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ERROR ANALYSIS OF A FINITE DIFFERENCE SCHEME FOR THE EPITAXIAL THIN FILM MODEL WITH SLOPE SELECTION WITH AN IMPROVED CONVERGENCE CONSTANT

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Abstract. In this paper we present an improved error analysis for a finite difference scheme for solving the 1-D epitaxial thin film model with slope selection. The unique solvability and unconditional energy stability are assured by the convex nature of the splitting scheme. A uniform-in-time H^m bound of the numerical solution is acquired through Sobolev estimates at a discrete level. It is observed that a standard error estimate, based on the discrete Gronwall inequality, leads to a convergence constant of the form $\exp(CT\varepsilon^{-m})$, where m is a positive integer, and ε is the corner rounding width, which is much smaller than the domain size. To improve this error estimate, we employ a spectrum estimate for the linearized operator associated with the 1-D slope selection (SS) gradient flow. With the help of the aforementioned linearized spectrum estimate, we are able to derive a convergence analysis for the finite difference scheme, in which the convergence constant depends on ε^{-1} only in a polynomial order, rather than exponential.

Key words. Epitaxial thin film growth, finite difference, convex splitting, uniform-in-time H^m stability, linearized spectrum estimate, discrete Gronwall inequality.

1. Introduction

The epitaxial thin film growth model with slope selection, also known as the regularized Cross-Newell equation [15, 23], has been used as a model for thin film roughening and coarsening [30, 31, 32, 33, 34, 35, 36, 37, 38, 42, 41, 50]. This equation contains a continuum-level description of the Ehrlich-Schwoebel barrier, which leads to an uphill adatom "current" and ultimately the formation of hill and valley structures [31, 37]. The model may be viewed as a gradient flow with respect to the Aviles-Giga-type energy functional [3, 29, 34, 37], which is given by

$$E(\phi) := \int_\Omega \left(\frac{1}{4}\varepsilon^{-1} \left((\partial\phi_x)^2 - 1 \right)^2 + \frac{\varepsilon}{2} (\partial_x^2 \phi)^2 \right) \mathrm{d}x, \tag{1}$$

where $\Omega = (0, L)$, $\phi : \Omega \to \mathbb{R}$ is the height of the film, and $\varepsilon > 0$ is a positive constant that is much smaller that the domain size L. As is standard, we assume that ϕ is periodic. The chemical potential is defined to be the variational derivative of the energy (1), *i.e.*,

$$\mu := \delta_\phi E = \varepsilon^{-1} \left[-\partial_x (|\partial_x \phi|^2 \partial_x \phi) + \partial_x^2 \phi \right] + \varepsilon \partial_x^4 \phi. \tag{2}$$

The linear term $\varepsilon\partial_x^4\phi$ models surface diffusion. The remainder of the terms in the chemical potential model the Ehrlich-Schwoebel barrier, which gives rise to "facets" on the film surface. The parameter $\varepsilon > 0$ describes the strength of the surface diffusion. More surface diffusion leads to more corner rounding at the junction of two facets. The epitaxial thin film model with slope selection is the L^2 gradient flow associated with the energy (1):

$$\partial_t \phi = -\mu = \varepsilon^{-1} \left[\partial_x \left((\partial_x \phi)^3 \right) - \partial_x^2 \phi \right] - \varepsilon \partial_x^4 \phi. \tag{3}$$

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We will refer to this equation as the slope selection (SS) equation. It is easy to see that the SS equation (3) is mass conservative, and the energy (1) is non-increasing in time along the solution trajectories of (3). Interestingly, one will also observe that, at least in one spatial dimension, the slope function, $\partial_x \phi$ satisfies a Cahn-Hilliard equation:

$$\partial_t \left(\partial_x \phi\right) = \varepsilon^{-1} \partial_x^2 \left[\left(\partial_x \phi\right)^3 - \partial_x \phi\right] - \varepsilon \partial_x^4 \left(\partial_x \phi\right). \tag{4}$$

Energy stability is an important issue for long-time numerical simulation. Convex-splitting time discretization schemes, popularized by Eyre's work [18], have some desirable properties, including unique solvability and unconditional energy stability. See the related works for the Cahn-Hilliard equation [17, 26], the phase field crystal (PFC) and modified phase field crystal (MPFC) equations [4, 5, 28, 46, 47, 49], the Cahn-Hilliard-Hele-Shaw (CHHS) and related models [9, 14, 16, 22, 39, 48], et cetera. In particular, for the epitaxial thin film growth models, the authors recall the first order convex splitting scheme reported in [45], the second order splitting scheme in [43], and their extensions to the no-slope-selection model [8, 10].

We are focused on error estimates and convergence analyses for the convex splitting scheme applied to the 1-D SS model in this work. Given any fixed final time T, such an error estimate could be derived through a standard process of consistency and stability analyses; the convergence constant is independent of the time step s and spatial grid size h. However, a careful calculation shows that, this constant depends singularly on T and the reciprocal of the surface diffusion parameter ε: the specific form is $\exp\left(C\varepsilon^{-m}T\right)$, where m is a positive integer. As usual, this form comes from the application of a discrete Gronwall inequality in the analysis.

On the other hand, the authors observe that, there have been a few works on the improved convergence constant for the Cahn-Hilliard flow. In particular, Feng and Prohl [21] proved – for a first-order-in-time backward Euler scheme coupled with a mixed finite element spatial discretization scheme – that the convergence constant is of order $\exp\left(C_0 T\right)\varepsilon^{-m_0}$, for some positive integer m_0 and a constant C_0 independent of ε. In other words, the exponential dependence on ε^{-1} may be replaced by a polynomial dependence. Two more recent works of Feng, Li and Xing [19, 20] applied a similar technique to analyze the first-order-in-time, discontinuous Galerkin schemes for the Allen-Cahn and Cahn-Hilliard equations. Both the backward Euler and convex splitting temporal discretizations were included in their recent works. Such an elegant improvement was based on a subtle spectrum analysis for the linearized Cahn-Hilliard operator (with certain given structure assumptions of the solution), provided in earlier PDE analyses [1, 2, 11, 12, 13].

In this article, we extend this idea and utilize the related methodology to derive a similar estimate for the first order convex splitting, finite difference scheme applied to the 1-D SS equation. The multi-dimensional SS equation is much more challenging than the Cahn-Hilliard equation, due to the higher degree of nonlinearity of the 4-Laplacian term. Meanwhile, we observe that, the one-dimensional SS equation takes a very similar structure as the corresponding Cahn-Hilliard one, and the linearized spectrum estimate can be derived in the same manner. This estimate plays an essential role in the error estimate with an improved constant.

Our analysis will proceed in the following way: to start with, the leading order energy stability yields an H^2 estimate of the numerical solution, independent on the final time. Subsequently, a uniform-in-time H^m (with $m \geq 3$) bound of the numerical solution may be derived with the help of higher order energy estimates and repeated application of Sobolev inequalities at the discrete level. These bounds are dependent on the initial H^m data and ε^{-1}

(in a polynomial form), but are independent of the final time T. Since this bound is available for the numerical solution for any $m \geq 3$, a subtle observation implies that $\|\phi^{n+1} - \phi^n\|_{H^k}$ (where ϕ^n is the fully discrete numerical approximation at the time instant t^n and k is an integer) is $O(s)$, with s the time step size. In addition, the constant appearing in $O(s)$ turns out to be independent of T. In other words, we are able to derive a uniform-in-time $O(s)$ estimate for $\|\phi^{n+1} - \phi^n\|_{H^k}$, independent of the convergence analysis.

Meanwhile, we observe that the existing works [20, 21] (for the CH equation with improved convergence constant) dealt with finite element approximations in space. For a finite difference scheme, in which the numerical solution is evaluated at collocation grid points, we estimate the difference between the discrete H^k norm of the numerical error function and the continuous H^k norm of its continuous interpolation, with the help of the discrete and continuous Fourier analysis. This Fourier analysis also enables us to perform an estimate for the difference between the discrete ℓ^2 inner product associated with the nonlinear term and its continuous interpolation, appropriately defined. Consequently, some aliasing error control techniques have to be applied, such as those derived in [25].

Both the numerical scheme and the exact solution are evaluated at the time instant t^{n+1}. With all the preliminary estimates available, we could apply the spectrum analysis for the linearized SS operator, and arrive at a discrete ℓ^2 error estimate of size $O(s+h^2)$, where the convergence constant is of the form as $\exp\left(C_0^* T\right)\varepsilon^{-m_0}$, with C_0^* independent of ε.

In Section 2 we review the first order convex splitting numerical scheme, combined with the finite difference approximation in space. The unique solvability, unconditional energy stability and a uniform-in-time (discrete) H^2 stability are established. In Section 3, we present the higher order H^m (for $m \geq 3$) numerical stability analysis of the approximate solution. As a result, a uniform-in-time estimate for $\|\phi^{n+1} - \phi^n\|_{H^k}$ is provided. In Section 4 we present the discrete ℓ^2 error estimate of size $O(s+h^2)$, with the convergence constant dependent on ε^{-1} in a polynomial form. Some concluding remarks are given in Section 5.

2. The numerical scheme and the leading H^2 estimate

2.1. The finite difference approximation. The domain is given by $\Omega = (0, L)$, and we take a uniform mesh with $h = \frac{L}{N}$. The height function ϕ is evaluated at cell center points $x_i = (i - 1/2)\cdot h$, $i = 1, \cdots, N$. For the numerical approximation we write $\phi_i = \phi(x_i)$. Edge centered functions are represented by $f_{i+1/2} = f(x_{i+1/2})$, $i = 0, \cdots, N$. We assume that grid functions are periodic. In the case of cell-centered functions, this means that

$$\phi_{i+q\cdot N} = \phi_i, \quad \forall\ i, q \in \mathbb{Z}, \tag{5}$$

and a similar expression holds for periodic edge-centered functions.

The center-to-edge and edge-to-center differences are defined, respectively, via

$$D\phi_{i+1/2} = \frac{\phi_{i+1} - \phi_{i-1}}{h} \quad \text{and} \quad df_i = \frac{f_{i+1/2} - f_{i-1/2}}{h}, \tag{6}$$

where ϕ_i is a cell-centered function and $f_{i+1/2}$ is an edge-centered function. The second difference is defined as

$$D^2\phi_i = d(D\phi)_i = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{h^2}. \tag{7}$$

Subsequent differences of cell-centered functions ϕ can be defined recursively via

$$D^{2k+1}\phi_{i+1/2} = D(D^{2k}\phi)_{i+1/2} \quad \text{and} \quad D^{2k+2}\phi_i = D^2(D^{2k}\phi)_i. \tag{8}$$

To define the energy at the discrete level, we introduce some more notation. Given any periodic, cell-centered grid functions ϕ and ψ, the discrete ℓ^2 inner product and norm is given by

$$\|\phi\|_2 = \sqrt{\langle \phi, \phi \rangle}, \quad \text{with} \quad \langle \phi, \psi \rangle = h \sum_{i=1}^{N} \phi_i \psi_i. \tag{9}$$

Similarly, for periodic grid edge-centered grid functions f and g , the discrete ℓ^2 inner product and norm becomes

$$\|f\|_2 = \sqrt{\langle f, f \rangle_e}, \quad \text{with} \quad \langle f, g \rangle_e = h \sum_{i=1}^{N} f_{i-1/2} g_{i-1/2}. \tag{10}$$

The following summation-by-parts formulas are available for periodic grid functions; see [5, 9, 26, 47] for the derivations:

$$\langle \phi, df \rangle = - \langle D\phi, f \rangle_e , \tag{11}$$

$$\begin{aligned} &\left\langle \phi, D^2\psi \right\rangle = - \langle D\phi, D\psi \rangle_e , \quad \left\langle \phi, D^4\psi \right\rangle = \left\langle D^2\phi, D^2\psi \right\rangle , \\ &\left\langle \phi, D^6\psi \right\rangle = - \left\langle D^3\phi, D^3\psi \right\rangle_e , \quad \left\langle D^2\phi, D^6\psi \right\rangle = \left\langle D^4\phi, D^4\psi \right\rangle , \\ &\left\langle D^4\phi, D^6\psi \right\rangle = - \left\langle D^5\phi, D^5\psi \right\rangle_e . \end{aligned} \tag{12}$$

In addition, we introduce the discrete ℓ^p $(1 \le p < +\infty)$ and ℓ^∞ norms for cell-centered grid functions ψ:

$$\|\psi\|_p = (h \sum_{i=1}^{N} |\psi_i|^p)^{1/p}, \quad \|\psi\|_\infty = \max_{1 \le i \le N} |\psi_i|. \tag{13}$$

Similar definitions hold for edge-centered functions. The correct usage should be clear from the context.

