{2,2}$  of (3.13) is trivial:

$$J_{2,2} \ge 0. \tag{3.18}$$

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Then, we arrive at

$$-J_2 \le C_8 \|e^{k+1}\|_2^2 + \frac{3}{4} \varepsilon^2 \|\Delta_h e^{k+1}\|_2^2.$$
(3.19)

Finally, a combination of (3.8), (3.9), (3.10), (3.11), (3.12), and (3.19) yields that

$$\frac{3}{4s} \left( \|e^{k+1}\|_{2}^{2} - \|e^{k}\|_{2}^{2} \right) - \frac{1}{4s} \left( \|e^{k}\|_{2}^{2} - \|e^{k-1}\|_{2}^{2} \right) + \frac{1}{2s} \|e^{k+1} - e^{k}\|_{2}^{2} 
- \frac{1}{2s} \|e^{k} - e^{k-1}\|_{2}^{2} + \frac{As}{2} \left( \|\Delta_{h}e^{k+1}\|_{2}^{2} - \|\Delta_{h}e^{k}\|_{2}^{2} \right) + \varepsilon^{2} \|\Delta_{h}e^{k+1}\|_{2}^{2} 
\leq \frac{1}{2} \|\tau^{k}\|_{2}^{2} + \frac{1}{2} \|e^{k+1}\|_{2}^{2} + C_{8} \|e^{k+1}\|_{2}^{2} + \frac{3}{4} \varepsilon^{2} \|\Delta_{h}e^{k+1}\|_{2}^{2} 
- \|\nabla_{h}^{\mathsf{v}}e^{k+1}\|_{2}^{2} - 2\|\nabla_{h}^{\mathsf{v}}e^{k}\|_{2}^{2} - \|\nabla_{h}^{\mathsf{v}}(e^{k+1} - e^{k-1})\|_{2}^{2} 
+ 4\varepsilon^{-2} \|e^{k+1}\|_{2}^{2} + 288\varepsilon^{-2} \|e^{k}\|_{2}^{2} + 72\varepsilon^{-2} \|e^{k-1}\|_{2}^{2} 
+ \frac{1}{16} \varepsilon^{2} \left( \|\Delta_{h}e^{k+1}\|_{2}^{2} + \|\Delta_{h}e^{k}\|_{2}^{2} + \|\Delta_{h}e^{k-1}\|_{2}^{2} \right).$$
(3.20)

A summation in time implies that

$$\frac{3}{4s} \left( \|e^{k+1}\|_{2}^{2} - \|e^{1}\|_{2}^{2} \right) - \frac{1}{4s} \left( \|e^{k}\|_{2}^{2} - \|e^{0}\|_{2}^{2} \right) + \frac{1}{2s} \|e^{k+1} - e^{k}\|_{2}^{2} 
- \frac{1}{2s} \|e^{1} - e^{0}\|_{2}^{2} + \frac{As}{2} \left( \|\Delta_{h}e^{k+1}\|_{2}^{2} - \|\Delta_{h}e^{0}\|_{2}^{2} \right) + \frac{3}{16} \varepsilon^{2} \sum_{\ell=1}^{k} \|\Delta_{h}e^{\ell+1}\|_{2}^{2} 
\leq \frac{1}{2} \sum_{\ell=1}^{n} \|\tau^{\ell}\|_{2}^{2} + \sum_{\ell=1}^{k} \left( \frac{1}{2} + C_{8} + 4\varepsilon^{-2} \right) \|e^{\ell+1}\|_{2}^{2} 
+ 72\varepsilon^{-2} \sum_{\ell=1}^{k} \left( 4\|e^{\ell}\|_{2}^{2} + \|e^{\ell-1}\|_{2}^{2} \right) + \frac{1}{16} \varepsilon^{2} \sum_{\ell=1}^{k} \left( \|\Delta_{h}e^{\ell}\|_{2}^{2} + \|\Delta_{h}e^{\ell-1}\|_{2}^{2} \right).$$
(3.21)

In turn, an application of discrete Gronwall inequality yields the desired convergence result (3.1). This completes the proof of Theorem 3.6.

## 4 | PRECONDITIONED DESCENT SOLVERS

#### 4.1 | Preconditioned steepest descent

In this section, we describe a preconditioned steepest descent (PSD) algorithm following the practical and theoretical framework in [20]. The nonlinear, fully discrete scheme (2.10) at a fixed time level may be expressed as

$$\mathcal{N}_h[\phi] = f, \tag{4.1}$$

with

$$\mathcal{N}_{h}[\phi] = \phi^{k+1} - \frac{2s}{3} \nabla_{h}^{\mathsf{v}} \cdot (|\nabla_{h}^{\mathsf{v}} \phi^{k+1}|^{2} \nabla_{h}^{\mathsf{v}} \phi^{k+1}) + \frac{2s(\varepsilon^{2} + As)}{3} \Delta_{h}^{2} \phi^{k+1}, \qquad (4.2)$$

and

$$f = \frac{4}{3}\phi^{k} - \frac{1}{3}\phi^{k-1} - \frac{2s}{3}\Delta_{h}^{\mathsf{v}}(2\phi^{k} - \phi^{k-1}) + \frac{2As^{2}}{3}\Delta_{h}^{2}\phi^{k}.$$
(4.3)

The problem can be recast as a minimization problem: For any  $\phi \in C_{per}$ , the following energy functional is introduced:

$$E_{h}[\phi] = \frac{1}{2} \|\phi\|_{2}^{2} + \frac{2s}{12} \|\nabla_{h}^{\mathsf{v}}\phi\|_{4}^{4} + \frac{2s(\varepsilon^{2} + As)}{6} \|\Delta_{h}\phi\|_{2}^{2} - (f,\phi).$$
(4.4)

One observes that the fully discrete scheme (4.1) is the discrete variation of the strictly convex energy (4.4) set equal to zero. In particular, the discrete variation is

$$\delta_{\phi} E_h[\phi] = \mathcal{N}_h[\phi] - f.$$

The main idea of the PSD solver is to use a linearized version of the nonlinear operator as a preconditioner, or in other words, as a metric for choosing the search direction. A linearized version of the nonlinear operator  $\mathcal{N}_h$ , denoted as  $\mathcal{L}_h$ :  $\mathring{\mathcal{C}}_{per} \rightarrow \mathring{\mathcal{C}}_{per}$ , is defined as follows:

$$\mathcal{L}_h[\psi] := \psi - \gamma s \Delta_h \psi + \frac{2s(\varepsilon^2 + As)}{3} \Delta_h^2 \psi,$$

where  $\gamma \ge 0$  is a parameter chosen to optimize the performance of the pre-conditioner. Clearly, this is a positive, symmetric operator, and we use this as a preconditioner for the method. Specifically, this "metric" is used to find an appropriate search direction for the steepest descent solver [20]. Given the current iterate  $\phi^n \in C_{per}$ , we define the following *search direction* problem: find  $d^n \in \mathring{C}_{per}$  such that

$$\mathcal{L}_h[d^n] = f - \mathcal{N}_h[\phi^n] := r^n,$$

where  $r^n$  is the nonlinear residual of the  $n^{\text{th}}$  iterate  $\phi^n$ . This last equation can be solved efficiently using the Fast Fourier Transform (FFT).