2.2. The fully discrete numerical scheme. Let ϕ be a cell-centered grid function approximating the height of the thin film. The discrete energy is defined via

$$F(\phi) := \varepsilon^{-1} \left(\frac{1}{4} \|D\phi\|_4^4 - \frac{1}{2} \|D\phi\|_2^2 + \frac{1}{4} \right) + \frac{\varepsilon}{2} \|D^2\phi\|_2^2. \tag{14}$$

This is consistent with the continuous energy (1) as $h \to 0$. The convex-concave decomposition of the energy (14) is obvious: $F(\phi) = F_c(\phi) - F_e(\phi)$, with

$$F_c(\phi) = \varepsilon^{-1} \left(\frac{1}{4} \|D\phi\|_4^4 + \frac{1}{4} \right) + \frac{\varepsilon}{2} \|D^2\phi\|_2^2, \quad F_e(\phi) = \frac{1}{2\varepsilon} \|D\phi\|_2^2. \tag{15}$$

Let $M \in \mathbb{Z}^+$, and set $s := T/M$, where T is the final time. The first order convex splitting scheme is formulated in [45]:

$$\frac{\phi_i^{n+1} - \phi_i^n}{s} = \varepsilon^{-1} \left(d \left[(D\phi^{n+1})^3 \right]_i - D^2\phi_i^n \right) - \varepsilon D^4 \phi_i^{n+1}. \tag{16}$$

The local truncation error of this scheme is $O(s + h^2)$: first order in time, second order in space.

Because of the convex splitting, scheme (16) is unconditionally uniquely solvable and unconditionally energy stable:

$$F(\phi^n) \le F(\phi^{n-1}) \le \cdots \le F(\phi^0) := \tilde{C}_0, \tag{17}$$

for all $n \ge 0$.

2.3. A few related estimates for the finite difference approximation. For simplicity of presentation, we assume N is odd. The general case can be analyzed in a similar manner to what follows but with a few more technical details. In particular, set $N = 2K + 1$. For any periodic cell-centered grid function f, its discrete Fourier representation is given by

$$f_j = \sum_{\ell=-K}^{K} \hat{f}_\ell^N \mathrm{e}^{2\ell\pi i x_j/L}, \tag{18}$$

where $\hat{f}_\ell^N$ is the discrete Fourier transform coefficient. The extension of the grid function to a smooth periodic function is conveniently obtained via Fourier interpolation:

$$f_{\mathbf{F}}(x) = \sum_{\ell=-K}^{K} \hat{f}_\ell^N \mathrm{e}^{2\ell\pi i x/L}. \tag{19}$$

In other words, replace x_j with x. For edge-centered functions, we have analogous formulas.

The following preliminary estimates are crucial to the analyses in later sections; their proofs will be given in Appendices A and B:

Lemma 2.1. *For any periodic cell-centered grid function f, we have*

$$\kappa_j \left\|\partial_x^j f_{\mathbf{F}}\right\| \le \left\|D^j f\right\|_2 \le \left\|\partial_x^j f_{\mathbf{F}}\right\|, \quad \forall 0 \le j \le k, \tag{20}$$

$$\|f_{\mathbf{F}}\|_{H^k} \le C\left(|\overline{f}| + \left\|D^k f\right\|_2\right), \quad \text{with } \overline{f} = h\sum_{i=1}^{N} f_i, \tag{21}$$

$$\left\|D^3 f\right\|_2 \le C_1 \left\|D^5 f\right\|_2, \tag{22}$$

$$\|Df\|_\infty \le C\|D^2 f\|_2, \tag{23}$$

$$\|D^j f\|_\infty \le C\|D^{j+1} f\|_2, \quad 1 \le j \le k, \tag{24}$$

$$\|D^3 f\|_2 \le C\|D^2 f\|_2^{2/3} \cdot \|D^5 f\|_2^{1/3}, \tag{25}$$

$$\|D^2 f\|_\infty \le C\|D^2 f\|_2^{5/6} \cdot \|D^5 f\|_2^{1/6}, \tag{26}$$

where $0 < \kappa_j \le 1$, $0 \le j \le k$, and $C > 0$ is a constant that is independent of h.

Lemma 2.2. *For a cell-centered grid function f, we have*

$$0 \le \|\partial_x f_{\mathbf{F}}\|^2 - \|Df\|_2^2 \le Ch^2 \|f_{\mathbf{F}}\|_{H^2}^2, \tag{27}$$

$$0 \le \left\|\partial_x^2 f_{\mathbf{F}}\right\|^2 - \left\|D^2 f\right\|_2^2 \le Ch^2 \|f_{\mathbf{F}}\|_{H^3}^2, \tag{28}$$

$$\|\partial_x^k(\partial_x f_{\mathbf{F}} - (Df)_{\mathbf{F}})\| \le Ch^2\|\partial_x^{k+3} f_{\mathbf{F}}\|, \quad \forall k \ge 0, \tag{29}$$

where $C > 0$ is a constant that is independent of h.

To analyze the finite difference scheme over a uniform grid, we have to estimate the discrete inner product involving the nonlinear terms. To achieve this, some tools in Fourier pseudo-spectral analysis are needed. Denote $\mathcal{B}^K$ as the space of trigonometric polynomials of degree up to K (note that $N = 2K+1$). For a continuous L-periodic function $\mathbf{f}$ – or more generally, for $\mathbf{f} \in L^2(0, L)$ – with the Fourier series $\mathbf{f}(x) = \sum_{\ell=-\infty}^{\infty} \hat{\mathbf{f}}_\ell \mathrm{e}^{2\ell\pi \mathrm{i} x/L}$, its projection onto the space $\mathcal{B}^K$ is the following truncated series

$$\mathcal{P}_N \mathbf{f}(x) = \sum_{\ell=-K}^{K} \hat{\mathbf{f}}_\ell \mathrm{e}^{2\ell\pi \mathrm{i} x/L}. \tag{30}$$

On the other hand, suppose that $\mathbf{f}$ is a continuous L-periodic function, which may or may not be in $\mathcal{B}^K$, we introduce the periodic cell-centered grid function $f_i = \mathbf{f}(x_i)$, which we refer to as the grid projection of $\mathbf{f}$. Moreover, the interpolation operator $\mathcal{I}_N\mathbf{f} \in \mathcal{B}^K$ is defined as

$$\mathcal{I}_N\mathbf{f}(x) = f_{\mathbf{F}}(x). \tag{31}$$

Clearly $\mathcal{I}_N\mathbf{f} \neq \mathbf{f}$, unless $\mathbf{f} \in \mathcal{B}^K$. If $\mathbf{f} \notin \mathcal{B}^K$ there is aliasing error; and the Fourier coefficients of $\mathbf{f}$ and $\mathcal{I}_N\mathbf{f}$ are different. See the related references [6, 24, 27, 44], et cetera. On the other hand, a standard approximation analysis shows that, as long as $\mathbf{f} \in H^m_{\text{per}}(0,L)$, the convergence of the derivatives of the projection and interpolation is given by

$$\|\mathbf{f}(x) - \mathcal{P}_N\mathbf{f}(x)\|_{H^k} \le Ch^{m-k}\|\mathbf{f}\|_{H^m}, \quad 0 \le k \le m, \tag{32}$$

$$\|\mathbf{f}(x) - \mathcal{I}_N\mathbf{f}(x)\|_{H^k} \le Ch^{m-k}\|\mathbf{f}\|_{H^m}, \quad 0 \le k \le m,\, m > \frac{d}{2}, \tag{33}$$

where $C > 0$ is an h-independent constant. See the related discussion on trigonometric approximation theory in [7]; a similar aliasing error control result is also available in a more recent work [25].

The following results play a very important role in the nonlinear inner product analysis; their proofs will be given in Appendices C and D.

Lemma 2.3. *Suppose $\mathbf{f},\mathbf{g} \in C_{\text{per}}(0,L)$ with edge-centered grid projections denoted by f, g, respectively.*

(1) If $\mathbf{f},\mathbf{g} \in \mathcal{B}^K$, we have

$$\langle f, g\rangle_e = (\mathbf{f},\mathbf{g})\,. \tag{34}$$

(2) More generally, the following estimates are valid:

$$|\langle f, g\rangle_e - (\mathbf{f},\mathbf{g})| \le Ch^4\left(\|\mathbf{f}\|_{H^4}\cdot\|\mathbf{g}\|_{H^2} + \|\mathbf{f}\|_{H^2}\cdot\|\mathbf{g}\|_{H^4}\right),\ \mathbf{f},\mathbf{g} \in H^4_{\text{per}}(0,L), \tag{35}$$

$$|\langle f, g\rangle_e - (\mathbf{f},\mathbf{g})| \le Ch^2\,\|\mathbf{f}\|_{H^2}\cdot\|\mathbf{g}\|_{H^2}\,,\ \mathbf{f},\mathbf{g} \in H^2_{\text{per}}(0,L), \tag{36}$$

where $C > 0$ is a constant that is independent of h.

Lemma 2.4. *Suppose f_j, $1 \le j \le 4$, are periodic cell-centered grid functions, with representations as in (18). Denote their continuous Fourier interpolants by $f_{\mathbf{F},j} =: \mathbf{f}_j$, $1 \le j \le 4$, obtained via (19). Then we have the following estimate:*

$$\begin{aligned}&\Big|\langle Df_1\cdot Df_2, Df_3\cdot Df_4\rangle_e - \ (\partial_x\mathbf{f}_1\cdot\partial_x\mathbf{f}_2, \partial_x\mathbf{f}_3\cdot\partial_x\mathbf{f}_4)\Big|\\ &\qquad\qquad \le Ch^2(\|\mathbf{f}_1\|^2_{H^3} + \|\mathbf{f}_2\|^2_{H^3})(\|\mathbf{f}_3\|^2_{H^3} + \|\mathbf{f}_4\|^2_{H^3}),\end{aligned} \tag{37}$$

where $C > 0$ is a constant that is independent of h.