We then obtain the next iterate as

$$\phi^{n+1} = \phi^n + \alpha_n d^n, \tag{4.5}$$

where  $\alpha_n \in \mathbb{R}$  is the unique solution to the steepest descent line minimization problem

$$\alpha_n := \underset{\alpha \in \mathbb{R}}{\operatorname{argmin}} E_h[\phi^n + \alpha d^n] = \underset{\alpha \in \mathbb{R}}{\operatorname{argzero\delta}} \delta_{\phi} E_h[\phi^n + \alpha d^n](d^n).$$
(4.6)

The theoretical analysis in [20] suggests that the iteration sequence  $\phi^n$  converges geometrically to  $\phi^{k+1}$ , with  $\phi^{k+1}$  the exact numerical solution of scheme (2.10) at time level k + 1, that is,  $\mathcal{N}_h[\phi^{k+1}] = f$ . Importantly, the analysis implies a convergence rate that is independent of h.

*Remark* 4.1 The energy stable Crank-Nicolson (CN-ES) scheme for the SS equation (1.3), proposed and analyzed in [19], takes the following (spatially continuous) form:

$$\begin{aligned} \frac{\Phi^{k+1} - \Phi^{k}}{s} &= \chi(\nabla \Phi^{k+1}, \nabla \Phi^{k}) - \Delta \left(\frac{3}{2} \Phi^{k} - \frac{1}{2} \Phi^{k-1}\right) - \frac{\varepsilon^{2}}{2} \Delta^{2} \left(\Phi^{k+1} + \Phi^{k}\right), \\ \chi(\nabla \Phi^{k+1}, \nabla \Phi^{k}) &:= \frac{1}{4} \nabla \cdot \left( (|\nabla \Phi^{k+1}|^{2} + |\nabla \Phi^{k}|^{2}) \nabla (\Phi^{k+1} + \Phi^{k}) \right). \end{aligned}$$

$$(4.7)$$

In this numerical approach, every term in the chemical potential is evaluated at time instant  $t^{k+1/2}$ .

Both the CN-ES scheme (4.7) and the BDF2-ES scheme (2.10) require a nonlinear solver, while the nonlinear term in (4.7) takes a more complicated form than (2.10), which comes from different time instant approximations. As a result, a stronger convexity of the nonlinear term in the BDF one (2.10) is expected to improve the numerical efficiency in the nonlinear iteration.

Such a numerical comparison has been undertaken for the Cahn-Hilliard (CH) model in recent works: the analogous CN-ES and BDF2-ES numerical schemes for the CH equation, proposed in [39, 23], respectively, were tested using a similar numerical setup. The numerical experiments have indicated that, since the nonlinear term in the BDF2-ES approach has a stronger convexity than the one in the CN-ES scheme, a 20 to 25% improvement of the computational efficiency is generally available for the CH model.

For the numerical comparison between the present BDF2-ES and CN-ES approaches for the SS equation (1.3), namely (2.10), and (4.7), respectively, such an efficiency improvement is expected to be even greater. This expectation comes from a subtle fact that, the modified CN approximation to the four-Laplacian term,  $\chi(\nabla \phi^{k+1}, \nabla \phi^k)$ , does not correspond to a convex energy functional, because of the vector gradient form (other than a scalar form) in the four-Laplacian expansion. As a consequence, the PSD algorithm proposed in this section fails to have theoretical justification as a solver for (4.7). An application of the Polak-Ribiére variant of NCG method [21] to solve for (4.7), as reported in [19], has shown fairly poor numerical performance, although this may be improved by some preconditioning strategy. See more details in Section 5.

### 4.2 | Preconditioned nonlinear conjugate gradient solvers

The preconditioned nonlinear conjugate gradient (PNCG) algorithm is given by the following recursive formulae [42]:

$$r^{n} = f - \mathcal{N}_{h}[\phi^{n}]; \tag{4.8}$$

$$y_n = \mathcal{L}_h^{-1}[r^n]; \tag{4.9}$$

$$d^{n} = \begin{cases} y^{0} & n = 0\\ y^{n} + \beta_{n} d^{n-1} & n \ge 1 \end{cases};$$
(4.10)

$$\phi^{n+1} = \phi^n + \alpha_n d^n, \quad \alpha_n = \underset{\alpha \in \mathbb{R}}{\operatorname{argzero\delta}} E_h[\phi^n + \alpha d^n](d^n)$$
(4.11)

There are several different ways to choose the parameter  $\beta_n$ . We use the following in our tests:

Fletcher-Reeves [43]:

$$\beta_n^{\text{FR}} = \frac{(r^n)^T y^n}{(r^{n-1})^T y^{n-1}}.$$
(4.12)

Polak-Ribière [44]:

$$\beta_n^{\text{PR}} = \frac{(r^n)^T (y^n - y^{n-1})}{(r^{n-1})^T y^{n-1}}.$$
(4.13)

PNCG1:

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$$\beta_{n+1} = \max\left\{0, \beta_{n+1}^{PR}\right\}.$$
(4.14)

PNCG2 [45]:

$$\beta_{n+1} = \max\left\{0, \min\left\{\beta_{n+1}^{\text{FR}}, \beta_{n+1}^{\text{PR}}\right\}\right\},\tag{4.15}$$

called the hybrid conjugate gradient algorithm in [45].

## **5 | NUMERICAL EXPERIMENTS**

#### 5.1 | Convergence test and the complexity of the preconditioned solvers

In this subsection, we demonstrate the accuracy and complexity of the preconditioned solvers. We present the results of the convergence test and perform some sample computations to investigate the effect of the time step *s* and stabilized parameter *A* for the energy  $F_h(\phi)$ .

To simultaneously demonstrate the spatial accuracy and the efficiency of the solver, we perform a typical time-space convergence test for the fully discrete scheme (2.10) for the slope selection model. As in [19, 22, 46], we perform the Cauchy-type convergence test using the following periodic initial data [19]:

$$u(x, y, 0) = 0.1 \sin^2\left(\frac{2\pi x}{L}\right) \cdot \sin\left(\frac{4\pi(y - 1.4)}{L}\right)$$
$$- 0.1 \cos\left(\frac{2\pi(x - 2.0)}{L}\right) \cdot \sin\left(\frac{2\pi y}{L}\right), \tag{5.1}$$

with  $\Omega = [0, 3.2]^2$ ,  $\varepsilon = 0.1$ , s = 0.01h, A = 1/16, and T = 0.32. We use a linear refinement path, that is, s = Ch. At the final time T = 0.32, we expect the global error to be  $\mathcal{O}(s^2) + \mathcal{O}(h^2) = \mathcal{O}(h^2)$ , in either the  $\ell^2$  or  $\ell^\infty$  norm, as  $h, s \to 0$ . The Cauchy difference is defined as  $\delta_{\phi} := \phi_{h_f} - \mathcal{I}_c^f(\phi_{h_c})$ , where  $\mathcal{I}_c^f$  is a bilinear interpolation operator (which is similar to the 2D case in [20, [24] and the 3D case in [47]). This requires a relatively coarse solution, parametrized by  $h_c$ , and a relatively fine solution, parametrized by  $h_f$ , in particular  $h_c = 2h_f$ , at the same final time. The  $\ell^2$  norms of Cauchy difference and the convergence rates can be found in Table 1. The results confirm our expectation for the second-order convergence in both space and time.