2.4. A uniform-in-time H^2 bound of the numerical solution. We note that the discrete energy (14) could be rewritten as

$$F(\phi) := \frac{1}{4}\varepsilon^{-1}h\sum_{i=1}^{N}\left((D\phi)_{i-1/2} - 1\right)^2 + \frac{\varepsilon}{2}\|D^2\phi\|_2^2. \tag{38}$$

Therefore, the energy estimate (17) yields the following result

$$\|D^2\phi^n\|_2^2 \le \frac{2\tilde{C}_0}{\varepsilon}, \quad \forall\ n \ge 0. \tag{39}$$

Meanwhile, we see that the numerical scheme (16) is mass conserving:

$$\overline{\phi^k} = \overline{\phi^0} = \beta_0, \quad \forall\, k \geq 0, \qquad \text{with} \qquad \overline{f} = h \sum_{i=0}^{N-1} f_i. \tag{40}$$

Without loss of generality, we may assume that $\beta_0 = 0$. In turn, an application of elliptic regularity indicates that

$$\left\|\phi_{\mathbf{F}}^k\right\|_{H^2}^2 \leq C_0 \left\|\partial_x^2 \phi_{\mathbf{F}}^k\right\|^2 \leq C\|D^2\phi^k\|_2^2 \leq \frac{2C\tilde{C}_0}{\varepsilon}, \tag{41}$$

for any $k \geq 0$, with the estimate (20) applied in the second step.

As a consequence, the following $\ell^\infty(0,T;H^2)$ bound of the numerical solution is valid: if the initial data are sufficiently regular, say $\phi_0 \in H^2_{\text{per}}(0,L)$, then

$$\|\phi_{\mathbf{F}}\|_{\ell^\infty(0,T;H^2)} := \max_{0\leq m\leq M} \|\phi_{\mathbf{F}}^m\|_{H^2} \leq \hat{C}_{2,\varepsilon} := C\varepsilon^{-k_2}, \quad \text{with } k_2 = 1. \tag{42}$$

3. Higher order estimates of the numerical scheme

3.1. $\ell^\infty(0,T;H^m)$ **$(m \geq 3)$ bound of the scheme.** The leading order H^2 bound (42) is not sufficient to assure an error estimate with the desired improved convergence constant. In this section, we establish a uniform-in-time H^m bound, for any $m \geq 3$, of the numerical solution. Such a bound depends on ε^{-1} in a polynomial form.

Theorem 3.1. *For the numerical solution given by (16), with $\phi_0 \in H^3_{\text{per}}(0,L)$, we have*

$$\|\phi_{\mathbf{F}}\|_{\ell^\infty(0,T;H^3)} := \max_{0\leq m\leq M} \|\phi_{\mathbf{F}}^m\|_{H^3} \leq \hat{C}_{3,\varepsilon} := C\varepsilon^{-k_3}, \tag{43}$$

where k_3 is a positive integer and $C > 0$ is a constant independent of s, h, T, and ε.

Proof. Taking a discrete inner product of (16) with $-2D^6\phi^{n+1}$ gives

$$\begin{aligned}\left\|D^3\phi^{n+1}\right\|_2^2 - \left\|D^3\phi^n\right\|_2^2 + \left\|D^3(\phi^{n+1}-\phi^n)\right\|_2^2 + 2\varepsilon s\left\|D^5\phi^{n+1}\right\|_2^2 \\ = 2\varepsilon^{-1}s\left\langle D^6\phi^{n+1}, D^2\phi^n\right\rangle - 2\varepsilon^{-1}s\left\langle D^6\phi^{n+1}, d\left[(D\phi^{n+1})^3\right]\right\rangle.\end{aligned} \tag{44}$$

using the summation-by-parts formulas in (12).

For the term associated with the concave diffusion, the preliminary estimate (25) indicates that

$$\left\|D^3\phi^n\right\|_2 \leq C\left\|D^2\phi^n\right\|^{2/3} \cdot \left\|D^5\phi^n\right\|^{1/3} \leq C\hat{C}_{2,\varepsilon}^{2/3} \cdot \left\|D^5\phi^n\right\|^{1/3}, \tag{45}$$

with the uniform-in-time H^2 analysis (39) applied in the last step. Therefore, the following bound is available:

$$\begin{aligned}\left\langle D^6\phi^{n+1}, D^2\phi^n\right\rangle = & -\left\langle D^5\phi^{n+1}, D^3\phi^n\right\rangle_e \leq \left\|D^5\phi^{n+1}\right\|_2 \cdot \left\|D^3\phi^n\right\|_2 \\ & \leq C\hat{C}_{2,\varepsilon}^{2/3} \cdot \left\|D^5\phi^n\right\|_2^{1/3} \cdot \left\|D^5\phi^{n+1}\right\|_2 \\ & \leq C\varepsilon^{-4}\hat{C}_{2,\varepsilon}^2 + \frac{1}{8}\varepsilon^2(\left\|D^5\phi^{n+1}\right\|_2^2 + \left\|D^5\phi^n\right\|_2^2),\end{aligned} \tag{46}$$

with Young's inequality applied in the last step.

For the nonlinear term, summation-by-parts gives

$$\begin{aligned}-\left\langle D^6\phi^{n+1}, d\left[(D^{n+1})^3\right]\right\rangle = & \left\langle D^5\phi^{n+1}, D\left\{d\left[(D\phi^{n+1})^3\right]\right\}\right\rangle_e \\ & \leq \left\|D^5\phi^{n+1}\right\|_2 \cdot \left\|D\left\{d\left[(D^{n+1})^3\right]\right\}\right\|_2.\end{aligned} \tag{47}$$

Meanwhile, a careful expansion yields

$$D\left\{d\left[(D\phi)^3\right]\right\}_{i+1/2} = 3\left(D\phi_{i+1/2}\right)^2 D^3\phi_{i+1/2} + \left(D\phi_{i+3/2} + 2D\phi_{i+1/2}\right)\left(D^2\phi_{i+1}\right)^2 + \left(D\phi_{i-1/2} + 2D\phi_{i+1/2}\right)\left(D^2\phi_i\right)^2. \tag{48}$$

In turn, an application of the discrete Hölder inequality shows that

$$\left\|D\left\{d\left[(D\phi^{n+1})^3\right]\right\}\right\|_2 \le C\Big(\left\|D\phi^{n+1}\right\|_\infty^2 \cdot \left\|D^3\phi^{n+1}\right\|_2 + \left\|D\phi^{n+1}\right\|_\infty \cdot \left\|D^2\phi^{n+1}\right\|_\infty \cdot \left\|D^2\phi^{n+1}\right\|_2\Big). \tag{49}$$

Furthermore, the following estimates could be carried out, with the help of preliminary estimates (23), (25) and (26) in Lemma 2.1:

$$\|D^2\phi^{n+1}\|_2 \le \hat{C}_{2,\varepsilon}, \tag{50}$$

$$\|D^3\phi^{n+1}\|_2 \le C\|D^2\phi^{n+1}\|_2^{2/3} \cdot \|D^5\phi^{n+1}\|_2^{1/3} \le C\hat{C}_{2,\varepsilon}^{2/3} \cdot \|D^5\phi^{n+1}\|_2^{1/3}, \tag{51}$$

$$\|D\phi^{n+1}\|_\infty \le C\|D^2\phi^{n+1}\|_2 \le C\hat{C}_{2,\varepsilon}, \tag{52}$$

$$\|D^2\phi^{n+1}\|_\infty \le C\|D^2\phi^{n+1}\|_2^{5/6} \cdot \|D^5\phi^{n+1}\|_2^{1/6} \le C\hat{C}_{2,\epsilon}^{5/6} \cdot \|D^5\phi^{n+1}\|_2^{1/6}. \tag{53}$$

As a result, a substitution of the above inequalities into (49) leads to

$$\left\|D\left\{d\left[(D\phi^{n+1})^3\right]\right\}\right\|_2 \le C(\hat{C}_{2,\varepsilon}^{8/3} \cdot \|D^5\phi^{n+1}\|_2^{1/3} + \hat{C}_{2,\varepsilon}^{17/6} \cdot \|D^5\phi^{n+1}\|_2^{1/6}). \tag{54}$$

Going back to (47), we arrive at

$$\begin{aligned} -\left\langle D^6\phi^{n+1}, d\left[(D\phi^{n+1})^3\right]\right\rangle &\le C(\hat{C}_{2,\varepsilon}^{8/3} \cdot \|D^5\phi^{n+1}\|_2^{4/3} + \hat{C}_{2,\varepsilon}^{17/6} \cdot \|D^5\phi^{n+1}\|_2^{7/6}) \\ &\le C\varepsilon^{-4}\hat{C}_{2,\varepsilon}^{8} + \frac{1}{8}\varepsilon^2\|D^5\phi^{n+1}\|_2^2, \end{aligned} \tag{55}$$

with the Young inequality applied in the last step.

Subsequently, a substitution of (46) and (55) into (44) results in

$$\left\|D^3\phi^{n+1}\right\|_2^2 - \left\|D^3\phi^n\right\|_2^2 + \frac{3}{2}\varepsilon s\left\|D^5\phi^{n+1}\right\|_2^2 \le C_3 s + \frac{1}{4}\varepsilon s\left\|D^5\phi^n\right\|_2^2, \tag{56}$$

with $C_3 = C\varepsilon^{-5}\hat{C}_{2,\varepsilon}^8$. By denoting

$$G^n \quad := \quad \left\|D^3\phi^n\right\|_2^2 + \frac{1}{4}\varepsilon s\left\|D^5\phi^n\right\|_2^2, \tag{57}$$

we obtain

$$G^{n+1} - G^n + \frac{5}{4}\varepsilon s\left\|D^5\phi^{n+1}\right\|_2^2 \le C_3 s. \tag{58}$$

Meanwhile, the discrete elliptic regularity (22) indicates that

$$C_4 G^{n+1} \le \frac{5}{4}\left\|D^5\phi^{n+1}\right\|_2^2, \quad \text{provided that } \varepsilon s \le 1, \tag{59}$$

with $C_4 = C_1^{-2}$. Then we get

$$G^{n+1} - G^n + C_4\varepsilon s G^{n+1} \le C_3 s. \tag{60}$$

An application of induction (in time index) results in

$$G^{n+1} = (1 + C_4 s\varepsilon)^{-(n+1)}G^0 + \frac{C_3}{C_4\varepsilon} \le G^0 + \frac{C_3}{C_4\varepsilon} := \tilde{C}_3, \tag{61}$$

where $\tilde{C}_3$ is a global-in-time constant. Finally, (43) is a direct consequence of (61) and the elliptic regularity (21):

$$\left\|\phi_{\mathbf{F}}^k\right\|_{H^3} \le C \left\|D^3\phi^k\right\|_2 \le C + (G^k)^{1/2} \le C\tilde{C}_3^{1/2} := \hat{C}_{3,\varepsilon}. \tag{62}$$

Note that $\hat{C}_{3,\varepsilon}$ depends on ε^{-1} in a polynomial form, since $\hat{C}_{2,\varepsilon}$ does. This completes the proof. □

Using similar tools, a uniform-in-time H^{m_0} bound for the numerical solution could be established, for any $m_0 \ge 3$, by taking an inner product with (16) by $(-D^2)^{m_0}\phi^{n+1}$. The details are left for interested readers.