In the second part of this test, we demonstrate the complexity of the preconditioned solvers with initial data (5.1). In Figure 1, we plot the semilog scale of the relative residuals versus preconditioned

**TABLE 1** Errors, convergence rates, average iteration numbers and average CPU time (in seconds) for each time step

				PSD		PNCG1		PNCG2	
$h_c$	$h_f$	$\ \delta_{\phi}\ _2$	Rate	# <sub>iter</sub>	$T_{cpu}(h_f)$	# <sub>iter</sub>	$T_{cpu}(h_f)$	# <sub>iter</sub>	$T_{cpu}(h_f)$
$\frac{3.2}{16}$	$\frac{3.2}{32}$	$1.3938\times 10^{-2}$	_	11	.0019	9	.0016	9	.0015
$\frac{3.2}{32}$	$\frac{3.2}{64}$	$1.7192 \times 10^{-3}$	3.02	10	.0103	9	.0093	8	.0085
$\frac{3.2}{64}$	$\frac{3.2}{128}$	$3.8734\times10^{-4}$	2.15	08	.0529	8	.0486	7	.0454
$\frac{3.2}{128}$	$\frac{3.2}{256}$	$9.4766 \times 10^{-5}$	2.03	07	.2512	7	.2038	6	.2046
$\frac{3.2}{256}$	$\frac{3.2}{512}$	$2.3564\times10^{-5}$	2.01	07	1.6650	7	1.6268	6	1.5207

Parameters are given in the text, and the initial data is defined in (5.1). The refinement path is s = .01h

solvers' iteration numbers for various values of h and  $\varepsilon$  at T = .02, with time step  $s = 10^{-3}$ . The other common parameters are set as A = 1/16,  $\Omega = [0, 3.2]^2$ . The figures in the top row of Figure 1 indicate that the convergence rate (as gleaned from the error reduction) is nearly uniform and nearly independent of h for a fixed  $\varepsilon$ . And the plots in the bottom row of Figure 1 show that the number of preconditioned solvers' iterations increases with a decreasing value of  $\varepsilon$ , which confirms the theoretical results that the PSD solver is dependent on parameter  $\varepsilon$  in [20]. Figure 1 confirms the expected geometric convergence rate of the PSD solver predicted by the theory in [20]. Moreover, the number of the interaction steps in Figure 1 also indicate that PNCG2 is the most efficient one and PNCG1 is better than PSD, especially when  $\varepsilon$  is small.

In the third part of this test, we perform CPU time comparison between the proposed preconditioned solvers and the PSD solver with random initial data. The initial data for the simulations are taken as essentially random:





**FIGURE 1** Complexity tests showing the solvers' performance for changing values of *h* and  $\varepsilon$ . Top row: *h*-independence with  $\varepsilon = 0.1$ ; Bottom row:  $\varepsilon$ -dependence with h = 3.2/512. The rest of the parameters are given in the text. (a) Energy profiles with various *s* (b) evolutions of energy w.r.t various *A* [Color figure can be viewed at wileyonlinelibrary.com]



**TABLE 2** The average iteration numbers and total CPU time (in seconds) for the preconditioned methods with fixed time steps s = .001

Methods	PSD	PNCG1	PNCG2
# <sub>iter</sub>	20	14	13
$T_{\rm cpu}({\rm s})$	4406.1764	3212.2898	3035.4369
Speedup	_	1.37	1.45

Parameters are given in the text.

where the  $r_{i,j}$  are uniformly distributed random numbers in [0, 1]. The parameters for the comparison simulations are  $\Omega = [0, 12.8]^2$ ,  $\varepsilon = 3 \times 10^{-2}$ , h = 12.8/512, s = .001, and T = 1. The average iteration numbers, total CPU time (in seconds) and speedups for the preconditioned methods can be found in Table 2. The Table 2 indicates that the PNCG1 solver and PNCG2 solver have provided a  $1.37 \times \text{and } 1.45 \times \text{speedup over PSD solver, respectively.}$ 

In the last part of this test, we investigate the effect of the parameters *s* and *A* for the energy  $F_h(\phi)$  with initial data (5.1). As the proposed solvers give the same results, we only present the results from PSD solver in the rest of the article. The evolutions of the energy with various time steps *s* and stabilized parameter *A* are given in Figure 2. As can be seen in Figure 2a, the larger time steps produce inaccurate or nonphysical solutions. In turn, Figure 2a indicates the proper time steps and provides the motivation of using adaptive time stepping strategy. Figure 2b shows that the proposed scheme and PSD solver is not that sensitive to the stabilized parameter *A* when  $A \leq 1$ . Meanwhile, for large values of *A*, such as A = 5 and A = 20, the accuracy loss becomes significant.

### 5.2 | Long-time coarsening, energy dissipation and mass conservation

Coarsening processes in thin film system can take place on very long-time scales [48]. In this subsection, we perform a long-time simulation for the SS equation. Such a test, which has been performed in many existing articles, can confirm the expected coarsening rates and serve as a benchmarks for the proposed solver; see, for example, [19, 20, 22].



**FIGURE 2** The effect of time steps *s* and stabilized parameter *A* for the energy  $F_h(\phi)$ . Left: the effect of time step *s*. The other parameters are  $\Omega = [0, 3.2]^2$ ,  $\varepsilon = 3.0 \times 10^{-2}$ , h = 3.2/512, and A = 1/16; Right: the effect of stabilized parameter *A*. The other parameters are  $\Omega = [0, 3.2]^2$ ,  $\varepsilon = 3.0 \times 10^{-2}$ , h = 3.2/512 and A = 1/16; Right: the effect of stabilized parameter *A*. The other parameters are  $\Omega = [0, 3.2]^2$ ,  $\varepsilon = 3.0 \times 10^{-2}$ , h = 3.2/512 and s = 0.001. (a) t = 10 (b) t = 100 (c) t = 500 (d) t = 2000 (e) t = 4000 (f) t = 10000 [Color figure can be viewed at wileyonlinelibrary.com]



FIGURE 3 Time snapshots of the evolution with preconditioned solvers for the epitaxial thin film growth model at t = 10, 100, 500, 2000, 4000 and 10000. Left: contour plot of u, Right: contour plot of  $\Delta u$ . The parameters are  $\varepsilon = 0.03, \Omega = [12.8]^2, s = 0.001, h = 12.8/512$  and A = 1/16. These simulation results are consistent with earlier work on this topic in [13, 41, 43, 46]. (a) Energy evolution (b) Roughness evolution [Color figure can be viewed at wileyonlinelibrary.com]