Theorem 3.2. *For the numerical solution given by (16), with $\phi_0 \in H_{\mathrm{per}}^{m_0}(0,L)$, we have*

$$\|\phi_{\mathbf{F}}\|_{\ell^\infty(0,T;H^{m_0})} := \max_{0\le m\le M} \|\phi_{\mathbf{F}}^m\|_{H^{m_0}} \le \hat{C}_{m_0,\varepsilon} := C\varepsilon^{-k_{m_0}}, \tag{63}$$

where k_{m_0} is a positive integer and $C>0$ is a positive constant that is independent of s, h, T, and ε.

Remark 3.1. *The global-in-time H^3 bound for the numerical solution, $C\tilde{C}_3^{1/2}$ in (62), depends singularly on ε. In more details, we have $C_3 = O(\varepsilon^{-13})$, $\tilde{C}_3 = O(\varepsilon^{-14})$, so that $k_3 = 7$. In addition, a careful calculation shows that $k_4 = 9$, $k_5 = 11$, ..., $k_{m_0} = 2m_0 + 1$.*

3.2. Estimates for $\left\|(\phi^{n+1}-\phi^n)_{\mathbf{F}}\right\|_{H^k}$. The following estimate is needed in later analysis.

Theorem 3.3. *Suppose that $\phi_0 \in H_{\mathrm{per}}^{k+4}(0,T)$. The numerical solution for (16) satisfies*

$$\max_{0\le n\le M-1} \|(\phi^{n+1}-\phi^n)_{\mathbf{F}}\|_{H^k} \le \hat{D}_{k,\varepsilon} s, \tag{64}$$

where $\hat{D}_{k,\varepsilon} := C\varepsilon^{n_k}$, n_k is a positive integer, and $C>0$ is a constant independent of s, h, T, and ε.

Proof. Let us define the cell centered chemical potential

$$\mu^{n+1} := -\varepsilon^{-1}\left(d\left[(D\phi^{n+1})^3\right] - D^2\phi^n\right) + \varepsilon D^4\phi^{n+1}.$$

Subsequently, the following estimates can be derived, with a repeated application of the uniform bound (63): with repeated applications of discrete Hölder and Sobolev inequalities:

$$\begin{aligned}
&\left\|D^k\left\{d\left[(D\phi^{n+1})^3\right]\right\}\right\|_2 \\
\le\;& C \sum_{i_1+i_2+i_3=k+4} \left\|D^{i_1}\phi^{n+1}\right\|_\infty \cdot \left\|D^{i_2}\phi^{n+1}\right\|_\infty \cdot \left\|D^{i_3}\phi^{n+1}\right\|_2 \\
\le\;& C \sum_{i_1+i_2+i_3=k+4} \left\|D^{i_1+1}\phi^{n+1}\right\|_2 \cdot \left\|D^{i_2+1}\phi^{n+1}\right\|_2 \cdot \left\|D^{i_3}\phi^{n+1}\right\|_2 \\
\le\;& C\tilde{\hat{C}}_{k,\varepsilon} := C \sum_{i_1+i_2+i_3=k+4} \hat{C}_{i_1+1,\varepsilon} \cdot \hat{C}_{i_2+1,\varepsilon} \cdot \hat{C}_{i_3,\varepsilon},
\end{aligned} \tag{65}$$

$$\left\|D^k(D^2\phi^n)\right\|_2 = \|D^{k+2}\phi^n\|_2 \le \hat{C}_{k+2,\varepsilon}, \tag{66}$$

$$\left\|D^k(D^4\phi^{n+1})\right\|_2 = \|D^{k+4}\phi^{n+1}\|_2 \le \hat{C}_{k+4,\varepsilon}. \tag{67}$$

In particular, we note that, in the analysis of the nonlinear term (65), a similar discrete expansion as (48) has been performed, with a discrete Hölder inequality applied, and the preliminary estimate (24) was also utilized. In turn, the numerical scheme (16) shows that

$$\begin{aligned} \|(\phi^{n+1}-\phi^n)_{\mathbf{F}}\|_{H^k} &\le Cs\|D^k\mu^{n+1}\|_2 \\ &\le Cs\Big(\left\|D^k\left\{d\left[(D\phi^{n+1})^3\right]\right\}\right\|_2 + \left\|D^{k+2}\phi^n\right\|_2 + \left\|D^{k+4}\phi^{n+1}\right\|_2\Big) \\ &\le \hat{D}_{k,\varepsilon}s, \end{aligned} \tag{68}$$

where $\hat{D}_{k,\varepsilon} := C\varepsilon^{-1}(\tilde{\hat{C}}_{k,\varepsilon}+1) + \varepsilon\hat{C}_{k+4,\varepsilon}$. We observe that the first step was based on the inequality (21) in Lemma 2.1, combined with the fact that $\overline{\phi^{n+1}-\phi^n}=0$. Also note that $\hat{D}_{k,\varepsilon}$ depends on ε^{-1} in a polynomial form, since both $\hat{C}_{k+2,\varepsilon}$ and $\hat{C}_{k+4,\varepsilon}$ do. This completes the proof. □

3.3. Some related estimates for the exact solution. We denote Φ as the exact solution of the SS equation (3), with a smooth initial data. The following estimates can be derived by performing standard energy estimates. The details are skipped for brevity.

Theorem 3.4. *Suppose that the initial data satisfy $\Phi(0)=\phi_0\in C^\infty_{\text{per}}(0,L)$. Then there is a unique global smooth solution Φ, and the following estimates are valid:*

$$\|\Phi\|_{L^\infty(0,T;H^{m_0})} \le \hat{C}^*_{m_0,\varepsilon} := C\varepsilon^{-k_{m_0}}, \quad \forall\, m_0\ge 2, \tag{69}$$

$$\|\partial_t\Phi\|_{L^\infty(0,T;H^k)} \le \hat{D}^*_{k,\varepsilon}, \quad \text{with} \quad \hat{D}^*_{k,\varepsilon} := C\varepsilon^{-n_k}, \quad \forall\, k\ge 0, \tag{70}$$

$$\left\|\partial_t^2\Phi\right\|_{L^\infty(0,T;H^k)} \le \hat{Q}^*_{k,\varepsilon}, \quad \text{with} \quad \hat{Q}^*_{k,\varepsilon} := C\varepsilon^{-m_k}, \quad \forall k\ge 0, \tag{71}$$

$$\max_{0\le n\le M-1}\left\|\Phi^{n+1}-\Phi^n\right\|_{H^k} \le s\hat{D}^*_{k,\varepsilon}, \quad \forall k\ge 0, \tag{72}$$

where k_{m_0} and n_k are positive integers and C is a positive constant independent of s, h, T, and ε.

Remark 3.2. *With the imposed periodic boundary condition, the SS equation (3) is infinitely smooth, both in space and time. This fact enables one to derive an H^m estimate of the solution, at both the analytic and numerical levels.*

Remark 3.3. *The estimates (70) and (71) are derived by taking temporal derivatives of (3) and using the $L^\infty(0,T;H^{m_0})$ estimate (69), so that the H^k norm of the first and second order temporal derivatives are converted into certain spatial H^m norms of the exact solution.*

The derivation of (72) is based on the following Taylor expansion (in time):

$$\Phi^{n+1}-\Phi^n = s\partial_t\Phi(\xi), \quad \text{with} \quad \xi\in(t^n,t^{n+1}), \tag{73}$$

combined with the established estimate (70).

Furthermore, consider the Fourier projection of the exact solution into the space $\mathcal{B}^K$, $\Phi_N(x,t)=\mathcal{P}_N\Phi(x,t)$. The following projection approximations, which we state without proof for the sake of brevity, are available:

$$\|\Phi_N\|_{L^\infty(0,T;H^k)} \le \|\Phi\|_{L^\infty(0,T;H^k)}, \tag{74}$$

$$\|\Phi_N-\Phi\|_{L^\infty(0,T;H^k)} \le Ch^{m-k}\|\Phi\|_{L^\infty(0,T;H^m)}, \tag{75}$$

$$\left\|\partial_t^\ell\Phi_N\right\|_{L^\infty(0,T;H^k)} \le \left\|\partial_t^\ell\Phi\right\|_{L^\infty(0,T;H^k)}, \quad \forall\,\ell\ge 1, \tag{76}$$

for any $0\le k\le m$. In particular, (76) comes from the fact that $\partial_t^\ell\Phi_N(x,t)$ turns out to be the Fourier projection of $\partial_t^\ell\Phi(x,t)$ onto $\mathcal{B}^K$.

We denote $\Phi_N^k(x) = \Phi_N(x, t^k)$. The following result is a consequence of Theorem 3.4 and the projection approximation estimates (74) and (76).

Theorem 3.5. *Suppose that $\Phi(0) = \phi_0 \in C^\infty_{\rm per}(0, L)$. The following estimates are valid for the projection of the solution Φ_N:*

$$\max_{0\le n\le M} \|\Phi_N^n\|_{H^{m_0}} \le \hat{C}^*_{m_0,\varepsilon} := C\varepsilon^{-k_{m_0}}, \tag{77}$$

$$\max_{0\le n\le M-1} \left\|\Phi_N^{n+1} - \Phi_N^n\right\|_{H^k} \le \hat{D}^*_{k,\varepsilon} s, \quad \hat{D}^*_{k,\varepsilon} := C\varepsilon^{-n_k}, \tag{78}$$

for any $m_0 \ge 1$ and $k \ge 0$, where k_{m_0}, n_k and m_k are positive integers and C is a constant independent of s, h, T, and ε.

4. Error analysis with an improved convergence constant

The numerical error function and its continuous extension are defined as

$$\tilde{\phi}_i^k = \Phi_N^k(x_i) - \phi_i^k, \quad \tilde{\phi}_{\mathbf{F}}^k(x) = \Phi_N^k(x) - \phi_{\mathbf{F}}^k(x), \tag{79}$$

with the formulas (18) and (19) applied in the extension. In more detail, we don't compare the numerical solution with the exact solution Φ directly; instead, we compare it with Φ_N, the Fourier projection of Φ. The advantage of this approach will be demonstrated later.

4.1. Statement of the main theorem.

The following theorem is the main result of this paper.

Theorem 4.1. *Suppose that the initial data $\phi_0 \in H^8_{\rm per}(\Omega)$ and that s and h satisfy the scaling laws*

$$s \le C\varepsilon^{J_1}, \quad h \le C\varepsilon^{J_2}, \tag{80}$$

where J_1 and J_2 are positive integers that are sufficiently large. Also assume that $\varepsilon \in (0, \varepsilon_0)$, with ε specified in Proposition 4.1. Then the following error estimate is valid:

$$\max_{1\le m\le M} \|\tilde{\phi}^m\|_2 \le \hat{R}^*(s + h^2), \quad \textit{with } \hat{R}^* = Ce^{C_0^* T}\varepsilon^{-J_0}, \tag{81}$$

where J_0 is a positive integer, C_0^* and C are positive constants that are independent of s, h and ε.

4.2. Consistency analysis and the equation for the error function.

Based on the projection approximation estimates (75) and (76), combined with the exact SS equation (3), we are able to derive the following estimate, whose proof is suppressed for simplicity:

$$\partial_t\Phi_N = \varepsilon^{-1}\left(((\partial_x\Phi_N)^3)_x - \partial_x^2\Phi_N\right) - \varepsilon\partial_x^4\Phi_N + \tau_0, \tag{82}$$

with $\|\tau_0(t)\| \le Ch^2\varepsilon^{-j_1}$ where $C > 0$ is a constant the is independent of t, ε, and N, and j_1 is a positive integer.

With the centered difference approximation taken in space, the following estimate is available:

$$\begin{aligned}\partial_t\Phi_N(x_i, t_n) = {}& \varepsilon^{-1}\left(d\left[(D\Phi_N)^3\right](x_i, t_n) - D^2\Phi_N(x_i, t_n)\right) \\ & - \varepsilon D^4\Phi_N(x_i, t_n) + \tau_1^n(x_i),\end{aligned} \tag{83}$$

with $\|\tau_1^n\| \le Ch^2\varepsilon^{-j_2}$. Subsequently, with a first order backward Euler temporal approximation taken, the following consistency estimate could be derived:

$$\begin{aligned}\frac{\Phi_N^{n+1}-\Phi_N^n}{s}(x_i) = {} & \varepsilon^{-1}\left(d\left[(D\Phi_N^{n+1})^3\right](x_i) - D^2\Phi_N^{n+1}(x_i)\right) \\ & - \varepsilon D^4\Phi_N^{n+1}(x_i) + \tau_2^{n+1}(x_i),\end{aligned} \tag{84}$$

where $\|\tau_2^{n+1}\|_2 \le C(s+h^2)\varepsilon^{-j_3}$.

For the numerical scheme (16), we rewrite it in an alternate form, to facilitate the error analysis presented later. The following consistency holds:

$$\frac{\phi^{n+1}-\phi^n}{s} = \varepsilon^{-1}\left(d\left[(D\phi^{n+1})^3\right] - D^2\phi^{n+1}\right) - \varepsilon D^4\phi^{n+1} + \tau_3^{n+1}, \tag{85}$$

where $\|\tau_3^{n+1}\|_2 \le C(s+h^2)\varepsilon^{-j_4}$.

Remark 4.1. *We note that the temporal discretization for both the approximate projection solution (84) and the numerical solution (85) is very different from the original numerical scheme (16). The purpose for these forms are to simplify the error analysis with an improved convergence constant, as will be observed later.*

The only truncation error estimate appearing in (82) come from the projection error, and the projection estimate (74) is applied to bound $\|\tau_0^{n+1}\|$. In (83), the finite difference truncation error is taken into consideration; we refer the readers the related references [5, 47] *for more detailed derivations. In the derivation of (84), the second order temporal derivative of the projection solution in involved in τ_2, in which the projection estimate (74) is applied.*

Similarly, for the numerical solution, the truncation error term τ_3 comes from the difference between $D^2\phi^{n+1}$ and $D^2\phi^n$, by a comparison with the numerical scheme (16). In turn, the quantity $\|D^2(\phi^{n+1}-\phi^n)\|_2$ could be controlled in the following way, with the help of Theorem 3.3:

$$\|D^2(\phi^{n+1}-\phi^n)\|_2 \le s\hat{D}_{2,\varepsilon}, \quad \textit{by taking } k=2 \textit{ in (64).} \tag{86}$$

Subtracting (84) from the reformulated numerical scheme (85) yields

$$\frac{\tilde{\phi}^{n+1}-\tilde{\phi}^n}{s} = \varepsilon^{-1}\left(d\left[(D\Phi_N^{n+1})^3 - (D\phi^{n+1})^3\right] - D^2\tilde{\phi}^{n+1}\right) - \varepsilon D^4\tilde{\phi}^{n+1} + \tau^{n+1} \tag{87}$$

where $\|\tau^{n+1}\|_2 \le C(s+h^2)\varepsilon^{-j_5}$.

4.3. A preliminary estimate for the numerical error term. By a comparison between (63) (in Theorem 3.2), (64) (in Theorem 3.3) and (77) – (78) (for the approximate projection solution) in Theorem 3.5, the following estimates are straightforward.

Lemma 4.1. *For the numerical error function, we have*

$$\max_{0\le n\le M} \|\tilde{\phi}_{\mathbf{F}}^n\|_{H^{m_0}} \le \hat{C}^{**}_{m_0,\varepsilon} := C\varepsilon^{-k_{m_0}}, \tag{88}$$

$$\max_{0\le n\le M-1} \|\tilde{\phi}_{\mathbf{F}}^{n+1} - \tilde{\phi}_{\mathbf{F}}^n\|_{H^k} \le \hat{D}^{**}_{k,\varepsilon}s, \quad \hat{D}^{**}_{k,\varepsilon} := C\varepsilon^{-n_k}, \tag{89}$$

for any $m_0 \ge 1$ and $k \ge 0$, where k_{m_0}, n_k and m_k are given integers and C is a constant independent of s, h, T, and ε.

Remark 4.2. *Note that these bounds for the numerical error function do not rely on the error and convergence analysis; all of them are final time independent.*

4.4. Review of the spectrum estimate for the linearized operator. The linearized spectrum estimate for the Cahn-Hilliard equation has been established in [1, 2, 11, 21]. We recall it here.

Proposition 4.1. *([21]) There exist $0 < \varepsilon_0 << 1$ and another positive constant C_0 such that the principle eigenvalue of the linearized Cahn-Hilliard operator satisfies*

$$\lambda_{CH} := \inf_{\psi \in H^1, \psi \neq 0} \frac{\varepsilon^{-1}\left(\left(3\Phi^2(t) - 1\right)\psi, \psi\right) + \varepsilon \left\|\nabla \psi\right\|^2}{\|\psi\|_{H^{-1}}^2} \geq -C_0, \tag{90}$$

for any $t \geq 0$, $\varepsilon \in (0, \varepsilon_0)$, where Φ is the exact solution to the Cahn-Hilliard problem.

For the 1-D SS model (3), we have a similar result, under the periodic boundary condition.

Proposition 4.2. *There exist $0 < \varepsilon_0 << 1$ and another positive constant C_0 such that the principle eigenvalue of the linearized SS operator satisfies*

$$\lambda_{SS} := \inf_{\psi \in H^2_{\mathrm{per}}(0,L),\ \psi \neq 0} \frac{\varepsilon^{-1}\left(\left(3(\partial_x\Phi)^2(t) - 1\right)\partial_x\psi, \partial_x\psi\right) + \varepsilon \left\|\partial_x^2 \psi\right\|^2}{\|\psi\|^2} \geq -C_0, \tag{91}$$

for any $t \geq 0$, $\varepsilon \in (0, \varepsilon_0)$, where Φ is the exact solution to the 1-D SS problem.

Remark 4.3. *The spectrum analysis (90) was derived for the linearized Cahn-Hilliard operator [1, 2, 11], under a homogeneous Neumann boundary condition. An extension of this analysis to the one with the periodic boundary condition is straightforward, and the details are skipped for the sake of brevity. Estimate (91) is a direct application of this extension in the one-dimensional case, upon observing that the slope function $\partial_x\Phi$ satisfies the Cahn-Hilliard equation.*

4.5. Error analysis: Proof of Theorem 4.1. Taking a discrete inner product of (87) with $2\tilde{\phi}^{n+1}$ gives

$$\begin{aligned} &\|\tilde{\phi}^{n+1}\|_2^2 - \|\tilde{\phi}^n\|_2^2 + \|\tilde{\phi}^{n+1} - \tilde{\phi}^n\|_2^2 + 2\varepsilon s\|D^2\tilde{\phi}^{n+1}\|_2^2 - 2s\varepsilon^{-1}\|D\tilde{\phi}^{n+1}\|_2^2 \\ &+ 2\varepsilon^{-1}s\left\langle (D\Phi_N^{n+1})^3 - (D\phi^{n+1})^3, D\tilde{\phi}^{n+1}\right\rangle_e = 2s\langle \tau^{n+1}, \tilde{\phi}^{n+1}\rangle, \end{aligned} \tag{92}$$

with repeated application of the summation-by-parts formulas.

The term associated with the truncation error has the following bound:

$$2\langle \tau^{n+1}, \tilde{\phi}^{n+1}\rangle \leq \|\tau^{n+1}\|_2^2 + \|\tilde{\phi}^{n+1}\|_2^2. \tag{93}$$

For the concave diffusion term, we apply (27) (in Lemma 2.2) and get

$$\|\partial_x\tilde{\phi}_{\mathbf{F}}^{n+1}\|^2 - \|D\tilde{\phi}^{n+1}\|_2^2 \leq Ch^2\|\tilde{\phi}_{\mathbf{F}}^{n+1}\|_{H^2}^2 \leq Ch^2\|\partial_x^2\tilde{\phi}_{\mathbf{F}}^{n+1}\|^2. \tag{94}$$

To obtain a sharper bound on the right hand side, we have

$$\|\partial_x^2\tilde{\phi}_{\mathbf{F}}^{n+1}\|^2 \leq C\|\tilde{\phi}_{\mathbf{F}}^{n+1}\|_{H^4} \cdot \|\tilde{\phi}_{\mathbf{F}}^{n+1}\| \leq C\hat{C}_{4,\varepsilon}^{**}\|\tilde{\phi}_{\mathbf{F}}^{n+1}\|, \tag{95}$$

with the preliminary estimate (88) (in Lemma 4.1) applied in the last step. This in turn yields

$$\|\partial_x\tilde{\phi}_{\mathbf{F}}^{n+1}\|^2 - \|D\tilde{\phi}^{n+1}\|_2^2 \leq C\hat{C}_{4,\varepsilon}^{**}h^2\|\tilde{\phi}_{\mathbf{F}}^{n+1}\| \leq \frac{\varepsilon}{8}\|\tilde{\phi}_{\mathbf{F}}^{n+1}\|^2 + C\varepsilon^{-1}h^4(\hat{C}_{4,\varepsilon}^{**})^2. \tag{96}$$

The surface diffusion term could be analyzed in the same manner, with the help of (28) (in Lemma 2.2). We state the result here; the details are skipped for the sake of brevity.

$$\|\partial_x^2\tilde{\phi}_{\mathbf{F}}^{n+1}\|^2 - \|D^2\tilde{\phi}^{n+1}\|_2^2 \leq C\hat{C}_{6,\varepsilon}^{**}h^2\|\tilde{\phi}_{\mathbf{F}}^{n+1}\| \leq \|\tilde{\phi}_{\mathbf{F}}^{n+1}\|^2 + Ch^4(\hat{C}_{6,\varepsilon}^{**})^2. \tag{97}$$

The rest work is focused on the following nonlinear inner product:

$$\begin{aligned} I_1^{(d)} &:= \langle (D\Phi_N^{n+1})^3 - (D\phi^{n+1})^3, D\tilde{\phi}^{n+1} \rangle_e \\ &= \langle (D\Phi_N^{n+1})^2 + D\Phi_N^{n+1} D\phi^{n+1} + (D\phi^{n+1})^2, (D\tilde{\phi}^{n+1})^2 \rangle_e . \end{aligned} \tag{98}$$

Meanwhile, we denote its continuous version as

$$I_1 := \left((\partial_x \Phi_N^{n+1})^2 + \partial_x \Phi_N^{n+1} \cdot \partial_x \phi_{\mathbf{F}}^{n+1} + (\partial_x \phi_{\mathbf{F}}^{n+1})^2, (\partial_x \tilde{\phi}_{\mathbf{F}}^{n+1})^2 \right). \tag{99}$$