FIGURE 4 The log-log plots of energy and roughness evolution and the corresponding linear regression for the simulation depicted in Figure 3. (a) t = 0 (b) t = 2 (c) t = 4 [Color figure can be viewed at wileyonlinelibrary.com]

The initial data for these simulations are taken as (5.2). Time snapshots of the evolution for the epitaxial thin film growth model can be found in Figure 3. The coarsening rates are given in Figure 4. The discrete film roughness is calculated as

$$W(t_n) = \sqrt{\frac{h^2}{L^2} \sum_{i,j=1}^m \left(\phi_{i,j}^n - \overline{\phi}\right)^2},$$
(5.3)

where *m* is the number of the grid points in the *x* and *y* direction, and  $\overline{\phi}$  is the discrete average value of  $\phi$  on the uniform grid. The log–log plots of roughness and energy evolution and the corresponding linear regression are presented in Figure 4. The linear regression in Figure 4 indicates that the surface roughness grows like  $t^{1/3}$ , while the energy decays like  $t^{-1/3}$ , which verify the one-third power laws predicted in [6]. More precisely, the linear fits have the form  $a_e t^{b_e}$  with  $a_e = 3.09870$ ,  $b_e = -.33554$ for energy evolution and  $a_m t^{b_m}$  with  $a_m = -5.35913$ ,  $b_m = .32555$  for roughness evolution. The linear regression is only taken up to t = 3000, as the system saturates at later times. These simulation results are consistent with earlier works on this topic in [8, 19, 20, 22].

### 5.3 | Direct comparison with other schemes

In this section, we compare the accuracy and performance of three other schemes to the one proposed in this article. The schemes are as follows:

#### 5.3.1 | Energy stable, order-two Backward Differentiation Formula (BDF2-ES) scheme

We first re-state the scheme proposed in this paper, which is labeled the BDF2-ES scheme:

$$\frac{3\phi^{k+1} - 4\phi^k + \phi^{k-1}}{2s} = \nabla_h^{\mathsf{v}} \cdot (|\nabla_h^{\mathsf{v}}\phi^{k+1}|^2 \nabla_h^{\mathsf{v}}\phi^{k+1}) - \Delta_h^{\mathsf{v}}(2\phi^k - \phi^{k-1}) - As\Delta_h^2(\phi^{k+1} - \phi^k) - \varepsilon^2 \Delta_h^2 \phi^{k+1}.$$
(5.4)

The associated nonlinear operator is

$$\mathcal{N}_{h}[\phi] = \phi - \frac{2s}{3} \nabla_{h}^{\mathsf{v}} \cdot (|\nabla_{h}^{\mathsf{v}}|^{2} \nabla_{h}^{\mathsf{v}} \phi) + \frac{2s(\varepsilon^{2} + As)}{3} \Delta_{h}^{2} \phi, \qquad (5.5)$$

and the linear preconditioner that we use is

$$\mathcal{L}_{h}[\phi] = \phi - \frac{s}{6} \Delta_{h} \phi + \frac{2s(\varepsilon^{2} + As)}{3} \Delta_{h}^{2} \phi.$$
(5.6)

#### 5.3.2 | Pure order-two Backward Differentiation Formula (BDF2) scheme

The BDF2 scheme is

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$$\frac{3\phi^{k+1} - 4\phi^k + \phi^{k-1}}{2s} = \nabla_h^{\mathsf{v}} \cdot (|\nabla_h^{\mathsf{v}}\phi^{k+1}|^2 \nabla_h^{\mathsf{v}}\phi^{k+1}) - \Delta_h^{\mathsf{v}}\phi^{k+1} - \varepsilon^2 \Delta_h^2 \phi^{k+1}.$$
(5.7)

The associated nonlinear operator is

$$\mathcal{N}_{h}[\phi] = \phi - \frac{2s}{3} \nabla_{h}^{\mathsf{v}} \cdot (|\nabla_{h}^{\mathsf{v}}|^{2} \nabla_{h}^{\mathsf{v}} \phi) + \frac{2s}{3} \Delta_{h}^{\mathsf{v}} \phi + \frac{2s\varepsilon^{2}}{3} \Delta_{h}^{2} \phi, \qquad (5.8)$$

and the linear preconditioner that we use is

$$\mathcal{L}_{h}[\phi] = \phi - \frac{s}{6} \Delta_{h} \phi + \frac{2s\epsilon^{2}}{3} \Delta_{h}^{2} \phi.$$
(5.9)

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We observe that the nonlinear operator is not unconditionally positive, because of the presence of the term  $+\frac{2s}{3}\Delta_{h}^{v}\phi$ , which has the wrong sign.

### 5.3.3 | Energy stable Crank-Nicolson (CN-ES) scheme

The energy stable Crank-Nicolson scheme was proposed in [19] and takes the following form:

$$\frac{\Phi^{k+1} - \Phi^{k}}{s} = \chi(\nabla \Phi^{k+1}, \nabla \Phi^{k}) - \Delta \left(\frac{3}{2}\Phi^{k} - \frac{1}{2}\Phi^{k-1}\right) - \frac{\varepsilon^{2}}{2}\Delta^{2}\left(\Phi^{k+1} + \Phi^{k}\right),$$
  
$$\chi(\nabla \Phi^{k+1}, \nabla \Phi^{k}) := \frac{1}{4}\nabla \cdot \left((|\nabla \Phi^{k+1}|^{2} + |\nabla \Phi^{k}|^{2})\nabla(\Phi^{k+1} + \Phi^{k})\right).$$
(5.10)

The corresponding nonlinear operator is

$$\mathcal{N}_{h}^{k}[\phi] = \phi - \frac{s}{4} \nabla_{h}^{\mathsf{v}} \cdot \left( (|\nabla_{h}^{\mathsf{v}} \phi|^{2} + |\nabla_{h}^{\mathsf{v}} \phi^{k}|^{2}) \nabla_{h}^{\mathsf{v}} (\phi + \phi^{k}) \right) + \frac{s\varepsilon^{2}}{2} \Delta_{h}^{2} \phi^{k+1}, \tag{5.11}$$

and the linear preconditioner that we use is

$$\mathcal{L}_{h}[\phi] = \phi - \frac{s}{4} \Delta_{h} \phi + \frac{s \varepsilon^{2}}{2} \Delta_{h}^{2} \phi.$$
(5.12)

#### 5.3.4 | Pure Crank-Nicolson (CN) scheme

The pure Crank-Nicolson scheme is based on an idea by Du and Nicolaides [49] and takes the following form:

$$\frac{\Phi^{k+1} - \Phi^{k}}{s} = \chi(\nabla \Phi^{k+1}, \nabla \Phi^{k}) - \frac{1}{2}\Delta \left(\Phi^{k+1} + \Phi^{k}\right) - \frac{\varepsilon^{2}}{2}\Delta^{2} \left(\Phi^{k+1} + \Phi^{k}\right),$$
  
$$\chi(\nabla \Phi^{k+1}, \nabla \Phi^{k}) := \frac{1}{4}\nabla \cdot \left((|\nabla \Phi^{k+1}|^{2} + |\nabla \Phi^{k}|^{2})\nabla(\Phi^{k+1} + \Phi^{k})\right).$$
(5.13)

This scheme is exactly energy stable, in the sense that

$$sF_{h}[\phi^{k+1}] + \|\phi^{k+1} - \phi^{k}\|^{2} = sF_{h}[\phi^{k}],$$

though it is not unconditionally uniquely solvable. The corresponding nonlinear operator is

$$\mathcal{N}_{h}^{k}[\phi] = \phi - \frac{s}{4} \nabla_{h}^{\mathsf{v}} \cdot \left( (|\nabla_{h}^{\mathsf{v}} \phi|^{2} + |\nabla_{h}^{\mathsf{v}} \phi^{k}|^{2} - 2) \nabla_{h}^{\mathsf{v}}(\phi + \phi^{k}) \right) + \frac{s\varepsilon^{2}}{2} \Delta_{h}^{2} \phi^{k+1}, \tag{5.14}$$

and the linear preconditioner that we use is

$$\mathcal{L}_{h}[\phi] = \phi - \frac{s}{4} \Delta_{h} \phi + \frac{s \varepsilon^{2}}{2} \Delta_{h}^{2} \phi, \qquad (5.15)$$

which is the same as that for the CN-ES scheme.



**FIGURE 5** Initial data and high-resolution approximate solutions at t = 2 and t = 4. A high-resolution solution is computed using the BDF2 scheme 5.7 with the initial data shown in the figure (t = 0). The parameters for the highresolution approximation are s = .00005 and h = 3.2/256. The other parameters are  $\Omega = (0, 3.2) \times (0, 3.2)$ and  $\varepsilon = 3.0 \times 10^{-2}$ . Significant coarsening occurs between t = 0 and t = 4 [Color figure can be viewed at wileyonlinelibrary.com]

#### 5.3.5 | Initial data and a high-resolution approximate solution at t = 4

A high-resolution solution is computed using the BDF2 Scheme 5.7 with the initial data shown in Figure 5 (t = 0). The parameters for the approximation are  $s = 5 \times 10^{-5}$  and h = 3.2/256. The other parameters are  $\Omega = (0, 3.2) \times (0, 3.2)$  and  $\varepsilon = 3.0 \times 10^{-2}$ . The time step size  $s = 5 \times 10^{-5}$  is 20 times smaller than what will be used in the comparison tests, and we will treat the approximation obtained here as the target solution.

#### 5.3.6 | Comparison results

For the comparison computations, we use the same parameters but with a larger time step size: s = 0.001and h = 3.2/256,  $\Omega = (0, 3.2) \times (0, 3.2)$  and  $\varepsilon = 3.0 \times 10^{-2}$ . To solve all of the schemes, we use the preconditioned steepest descent (PSD) and preconditioned nonlinear conjugate gradient (PNCG) solvers, even though in some cases the nonlinear operators are not necessarily guaranteed to be positive. For the PNCG solver, for simplicity, we use only the Polak-Ribière method.

The results of the tests are reported in Table 3, and they paint a complicated picture. The BDF2 scheme shows excellent accuracy and efficiency. Our new BDF2-ES scheme is slightly more efficient, but not as accurate. The accuracy of the BDF2-ES scheme improves greatly by setting the splitting parameter A = 0.

The Crank-Nicolson schemes also have excellent accuracy, but, as expected the CPU time per iteration for either CN scheme is much higher than for the BDF2 schemes, more than double that of the BDFs schemes. What is interesting is that the average number of iterations for the solvers for the CN schemes is smaller than for the BDF2 schemes, which is surprising, given the complicated structure of the nonlinear operators for the CN schemes. Clearly, the BDF schemes dominate in terms of efficiency per time step. But, when accuracy is considered in the calculus, the most efficient scheme, the new

Scheme	Solver	Error $t = 2$	Error $t = 4$	Ave. Iterations	Ave. CPU Time
BDF2	PSD	1.7720e - 07	4.1570e - 07	6.1307	.0452
BDF2	PNCG	1.7778e – 07	4.1705e - 07	5.4227	.0433
BDF2-ES, $A = 1/16$	PSD	5.9459e - 04	1.5551e - 03	6.0438	.0426
BDF2-ES, $A = 1/16$	PNCG	5.9459e - 04	1.5551e - 03	5.3738	.0408
BDF2-ES, $A = 0$	PSD	1.5988e - 05	2.3541e - 05	6.1043	.0432
BDF2-ES, $A = 0$	PNCG	1.5975e – 05	2.3523e - 05	5.4288	.0416
CN	PSD	2.2686e - 07	4.4921e - 07	5.3202	.1228
CN	PCNG	2.2693e - 07	4.5077e - 07	4.8117	.1150
CN-ES	PSD	7.3157e – 06	8.4747e – 06	5.2760	.1228
CN-ES	PNCG	7.3090e - 06	8.4596e - 06	4.7250	.1143

**TABLE 3** The errors, average iteration numbers, and average CPU time (in seconds) for the preconditioned methods with fixed time and space step sizes s = .001 and h = 3.2/256

The other parameters are  $\Omega = (0, 3.2) \times (0, 3.2)$  and  $\varepsilon = 3.0 \times 10^{-2}$ . The "errors," which are reported at times t = 2 and t = 4, are precisely the differences between the comparison approximations and the high-resolution target approximation computed using the BDF2 with the much smaller time step size  $s = 5 \times 10^{-5}$ 

BDF2-ES scheme, does not compare as favorably. The question remains, given a target accuracy, what is the CPU time per iteration that is required to achieve that accuracy? The answer to this question, and the test that will give that answer, we will save for a future work.

## **6 | CONCLUSIONS**

In this article, we have proposed and analyzed a second order accurate, unconditionally energy stable finite difference scheme for solving the two-dimensional epitaxial thin film model with Slope Selection (SS). The unique solvability, unconditional energy stability and optimal convergence analysis have been theoretically justified. In addition, a class of efficient preconditioned methods are applied to solve the nonlinear system. This framework can be easily generalized to the higher order in time BDF schemes. Various numerical results are also presented, including a second-order-in-time accuracy test, a complexity test and energy dissipation tests. We have also included a preliminary test comparing our new scheme with other existing schemes. In terms of efficiency per time iteration, the new scheme performs well. It also has good accuracy properties, though not the best of the schemes that we tested.