The difference $I_1^{(d)} - I_1$ can be analyzed with the help of Lemma 2.4. We see that $\Phi_N \in \mathcal{B}^K$, $\phi_{\mathbf{F}}$ and $\tilde{\phi}_{\mathbf{F}}$ are the continuous extensions of ϕ and $\tilde{\phi}$, respectively, so that an application of (37) leads to an estimate of the middle term:

$$\begin{aligned} &\left| \left\langle D\Phi_N^{n+1} D\phi^{n+1}, (D\tilde{\phi}^{n+1})^2 \right\rangle_e - \left(\partial_x \Phi_N^{n+1} \cdot \partial_x \phi_{\mathbf{F}}^{n+1}, (\partial_x \tilde{\phi}_{\mathbf{F}}^{n+1})^2 \right) \right| \\ &\quad \le C h^2 \|\tilde{\phi}_{\mathbf{F}}^{n+1}\|_{H^3}^2 (\|\Phi_N^{n+1}\|_{H^3}^2 + \|\phi_{\mathbf{F}}^{n+1}\|_{H^3}^2) \le C h^2 \|\tilde{\phi}_{\mathbf{F}}^{n+1}\|_{H^3}^2 (\hat{C}_{3,\varepsilon}^2 + (\hat{C}_{3,\varepsilon}^*)^2) \\ &\quad \le C h^2 \varepsilon^{-2k_3} \|\tilde{\phi}_{\mathbf{F}}^{n+1}\|_{H^3}^2 \le C h^2 \varepsilon^{-2k_3} \hat{C}_{6,\varepsilon}^{**} \|\tilde{\phi}_{\mathbf{F}}^{n+1}\| \\ &\quad \le \hat{R}_{0,\varepsilon}^* h^4 + \frac{\varepsilon}{12} \|\tilde{\phi}_{\mathbf{F}}^{n+1}\|^2, \quad \hat{R}_{0,\varepsilon}^* = C \varepsilon^{-4k_3 - 1} (\hat{C}_{6,\varepsilon}^{**})^2, \end{aligned} \tag{100}$$

in which the established estimates (63), (77) and (88), along with the Sobolev inequality $\|\tilde{\phi}_{\mathbf{F}}^{n+1}\|_{H^3}^2 \le C \hat{C}_{6,\varepsilon}^{**} \|\tilde{\phi}_{\mathbf{F}}^{n+1}\|$ (as derived in (97)), have been applied. The two other terms could be analyzed in the same way. Then we get

$$|I_1^{(d)} - I_1| \le 3 \hat{R}_{0,\varepsilon}^* h^4 + \frac{\varepsilon}{4} \|\tilde{\phi}_{\mathbf{F}}^{n+1}\|^2. \tag{101}$$

Before further analysis of the nonlinear term, we make an a-priori assumption about the numerical error.

4.5.1. An a-priori assumption up to time step t^n. We assume a-priori that the numerical error function has the desired convergence as given by (81), at time steps up to t^n.

$$\|\tilde{\phi}_{\mathbf{F}}^{\ell}\| \le \hat{R}^* \left(s + h^2 \right), \quad \text{with } \hat{R}^* = C e^{C_0^* T} \varepsilon^{-J_0}, \ \ell \le n. \tag{102}$$

For the continuous inner product I_1 in (99), we begin with the following identity:

$$\begin{aligned} (\partial_x \Phi_N^{n+1})^2 + \partial_x \Phi_N^{n+1} \cdot \partial_x \phi_{\mathbf{F}}^{n+1} + (\partial_x \phi_{\mathbf{F}}^{n+1})^2 = 3 (\partial_x \Phi_N^{n+1})^2 - 3 \partial_x \Phi_N^{n+1} \cdot \partial_x \tilde{\phi}_{\mathbf{F}}^{n+1} \\ + (\partial_x \tilde{\phi}_{\mathbf{F}}^{n+1})^2. \end{aligned} \tag{103}$$

This in turn shows that

$$I_1 \ge 3 \left((\partial_x \Phi_N^{n+1})^2, (\partial_x \tilde{\phi}_{\mathbf{F}}^{n+1})^2 \right) + \mathcal{I}E, \quad \mathcal{I}E = -3 \left((\partial_x \Phi_N^{n+1}), (\partial_x \tilde{\phi}_{\mathbf{F}}^{n+1})^3 \right). \tag{104}$$

Furthermore, we obtain

$$\begin{aligned} |\mathcal{I}E| &\le 3 \|\partial_x \Phi_N^{n+1}\|_{L^\infty} \cdot \|\partial_x \tilde{\phi}_{\mathbf{F}}^{n+1}\|_{L^3}^3 \le C \left\| \Phi_N^{n+1} \right\|_{H^2} \cdot \|\partial_x \tilde{\phi}_{\mathbf{F}}^{n+1}\|_{L^3}^3 \\ &\le C \hat{C}_{2,\varepsilon}^* \|\partial_x \tilde{\phi}_{\mathbf{F}}^{n+1}\|_{L^3}^3, \end{aligned} \tag{105}$$

with the estimate (69) applied in the last step. Meanwhile, based on the identity $\partial_x \tilde{\phi}_{\mathbf{F}}^{n+1} = \partial_x \tilde{\phi}_{\mathbf{F}}^{n} + \partial_x \left(\tilde{\phi}_{\mathbf{F}}^{n+1} - \tilde{\phi}_{\mathbf{F}}^{n} \right)$, the following analysis is performed:

$$\begin{aligned} \|\partial_x \tilde{\phi}_{\mathbf{F}}^{n+1}\|_{L^3}^3 &\le C \left(\|\partial_x \tilde{\phi}_{\mathbf{F}}^{n}\|_{L^3}^3 + \|\partial_x (\tilde{\phi}_{\mathbf{F}}^{n+1} - \tilde{\phi}_{\mathbf{F}}^{n})\|_{L^3}^3 \right) \\ &\le C \left(\|\partial_x \tilde{\phi}_{\mathbf{F}}^{n}\|_{L^3}^3 + \|\tilde{\phi}_{\mathbf{F}}^{n+1} - \tilde{\phi}_{\mathbf{F}}^{n}\|_{H^2}^3 \right) \\ &\le C \left(\|\partial_x \tilde{\phi}_{\mathbf{F}}^{n}\|_{L^3}^3 + s^3 (\hat{D}_{2,\varepsilon}^{**})^3 \right), \end{aligned} \tag{106}$$

with the preliminary estimate (89) applied in the last step. Moreover, the Sobolev inequalities indicate that

$$\begin{aligned} \|\partial_x \tilde{\phi}_{\mathbf{F}}^{n}\|_{L^3} \le C \|\tilde{\phi}_{\mathbf{F}}^{n}\|_{H^{7/6}} &\le C \|\tilde{\phi}_{\mathbf{F}}^{n}\|^{\frac{23}{30}} \cdot \|\tilde{\phi}_{\mathbf{F}}^{n}\|_{H^5}^{\frac{7}{30}} \\ &\le C (\hat{C}_{5,\varepsilon}^{**})^{\frac{7}{30}} (\hat{R}^*)^{\frac{23}{30}} (s+h^2)^{\frac{23}{30}}, \end{aligned} \tag{107}$$

in which the estimate (88) and the a-priori assumption (102) was recalled in the last step. Subsequently, a substitution of (106) and (107) into (105) yields

$$|\mathcal{I}E| \le \hat{R}_{2,\varepsilon}^* (s^{\frac{23}{10}} + h^{\frac{23}{5}}) + \hat{R}_{3,\varepsilon}^* s^3, \tag{108}$$

with $\hat{R}_{2,\varepsilon}^* = C \hat{C}_{2,\varepsilon}^* (\hat{C}_{5,\varepsilon}^{**})^{\frac{7}{10}} (\hat{R}^*)^{\frac{23}{10}}$, $\hat{R}_{3,\varepsilon}^* = C \hat{C}_{2,\varepsilon}^* (\hat{D}_{2,\varepsilon}^{**})^3$.

Finally, a combination of (92), (93), (96), (97), (101) and (108) leads to

$$\begin{aligned} &\|\tilde{\phi}^{n+1}\|_2^2 - \|\tilde{\phi}^{n}\|_2^2 - s\|\tau^{n+1}\|_2^2 \\ &\quad + 2s\Big(\varepsilon^{-1} \left(3 \left((\partial_x \Phi_N^{n+1})^2, (\partial_x \tilde{\phi}_{\mathbf{F}}^{n+1})^2 \right) - \|\partial_x \tilde{\phi}_{\mathbf{F}}^{n+1}\|^2 \right) + \varepsilon \|\partial_x^2 \tilde{\phi}_{\mathbf{F}}^{n+1}\|^2 \Big) \\ &\quad \le 2s\|\tilde{\phi}^{n+1}\|_2^2 + \hat{R}_{1,\varepsilon}^* s(s^2+h^4) + 2\varepsilon^{-1} s (\hat{R}_{2,\varepsilon}^* (s^{\frac{23}{10}} + h^{\frac{23}{5}}) + \hat{R}_{3,\varepsilon}^* s^3), \end{aligned} \tag{109}$$

with $\hat{R}_{1,\varepsilon}^* = C(\varepsilon^{-1} \hat{R}_{0,\varepsilon}^* + \varepsilon^{-2} (\hat{C}_{4,\varepsilon}^{**})^2 + \varepsilon (\hat{C}_{6,\varepsilon}^{**})^2)$. The linearized spectrum estimate (91) (reviewed in Proposition 4.2) implies that

$$\varepsilon^{-1} \left(3 \left((\partial_x \Phi_N^{n+1})^2, (\partial_x \tilde{\phi}_{\mathbf{F}}^{n+1})^2 \right) - \|\partial_x \tilde{\phi}_{\mathbf{F}}^{n+1}\|^2 \right) + \varepsilon \|\partial_x^2 \tilde{\phi}_{\mathbf{F}}^{n+1}\|^2 \ge -C_0 \|\tilde{\phi}^{n+1}\|^2. \tag{110}$$

Its substitution into (109) yields

$$\begin{aligned} \|\tilde{\phi}^{n+1}\|_2^2 - \|\tilde{\phi}^{n}\|_2^2 \quad &\le \quad (2C_0+2)s\|\tilde{\phi}^{n+1}\|_2^2 + \hat{R}_{4,\varepsilon}^* s(s^2+h^4) \\ &\quad + 2\varepsilon^{-1} s \hat{R}_{2,\varepsilon}^* (s^{\frac{23}{10}} + h^{\frac{23}{5}}), \end{aligned} \tag{111}$$

with $\hat{R}_{4,\varepsilon}^* = \varepsilon^{-2j_5} + \hat{R}_{1,\varepsilon}^* + 2\hat{R}_{3,\varepsilon}^* \varepsilon^{-1} s$. Under the condition that

$$\varepsilon^{-1} \hat{R}_{2,\varepsilon}^* s^{\frac{3}{10}} \le \frac{1}{2}, \ \varepsilon^{-1} \hat{R}_{2,\varepsilon}^* h^{\frac{3}{5}} \le \frac{1}{2}, \quad \text{i.e.} \quad \min(s,h) \le (\frac{\varepsilon}{2})^{\frac{10}{3}} (\hat{R}_{2,\varepsilon}^*)^{-\frac{10}{3}}, \tag{112}$$

we get

$$\|\tilde{\phi}^{n+1}\|_2^2 - \|\tilde{\phi}^{n}\|_2^2 \le (2C_0+2)s\|\tilde{\phi}^{n+1}\|_2^2 + \hat{R}_{5,\varepsilon}^* s(s^2+h^4), \tag{113}$$

with $\hat{R}_{5,\varepsilon}^* = 2\hat{R}_{4,\varepsilon}^* + 1$. Most importantly, observe that $2C_0+2$ is a constant independent of ε, and $\hat{R}_{5,\varepsilon}^*$ is independent of $\hat{R}^*$ appearing in (102). Clearly, $\hat{R}_{5,\varepsilon}^*$ depends on ε^{-1} in a polynomial form. An application of discrete Gronwall inequality to (113) results the desired error analysis:

$$\|\tilde{\phi}^{n+1}\|_2^2 \le C e^{(2C_0+2)T} \hat{R}_{5,\varepsilon}^* (s^2+h^4). \tag{114}$$

4.5.2. Recovery of the a-priori assumption (102). In turn, we can take $C_0^* = C_0 + 1$, and the integer index J_0 could be chosen according to the form of $\hat{R}_{5,\varepsilon}^*$, to recover the a-priori assumption (102) at time step t^{n+1}.