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#### **APPENDIX: A PROOF OF PROPOSITION 2.2**

For simplicity of presentation, in the analysis of  $\|\nabla_h \phi\|_6$ , we are focused on the estimate of  $\|D_x \phi\|_6$ . We suppose for simplicity that *m* is odd and we set m = 2K + 1. Due to the periodic boundary conditions for  $\phi$  and its cell-centered representation, it has the discrete Fourier representation

$$\phi_{i,j} = \sum_{k,\ell=-K}^{K} \hat{\phi}_{k,\ell}^{m} e^{2\pi i (kx_i + \ell y_j)/L}, \tag{A.1}$$

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

$$\phi_{\mathbf{F}}(x,y) = \sum_{k,\ell=-K}^{K} \hat{\phi}_{k,\ell}^{m} e^{2\pi i (kx+\ell y)/L}.$$
(A.2)

Similarly, we denote a grid function  $f_{i+\frac{1}{2}j+\frac{1}{2}} = \mathfrak{D}_x \phi_{i+\frac{1}{2}j+\frac{1}{2}} = A_y(D_x \phi)_{i+\frac{1}{2}j+\frac{1}{2}}$ . The periodic boundary conditions for *f* and its mesh location indicates the following discrete Fourier transformation:

$$f_{i+\frac{1}{2},j+\frac{1}{2}} = \sum_{k,\ell=-K}^{K} \hat{f}_{k,\ell}^{m} e^{2\pi i \left(kx_{i+\frac{1}{2}} + \ell y_{j+\frac{1}{2}}\right)/L},$$
(A.3)

with  $\hat{f}_{k,\ell}^m$  the discrete Fourier coefficients. Similarly, its extension to a continuous function is given by

$$f_{\mathbf{F}}(x,y) = \sum_{k,\ell=-K}^{K} \hat{f}_{k,\ell}^{m} \mathrm{e}^{2\pi i (kx+\ell y)/L}.$$
 (A.4)

Meanwhile, we also observe that  $\hat{\phi}_{0,0}^m = 0$  and  $\hat{f}_{0,0}^m = 0$ . The first identity comes from the fact that  $\overline{\phi} = 0$ , while the second one is due to the fact that  $\overline{f} = \overline{\mathfrak{D}}_x \overline{\phi} = 0$ , for any periodic grid function  $\phi$ .

The following preliminary estimates will play a very important role in the later analysis.

Lemma A.1 We have

$$\|\phi\|_2 = \|\phi_F\|,\tag{A.5}$$

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$$\frac{2}{\pi} \|\nabla \phi_{\mathbf{F}}\| \le \|\nabla_h \phi\|_2 \le \|\nabla \phi_{\mathbf{F}}\|, \quad \frac{4}{\pi^2} \|\Delta \phi_{\mathbf{F}}\| \le \|\Delta_h \phi\|_2 \le \|\Delta \phi_{\mathbf{F}}\|, \tag{A.6}$$

$$\|\partial_x f_{\mathbf{F}}\| \le \|\partial_x^2 \phi_{\mathbf{F}}\|, \quad \|\partial_y f_{\mathbf{F}}\| \le \|\partial_x \partial_y \phi_{\mathbf{F}}\|.$$
(A.7)

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

$$\sum_{i,j=1}^{m} |\phi_{i,j}|^2 = m^2 \sum_{k,\ell=-K}^{K} |\hat{\phi}_{k,\ell}^m|^2, \quad \|\phi_{\mathbf{F}}\|^2 = L^2 \sum_{k,\ell=-K}^{K} |\hat{\phi}_{k,\ell}^m|^2.$$
(A.8)

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

$$\|\phi\|_{2}^{2} = \|\phi_{\mathbf{F}}\|^{2} = L^{2} \sum_{k,\ell=-K}^{K} |\hat{\phi}_{k,\ell}^{m}|^{2}, \qquad (A.9)$$

so that (A.5) is proven.

For the comparison between  $f = \mathfrak{D}_x \phi$  and  $\partial_x \phi_F$ , we look at the following Fourier expansions:

$$f_{i+\frac{1}{2}j+\frac{1}{2}} = \frac{\phi_{i+1,j} - \phi_{i,j} + \phi_{i+1,j+1} - \phi_{i,j+1}}{2h} = \sum_{k,\ell=-K}^{K} \mu_{k,\ell} \hat{\phi}_{k,\ell}^m e^{2\pi i \left(kx_{i+\frac{1}{2}} + \ell y_{j+\frac{1}{2}}\right)/L}, \tag{A.10}$$

$$f_{\mathbf{F}}(x,y) = \sum_{k,\ell=-K}^{K} \mu_{k,\ell} \hat{\phi}_{k,\ell}^{m} e^{2\pi i (kx+\ell y)/L},$$
(A.11)

$$\partial_x \phi_{\mathbf{F}}(x, y) = \sum_{k,\ell=-K}^K \nu_k \hat{\phi}_{k,\ell}^m e^{2\pi i (kx+\ell y)/L},\tag{A.12}$$

with

$$\mu_{k,\ell} = -\frac{2i\sin\frac{k\pi h}{L}}{h}\cos(\ell\pi h), \quad \nu_k = -\frac{2k\pi i}{L}.$$
(A.13)

A comparison of Fourier eigenvalues between  $|\mu_{k,\ell}|$  and  $|\nu_k|$  shows that

$$\frac{2}{\pi}|v_k| \le |\mu_{k,\ell}| \le |v_k|, \quad \text{for} \quad -K \le k, \ell \le K, \tag{A.14}$$

which in turn leads to

$$\frac{2}{\pi} \|\partial_x \phi_{\mathbf{F}}\| \le \|\mathfrak{D}_x \phi\|_2 \le \|\partial_x \phi_{\mathbf{F}}\|. \tag{A.15}$$

A similar estimate could also be derived:

$$\frac{2}{\pi} \|\partial_{\mathbf{y}} \phi_{\mathbf{F}}\| \le \|\mathfrak{D}_{\mathbf{y}} \phi\|_2 \le \|\partial_{\mathbf{y}} \phi_{\mathbf{F}}\|.$$
(A.16)

A combination of (A.15) and (A.16) yields the first inequality of (A.6).

For the second estimate of (A.6), we look at similar Fourier expansions:

$$(\Delta_h \phi)_{i,j} = \sum_{k,\ell=-K}^{K} \left( \mu_k^2 + \mu_\ell^2 \right) \hat{\phi}_{k,\ell}^m e^{2\pi i (\ell x_i + m y_j)/L}, \tag{A.17}$$

$$\Delta \phi_{\mathbf{F}}(x,y) = \sum_{k,\ell=-K}^{K} \left( v_k^2 + v_\ell^2 \right) \hat{\phi}_{k,\ell}^m e^{2\pi i (kx+\ell y)/L}, \tag{A.18}$$

with  $\mu_k = -\frac{2i \sin \frac{k\pi h}{L}}{h}$ ,  $\mu_\ell = -\frac{2i \sin \frac{\ell\pi h}{L}}{h}$ . It is also clear that  $\frac{2}{\pi} |v_\ell| \le |\mu_\ell| \le |v_\ell|$ , for any  $-K \le \ell \le K$ . In turn, an application of Parseval's identity yields

$$\|\Delta_h \phi\|_2^2 = L^2 \sum_{k,\ell=-K}^K |\mu_k^2 + \mu_\ell^2|^2 |\hat{\phi}_{k,\ell}^m|^2, \qquad (A.19)$$

$$\|\Delta \phi_{\mathbf{F}}\|^{2} = L^{2} \sum_{k,\ell=-K}^{K} |v_{k}^{2} + v_{\ell}^{2}|^{2} |\hat{\phi}_{k,\ell}^{m}|^{2}.$$
(A.20)

The eigenvalue comparison estimate (A.14) implies the following inequality:

$$\frac{4}{\pi^2} |v_k^2 + v_\ell^2| \le |\mu_k^2 + \mu_\ell^2| \le |v_k^2 + v_\ell^2|, \quad \text{for} \quad -K \le k, \ell \le K.$$
(A.21)

As a result, inequality (A.6) comes from a combination of (A.19), (A.20) and (A.21).