Moreover, $\hat{R}^*$ is determined by this convergence result, so is $\hat{R}_{2,\varepsilon}^*$, given by $\hat{R}_{2,\varepsilon}^* = C\hat{C}_{2,\varepsilon}^* (\hat{C}_{5,\varepsilon}^{**})^{\frac{7}{10}} (\hat{R}^*)^{\frac{23}{10}}$. As a result, condition (112) for s and h could be converted into the form of (80). The proof of Theorem 4.1 is complete.

Remark 4.4. *The time step and mesh size have to satisfy the scaling law as indicated in (80): $s \le C\varepsilon^{J_1}$, $h \le C\varepsilon^{J_2}$. A preliminary calculation shows that $J_1 \ge 20$, $J_2 \ge 20$.*

Note that these two integer numbers have larger values than the ones reported in [19, 21]*, for a few reasons. The Allen-Cahn model covered in* [19] *has a well-known maximum principle, which in turn would greatly simplify the corresponding analysis. The Cahn-Hilliard model analyzed in* [21] *does not have the maximum principle, while its degree of nonlinearity is lower than the SS model, due to the fact that ϕ_x satisfies the SS equation, as given by (4). In addition, only an H^{-1} truncation error needs to be estimated in the Cahn-Hilliard model, in comparison with the L^2 truncation error presented in this article. This fact also makes the truncation error dependent on ε^{-1} in a higher degree polynomial form.*

In addition, the aliasing error estimates are needed in the finite difference analysis for the nonlinear error terms, which in turn requires higher regularity of the exact solution and numerical solution. This subtle fact also makes the numerical error dependent on ε^{-1} in a higher degree polynomial form; in comparison, the finite element approximations were applied in [19, 21]*, and no aliasing error needs to be estimated.*

Remark 4.5. *The authors are aware of the limitation of the 1-D SS equation (4). In fact, the multi-dimensional versions have been extensively studied in many recent articles* [36, 40, 43, 45]*, with local in time convergence analyses provided. However, all the estimates are involved with a convergence constant dependent on ε^{-1} in an exponential growth form, which comes from an application of discrete Gronwall inequality. The technique presented in this article could not be directly applied to the multi-dimensional SS model, because of a key fact that, the linearized spectrum estimate, as given by (4.2) for the 1-D equation, is not available for the multi-dimensional SS model.*

5. Conclusions

An improved error analysis is provided for an energy stable finite difference scheme to the 1-D slope selection equation. A uniform-in-time H^m bound of the numerical solution, for any $m \ge 3$, is obtained through Sobolev estimates at a discrete level. To avoid a convergence constant of the form $\exp(CT\varepsilon^{-m})$, we apply a spectrum estimate for the linearized operator associated with the 1-D SS gradient flow, so that an application of the discrete Gronwall inequality leads to a convergence constant dependent on ε^{-1} only in a polynomial order.

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Appendix A. Proof of Lemma 2.1

Proof. For the cell-centered grid function f and its smooth extension $f_{\mathbf{F}}$, given by (18) and (19), Parseval identity (at both the discrete and continuous levels) implies that

$$\|f\|_2^2 = \|f_{\mathbf{F}}\|_{L^2}^2 = L \sum_{\ell=-K}^{K} |\hat{f}_\ell^N|^2, \quad \text{since } hN = L. \tag{115}$$

For the comparison between the discrete and continuous gradient, we start with the following Fourier expansions:

$$Df_{j+1/2} = \sum_{\ell=-K}^{K} \mu_\ell \hat{f}_\ell^N \mathrm{e}^{2\ell\pi i x_{j+1/2}/L}, \quad \mu_\ell = -\frac{2i\sin\frac{\ell\pi h}{L}}{h}, \tag{116}$$

$$\partial_x f_{\mathbf{F}}(x) = \sum_{\ell=-K}^{K} \nu_\ell \hat{f}_\ell^N \mathrm{e}^{2\ell\pi i x/L}, \quad \nu_\ell = -\frac{2i\ell\pi}{L}. \tag{117}$$

In turn, an application of Parseval identity yields

$$\|Df\|_2^2 = L \sum_{\ell=-K}^{K} |\mu_\ell|^2 |\hat{f}_\ell^N|^2, \quad \|\partial_x f_{\mathbf{F}}\|_{L^2}^2 = L \sum_{\ell=-K}^{K} |\nu_\ell|^2 |\hat{f}_\ell^N|^2. \tag{118}$$

Comparison between $|\mu_\ell|$ and $|\nu_\ell|$ shows that

$$\frac{2}{\pi}|\nu_\ell| \le |\mu_\ell| \le |\nu_\ell|, \quad \text{for} \quad -\mathrm{K} \le \ell \le \mathrm{K}. \tag{119}$$

This indicates that

$$\frac{2}{\pi}\|\partial_x \phi_{\mathbf{F}}\|_{L^2} \le \|D\phi\|_2 \le \|\partial_x \phi_{\mathbf{F}}\|_{L^2}, \tag{120}$$

which gives (20) in Lemma 2.1, with $j = 1$. It can be proved analogously that

$$(2\pi^{-1})^j \|\partial_x^j \phi_{\mathbf{F}}\|_{L^2} \le \|D^j \phi\|_2 \le \|\partial_x^j \phi_{\mathbf{F}}\|_{L^2}, \quad \forall j \ge 1, \tag{121}$$

so that (20) has been established.

Estimate (22) is a direct consequence of (121), combined with the elliptic regularity at the continuous level:

$$\left\|D^3 f\right\|_2 \le \left\|\partial_x^3 f_{\mathbf{F}}\right\| \le C_1^* \left\|\partial_x^5 f_{\mathbf{F}}\right\| \le C_1^* (D_5)^{-1} \left\|D^5 f\right\|_2, \tag{122}$$

where C_1^* is the elliptic regularity constant at the continuous level. In turn, (22) is valid by taking $C_1 = C_1^*(D_5)^{-1}$.

Similarly, (21) could be derived as follows:

$$\|f_{\mathbf{F}}\|_{H^k} \le C\left(\int_\Omega f_{\mathbf{F}}\, dx + \|\partial_x^k f_{\mathbf{F}}\|\right) \le C\left(|\overline{f}| + \|D^k f_{\mathbf{F}}\|_2\right), \tag{123}$$

in which the elliptic regularity is applied in the first step, and the fact that $\int_\Omega f_{\mathbf{F}}\, dx = \overline{f}$ is observed in the second step, and the estimate (20) has also been recalled.

For (23), we define the edge-centered grid function $g_{i+1/2} = Df_{i+1/2}$ and denote its smooth extension as $g_{\mathbf{F}}$, with the extension formula given by (19). Based on the discrete Fourier expansion (116) for $g = Df$, we see that the continuous expansion for $g_{\mathbf{F}}$ becomes

$$g_{\mathbf{F}} = \sum_{\ell=-K}^{K} \mu_\ell \hat{f}_\ell^N \mathrm{e}^{2\ell\pi i x/L}, \quad \mu_\ell = -\frac{2i\sin\frac{\ell\pi h}{L}}{h}. \tag{124}$$

In turn, we have the following estimates for $\partial_x g_{\mathbf{F}}$:

$$\partial_x g_{\mathbf{F}} = \sum_{\ell=-K}^{K} \mu_\ell \cdot \frac{2\ell\pi i}{L} \cdot \hat{f}_\ell^N \mathrm{e}^{2\ell\pi i x/L}, \quad \text{so that} \tag{125}$$

$$\|\partial_x g_{\mathbf{F}}\|^2 = L \sum_{\ell=-K}^{K} |\mu_\ell|^2 \cdot \left|\frac{2\ell\pi i}{L}\right|^2 \cdot |\hat{f}_\ell^N|^2 \le L \sum_{\ell=-K}^{K} |\nu_\ell|^4 |\hat{f}_\ell^N|^2 = \|\partial_x^2 f_{\mathbf{F}}\|^2, \tag{126}$$

where the last step is based on the fact that $|\mu_\ell| \cdot \left|\frac{2\ell\pi i}{L}\right| \le |\nu_\ell|$, with ν_ℓ given by (117). Moreover, the discrete maximum norm of $g = Df$ could be analyzed as follows:

$$\|Df\|_\infty = \|g\|_\infty \le \|g_{\mathbf{F}}\|_{L^\infty} \le C\,\|\partial_x g_{\mathbf{F}}\| \le C\,\left\|\partial_x^2 f_{\mathbf{F}}\right\| \le C\,\left\|D^2 f\right\|_2. \tag{127}$$

We note that the second step comes from the fact that the edge-centered grid function g is the projection/evaluation of $g_{\mathbf{F}}$ to/at the grid points. The third step is based on the 1-D Sobolev embedding; (126) is applied in the fourth step; and the estimate (20) is recalled in the last step. This finishes the proof of (23).

Inequality (24) could be established in the same manner, we skip the details for the sake of brevity.

Estimates (25) and (26) could be derived with the help of the Sobolev inequalities, combined with (20):

$$\|Df\|_2 \le \|\partial_x^3 f_{\mathbf{F}}\| \le C\|\partial_x^2 f_{\mathbf{F}}\|^{2/3} \cdot \|\partial_x^5 f_{\mathbf{F}}\|^{1/3} \le C\|D^2 f\|_2^{2/3} \cdot \|D^5 f\|_2^{1/3}, \tag{128}$$

$$\|D^2 f\|_\infty \le C\|\partial_x^2 f_{\mathbf{F}}\|^{5/6} \cdot \|\partial_x^5 f_{\mathbf{F}}\|^{1/6} \le C\|D^2 f\|_2^{5/6} \cdot \|D^5 f\|_2^{1/6}, \tag{129}$$

with the first step in (129) derived in the same manner as (124)-(127).