For the estimate (A.7), we observe the following Fourier expansions:

$$\partial_x f_{\mathbf{F}}(x, y) = \sum_{k,\ell=-K}^{K} v_k \mu_{k,\ell} \hat{\phi}_{k,\ell}^m e^{2\pi i (kx+\ell y)/L}, \qquad (A.22)$$

$$\partial_x^2 \phi_{\mathbf{F}}(x, y) = \sum_{k,\ell=-K}^K v_k^2 \hat{\phi}_{k,\ell}^m e^{2\pi i (kx+\ell y)/L}, \qquad (A.23)$$

which in turn leads to (with an application of Parseval's identity)

$$\|\partial_{x} f_{\mathbf{F}}\|^{2} = L^{2} \sum_{k,\ell=-K}^{K} |v_{k} \mu_{k,\ell}|^{2} |\hat{\phi}_{k,\ell}^{m}|^{2}, \qquad (A.24)$$

$$\|\partial_x^2 \phi_{\mathbf{F}}\|^2 = L^2 \sum_{k,\ell=-K}^{K} |v_k|^4 |\hat{\phi}_{k,\ell}^m|^2.$$
(A.25)

Similarly, the following inequality could be derived, based on the eigenvalue comparison estimate (A.14):

$$|v_k \mu_{k,\ell}|^2 \le |v_k|^4$$
, for  $-K \le k, \ell \le K$ . (A.26)

Consequently, a combination of (A.24), (A.25) and (A.26) leads to the first inequality in (A.7). The second inequality,  $\|\partial_y f_F\| \le \|\partial_x \partial_y \phi_F\|$ , could be derived in the same manner. The proof of Lemma A.1 is complete.

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With the estimates in Lemma A.1, we are able to make the following derivations:

$$\|\phi\|_{H_{h}^{2}}^{2} = \|\phi\|_{2}^{2} + \|\nabla_{h}\phi\|_{2}^{2} + \|\Delta_{h}\phi\|_{2}^{2} \le \|\phi_{\mathbf{F}}\|^{2} + \|\nabla\phi_{\mathbf{F}}\|^{2} + \|\Delta\phi_{\mathbf{F}}\|^{2} \le \|\phi_{\mathbf{F}}\|_{H_{h}^{2}}^{2},$$
(A.27)

$$\|\phi_{\mathbf{F}}\|_{H_{h}^{2}}^{2} \leq B_{0} \|\Delta\phi_{\mathbf{F}}\|^{2}, \quad \left( \text{ elliptic regularity, since } \int_{\Omega} \phi_{\mathbf{F}} d \mathbf{x} = 0 \right),$$
(A.28)

so that 
$$\|\Delta_h \phi\|_2^2 \ge \frac{4}{\pi^2} \|\Delta \phi_{\mathbf{F}}\|^2 \ge \frac{4}{\pi^2 B_0} \|\phi_{\mathbf{F}}\|_{H_h^2}^2 \ge \frac{4}{\pi^2 B_0} \|\phi\|_{H_h^2}^2,$$
 (A.29)

so that (2.7) (in Proposition 2.2) is proved with  $C_1 = \frac{4}{\pi^2 B_0}$ .

Inequality (2.8) could be proved in a similar way. The following fact is observed:

$$\|\phi\|_{\infty} \le \|\phi_{\mathbf{F}}\|_{L^{\infty}} \le C \|\phi_{\mathbf{F}}\|_{H^{2}_{h}} \le C \|\phi\|_{H^{2}_{h}}, \tag{A.30}$$

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in which the first step is based on the fact that,  $\phi$  is the grid interpolation of the continuous function  $\phi_F$ , the second step comes from the Sobolev embedding, while the last step comes from the the estimates in Lemma A.1.

For the proof of (2.9), the last inequality in Proposition 2.2, the following lemma is needed, which gives a bound of the discrete  $\ell^p$  (with p = 4, 6) norm of the grid functions  $\phi$  and f, in terms of the continuous  $L^p$  norm of its continuous version  $f_F$ .

**Lemma A.2** For  $\phi \in C_{per}$ ,  $f \in \mathcal{V}_{per}$ , we have

$$\|\phi\|_{p} \leq \sqrt{\frac{p}{2}} \|\phi_{\mathbf{F}}\|_{L^{p}}, \quad \|f\|_{p} \leq \sqrt{\frac{p}{2}} \|f_{\mathbf{F}}\|_{L^{p}}, \quad \text{with } p = 4, 6.$$
 (A.31)

*Proof* For simplicity of presentation, we only present the analysis for  $||f||_p \le \sqrt{\frac{p}{2}} ||f_F||_{L^p}$ ; the analysis for  $\phi$  could be carried out in the same fashion. And also, we are focused on the case of p = 4. The case with p = 6 could be handled in a similar, yet more tedious way.

We denote the following grid function

$$g_{ij} = \left(f_{ij}\right)^2. \tag{A.32}$$

A direct calculation shows that

$$\|f\|_{4} = \left(\|g\|_{2}\right)^{\frac{1}{2}}.$$
(A.33)

Note that both norms are discrete in the above identity. Moreover, we assume the grid function g has a discrete Fourier expansion as

$$g_{i,j} = \sum_{k,\ell=-K}^{K} \hat{g}_{k,\ell}^{m} e^{2\pi i (kx_i + \ell y_j)}, \qquad (A.34)$$

and denote its continuous version as

$$G(x, y) = \sum_{k,\ell=-K}^{K} \hat{g}_{k,\ell}^{m} e^{2\pi i(kx+\ell y)} \in \mathcal{P}_{K}.$$
 (A.35)

With an application of the Parseval equality at both the discrete and continuous levels, we have

$$\|g\|_{2}^{2} = \|G\|^{2} = \sum_{k,\ell=-K}^{K} |\hat{g}_{k,\ell}^{m}|^{2}.$$
(A.36)

On the other hand, we also denote

$$H(x,y) = (f_{\mathbf{F}}(x,y))^2 = \sum_{k,\ell=-2K}^{2K} (\hat{h}^m)_{k,\ell} e^{2\pi i(\ell x + my)} \in \mathcal{P}_{2K}.$$
 (A.37)

The reason for  $H \in \mathcal{P}_{2K}$  is because  $f_{\mathbf{F}} \in \mathcal{P}_K$ . We note that  $H \neq G$ , since  $H \in \mathcal{P}_{2K}$ , while  $G \in \mathcal{P}_K$ , although H and G have the same interpolation values on at the numerical grid points  $(x_i, y_j)$ . In other words, g is the interpolation of H onto the numerical grid point and G is the continuous version of g in  $\mathcal{P}_K$ . As a result, collocation coefficients  $\hat{g}^m$  for G are not equal to  $\hat{h}^m$  for H, due to the aliasing error. In more detail, for  $-K \leq k, \ell \leq K$ , we have the following representations:

$$\hat{g}_{k,\ell}^{m} = \begin{cases}
(\hat{h}^{m})_{k,\ell} + (\hat{h}^{m})_{k+m,\ell} + (\hat{h}^{m})_{k,\ell+m} + (\hat{h}^{m})_{k+m,\ell+m}, k < 0, \ell < 0, \\
(\hat{h}^{m})_{k,\ell} + (\hat{h}^{m})_{k+m,\ell}, k < 0, \ell = 0, \\
(\hat{h}^{m})_{k,\ell} + (\hat{h}^{m})_{k+m,\ell} + (\hat{h}^{m})_{k,\ell-m} + (\hat{h}^{m})_{k+m,\ell-m}, k < 0, \ell > 0, \\
(\hat{h}^{m})_{k,\ell} + (\hat{h}^{m})_{k-m,\ell} + (\hat{h}^{m})_{k,\ell-m} + (\hat{h}^{m})_{k-m,\ell-m}, k > 0, \ell > 0, \\
(\hat{h}^{m})_{k,\ell} + (\hat{h}^{m})_{k-m,\ell}, k > 0, \ell = 0, \\
(\hat{h}^{m})_{k,\ell} + (\hat{h}^{m})_{k-m,\ell} + (\hat{h}^{m})_{k,\ell+m} + (\hat{h}^{m})_{k-m,\ell+m}, k > 0, \ell < 0, \\
(\hat{h}^{m})_{k,\ell} + (\hat{h}^{m})_{k,\ell+m}, k = 0, \ell < 0, \\
(\hat{h}^{m})_{k,\ell} + (\hat{h}^{m})_{k,\ell-m}, k = 0, \ell > 0.
\end{cases}$$
(A.38)

With an application of Cauchy inequality, it is clear that

$$\sum_{k,\ell=-K}^{K} \left| \hat{g}_{k,\ell}^{m} \right|^{2} \le 4 \left| \sum_{k,\ell=-2K}^{2K} (\hat{h}^{m})_{k,\ell} \right|^{2}.$$
(A.39)

Meanwhile, an application of Parseval's identity to the Fourier expansion (A.37) gives

$$\|H\|^{2} = \left|\sum_{k,\ell=-2K}^{2K} (\hat{h}^{m})_{k,\ell}\right|^{2}.$$
 (A.40)

Its comparison with (A.36) indicates that

$$||g||_2^2 = ||G||^2 \le 4||H||^2$$
, i.e.  $||g||_2 \le 2||H||$ , (A.41)

with the estimate (A.39) applied. Meanwhile, since  $H(x, y) = (f_F(x, y))^2$ , we have

$$\|f_{\mathbf{F}}\|_{L^4} = (\|H\|_{L^2})^{\frac{1}{2}}.$$
(A.42)

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Therefore, a combination of (A.33), (A.41) and (A.42) results in

$$\|f\|_{4} = \left(\|g\|_{2}\right)^{\frac{1}{2}} \le (2\|H\|_{L^{2}})^{\frac{1}{2}} \le \sqrt{2}\|f_{\mathbf{F}}\|_{L^{4}}.$$
(A.43)

This finishes the proof of (A.31) with p = 4, the inequality with p = 6 could be proved in the same fashion.

Now we proceed into the proof of (2.9) in Proposition 2.2.

*Proof* We begin with an application of (A.31) in Lemma A.2:

$$\|\mathfrak{D}_{x}\phi\|_{6} = \|f\|_{6} \le \sqrt{3}\|f_{\mathbf{F}}\|_{L^{6}}.$$
(A.44)

Meanwhile, using the fact that  $\overline{f_F} = 0$ , we apply the 2-D Sobolev inequality and get

$$\|f_{\mathbf{F}}\|_{L^{6}} \le B_{0}^{(1)} \|f_{\mathbf{F}}\|_{H^{1}} \le C(\|f_{\mathbf{F}}\| + \|\nabla f_{\mathbf{F}}\|).$$
(A.45)

Moreover, the estimates (A.5-A.7) (in Lemma A.1) indicate that

$$\|f_{\mathbf{F}}\| \le \|\partial_x \phi_{\mathbf{F}}\| \le \frac{\pi}{2} \|\nabla_h \phi\|_2, \tag{A.46}$$

$$\|\partial_{x}f_{\mathbf{F}}\| \leq \|\partial_{x}^{2}\phi_{\mathbf{F}}\| \leq M_{0}\|\Delta\phi_{\mathbf{F}}\| \leq \frac{\pi^{2}M_{0}}{4}\|\Delta_{h}\phi\|_{2}, \tag{A.47}$$

$$\|\partial_{\mathbf{y}}f_{\mathbf{F}}\| \le \|\partial_{\mathbf{x}}\partial_{\mathbf{y}}\phi_{\mathbf{F}}\| \le M_0\|\Delta\phi_{\mathbf{F}}\| \le \frac{\pi^2 M_0}{4}\|\Delta_h\phi\|_2, \tag{A.48}$$

so that 
$$||f_{\mathbf{F}}|| + ||\nabla f_{\mathbf{F}}|| \le \frac{\sqrt{2\pi^2 M_0}}{4} (||\nabla_h \phi||_2 + ||\Delta_h \phi||_2),$$
 (A.49)

in which the following elliptic regularity estimate is applied:

$$\|\partial_x^2 \phi_{\mathbf{F}}\|, \|\partial_x \partial_y \phi_{\mathbf{F}}\| \le M_0 \|\Delta \phi_{\mathbf{F}}\|.$$
(A.50)

Therefore, a substitution of (A.47), (A.49), and (A.45) into (A.44) results in

$$\|\mathfrak{D}_{x}\phi\|_{6} \leq \frac{\sqrt{6}\pi^{2}M_{0}B_{0}^{(1)}}{4}\|\phi\|_{H_{h}^{2}}.$$
(A.51)

The estimate for  $||D_y\phi||_6$  could be derived in the same fashion:

$$\|\mathfrak{D}_{y}\phi\|_{6} \leq \frac{\sqrt{6}\pi^{2}M_{0}B_{0}^{(1)}}{4}\|\phi\|_{H^{2}_{h}}.$$
(A.52)

As a consequence, (2.9) is valid, by setting  $C = \sqrt{2}B_0^{(1)}$ . The proof of Proposition 2.2 is complete.

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