The proof of Lemma 2.1 is complete. □

Appendix B. Proof of Lemma 2.2

Proof. The discrete Fourier expansion (18) for f and its continuous extension (19) yields

$$D^2 f_j = \sum_{\ell=-K}^{K} \lambda_\ell \hat{f}_\ell^N \mathrm{e}^{2\ell\pi i x_j/L}, \quad \lambda_\ell = -\left(\frac{2\sin\frac{\ell\pi h}{L}}{h}\right)^2, \tag{130}$$

$$\partial_x^2 f_{\mathbf{F}}(x) = \sum_{\ell=-K}^{K} \Lambda_\ell \hat{f}_\ell^N \mathrm{e}^{2\ell\pi i x/L}, \quad \Lambda_\ell = -\left(\frac{2\ell\pi}{L}\right)^2. \tag{131}$$

Subsequently, we apply the Parseval equality and get

$$\|\partial_x f_{\mathbf{F}}\|^2 - \|Df\|_2^2 = L \sum_{\ell=-K}^{K} \left(|\nu_\ell|^2 - |\mu_\ell|^2\right) \left|\hat{f}_\ell^N\right|^2, \quad \text{(by (118))}, \tag{132}$$

$$\left\|D^2 f\right\|_2^2 = L \sum_{\ell=-K}^{K} |\lambda_\ell|^2 \cdot \left|\hat{f}_\ell^N\right|^2, \quad \left\|\partial_x^2 f_{\mathbf{F}}\right\|^2 = L \sum_{\ell=-K}^{K} |\Lambda_\ell|^2 \cdot \left|\hat{f}_\ell^N\right|^2, \tag{133}$$

so that

$$\left\|\partial_x^2 f_{\mathbf{F}}\right\|^2 - \left\|D^2 f\right\|_2^2 = L \sum_{\ell=-K}^{K} \left(|\Lambda_\ell|^2 - |\lambda_\ell|^2\right) \left|\hat{f}_\ell^N\right|^2, \tag{134}$$

with μ_ℓ and ν_ℓ given by (116), (117). Furthermore, the following estimates are available:

$$|\nu_\ell| + |\mu_\ell| \le 2|\nu_\ell| = \frac{4\ell\pi}{L}, \quad |\lambda_\ell| + |\Lambda_\ell| \le 2|\Lambda_\ell| = 2\left(\frac{2\ell\pi}{L}\right)^2 \tag{135}$$

$$\sin\frac{\ell\pi h}{L} = \frac{\ell\pi h}{L} - \frac{\cos\eta}{6}\left(\frac{\ell\pi h}{L}\right)^3, \quad \text{with } \eta \in (0, \tfrac{\pi}{2}), \tag{136}$$

so that

$$0 \le |\nu_\ell| - |\mu_\ell| = \frac{2\ell\pi}{L} - \frac{2\sin\frac{\ell\pi h}{L}}{h} \le \frac{h^2}{3}\left(\frac{\ell\pi}{L}\right)^3, \tag{137}$$

$$0 \le \|\nu_\ell|^2 - |\mu_\ell|^2 = (|\nu_\ell| - |\mu_\ell|)\cdot(|\nu_\ell| + |\mu_\ell|) \le \frac{h^2}{24}\left(\frac{2\ell\pi}{L}\right)^4, \tag{138}$$

$$0 \le |\Lambda_\ell|^2 - |\lambda_\ell|^2 = (|\Lambda_\ell| - |\lambda_\ell|)\cdot(|\Lambda_\ell| + |\lambda_\ell|) \le \frac{h^2}{12}\left(\frac{2\ell\pi}{L}\right)^6, \tag{139}$$

where a Taylor expansion was performed in (136), and the fact that $|\lambda| = |\mu|^2$, $|\Lambda| = |\nu|^2$ was applied in (139). Going back to (132), (134), we arrive at

$$0 \le \|\partial_x f_{\mathbf{F}}\|^2 - \|Df\|_2^2 \le \frac{L}{24}\sum_{\ell=-K}^{K} h^2 \left(\frac{2\ell\pi}{L}\right)^4 \left|\hat{f}_\ell^N\right|^2 = \frac{h^2}{24}\left\|\partial_x^2 f_{\mathbf{F}}\right\|^2, \tag{140}$$

$$0 \le \left\|\partial_x^2 f_{\mathbf{F}}\right\|^2 - \left\|D^2 f\right\|_2^2 \le \frac{L}{12}\sum_{\ell=-K}^{K} h^2 \left(\frac{2\ell\pi}{L}\right)^6 \left|\hat{f}_\ell^N\right|^2 = \frac{h^2}{12}\left\|\partial_x^3 f_{\mathbf{F}}\right\|^2. \tag{141}$$

Inequality (29) could be similarly proven, by making a comparison between the Fourier expansions of Df and $\partial_x f_{\mathbf{F}}$, given by (116), (117), combined with the estimate (137). The details are skipped for the sake of brevity.

The proof of Lemma 2.2 is complete. □

Appendix C. Proof of Lemma 2.3

Proof. (1) In addition to (18) and (19), we set the discrete Fourier expansion for g and its continuous extension given by

$$g_i = \sum_{\ell=-K}^{K} \hat{g}_\ell^N \mathrm{e}^{2\ell\pi i x_i/L}, \quad \mathbf{g}(x) = g_{\mathbf{F}}(x) = \sum_{\ell=-K}^{K} \hat{g}_\ell^N \mathrm{e}^{2\ell\pi i x/L}. \tag{142}$$

In turn, we assume the Fourier expansion for the product function $\mathbf{f}\cdot\mathbf{g}$ as

$$(\mathbf{f}\cdot\mathbf{g})(x) = \sum_{\ell=-2K}^{2K} \hat{h}_\ell^N \mathrm{e}^{2\ell\pi i x/L}. \tag{143}$$

In particular, it is observed that $\mathbf{f}\cdot\mathbf{g} \in \mathcal{B}^{2K}$. Consequently, the discrete product function $f\cdot g$ turns out to be the projection of $\mathbf{f}\cdot\mathbf{g}$ at the numerical grid points:

$$(f\cdot g)_i = (\mathbf{f}\cdot\mathbf{g})(x_i) = \mathcal{I}_N\left(\mathbf{f}\cdot\mathbf{g}\right)(x_i). \tag{144}$$

A more careful expansion shows that

$$\overline{f\cdot g} = \int_\Omega \mathcal{I}_N(\mathbf{f}\cdot\mathbf{g})dx = \int_\Omega \mathbf{f}\cdot\mathbf{g}dx, \tag{145}$$

which is equivalent to (34). In more detail, the first step comes from the fact that $\mathcal{I}_N \mathbf{f} \cdot \mathbf{g} \in \mathcal{B}^K$, and the second step is based on the fact that, there is no aliasing error on the mode of $\ell = 0$, between $\mathbf{f} \cdot \mathbf{g} \in \mathcal{B}^{2K}$ and its projection onto $\mathcal{B}^K$.

(2) In the general case, we note that f and g are discrete interpolations of $\mathcal{I}_N \mathbf{f} \in \mathcal{B}^K$ and $\mathcal{I}_N \mathbf{g} \in \mathcal{B}^K$. By (34), we arrive at

$$\begin{aligned} |\langle f, g \rangle_e - (\mathbf{f}, \mathbf{g})| &= |(\mathcal{I}_N \mathbf{f}, \mathcal{I}_N \mathbf{g}) - (\mathbf{f}, \mathbf{g})| \le |(\mathcal{I}_N \mathbf{f} - \mathbf{f}, \mathcal{I}_N \mathbf{g})| + |(\mathbf{f}, \mathcal{I}_N \mathbf{g} - \mathbf{g})| \\ &\le \|\mathcal{I}_N \mathbf{f} - \mathbf{f}\| \cdot \|\mathcal{I}_N \mathbf{g}\| + \|\mathbf{f}\| \cdot \|\mathcal{I}_N \mathbf{g} - \mathbf{g}\| \\ &\le Ch^4 \left(\|\mathbf{f}\|_{H^4} \cdot \|\mathbf{g}\|_{H^2} + \|\mathbf{f}\|_{H^2} \cdot \|\mathbf{g}\|_{H^4} \right), \end{aligned} \tag{146}$$

which gives (35), with the Fourier spectral interpolation approximation (33) applied at the last step.

Estimate (35) could be established in the same fashion. The proof of Lemma 2.3 is complete. □

Appendix D. Proof of Lemma 2.4

Proof. We assume that f_j and its continuous extension $\mathbf{f}_j$ have the following Fourier expansions, $1 \le j \le 4$:

$$(f_j)_k = \sum_{\ell=-K}^{K} \hat{f}^N_{(j),\ell} \mathrm{e}^{2\ell\pi i x_k / L}, \quad \mathbf{f}_j(x) = \sum_{\ell}^{K} \hat{f}^N_{(j),\ell} \mathrm{e}^{2\ell\pi i x / L}. \tag{147}$$

We also denote periodic grid functions $(g_j)_{k+1/2} = (Df_j)_{k+1/2}$, and denote their continuous extensions as $\mathbf{g}_j$, $1 \le j \le 4$, using a similar formula as (18) – (19). A more detailed calculation shows that

$$(g_j)_{k+1/2} = \sum_{\ell=-K}^{K} \mu_\ell \hat{f}^N_{(j),\ell} \mathrm{e}^{2\ell\pi i x_{k+1/2} / L}, \quad \mathbf{g}_j(x) = \sum_{\ell}^{K} \mu_\ell \hat{f}^N_{(j),\ell} \mathrm{e}^{2\ell\pi i x / L}, \tag{148}$$

with μ_ℓ given by (116). Moreover, by a careful comparison between the Fourier coefficients of $\mathbf{g}_j$ and $\partial_x \mathbf{f}_j$, we could perform a similar analysis as in (116) – (121) and derive the following estimate:

$$2\pi^{-1} \|\partial_x^{k+1} \mathbf{f}_j\| \le \|\partial_x^k \mathbf{g}_j\| \le \|\partial_x^{k+1} \mathbf{f}_j\|, \quad \forall k \ge 0. \tag{149}$$

The details are skipped for the sake of brevity.

In addition, the following $O(h^2)$ consistency estimate could be derived, following (29) (in Lemma 2.2):

$$\|\partial_x^k (\partial_x \mathbf{f}_j - \mathbf{g}_j)\| \le Ch^2 \|\partial_x^{k+3} \mathbf{f}_j\|, \quad \forall k \ge 0. \tag{150}$$

Due to the fact that

(151) $g_j = Df_j$ is the interpolation of the continuos function $\mathbf{g}_j$, $1 \le j \le 4$,

we apply (36) (in Lemma 2.3) and conclude that

$$\begin{aligned} & |\langle Df_1 \cdot Df_2, Df_3 \cdot Df_4 \rangle_e - (\mathbf{g}_1 \mathbf{g}_2, \mathbf{g}_3 \mathbf{g}_4)| \\ \le \; & Ch^2 \|\mathbf{g}_1 \mathbf{g}_2\|_{H^2} \cdot \|\mathbf{g}_3 \mathbf{g}_4\|_{H^2} \le Ch^2 \|\mathbf{g}_1\|_{H^2} \cdot \|\mathbf{g}_2\|_{H^2} \cdot \|\mathbf{g}_3\|_{H^2} \cdot \|\mathbf{g}_4\|_{H^2} \\ \le \; & Ch^2 (\|\mathbf{g}_1\|^2_{H^2} + \|\mathbf{g}_2\|^2_{H^2})(\|\mathbf{g}_3\|^2_{H^2} + \|\mathbf{g}_4\|^2_{H^2}) \\ \le \; & Ch^2 (\|\mathbf{f}_1\|^2_{H^3} + \|\mathbf{f}_2\|^2_{H^3})(\|\mathbf{f}_3\|^2_{H^3} + \|\mathbf{f}_4\|^2_{H^3}), \end{aligned} \tag{152}$$

in which the estimate (149) (with $k = 4$) is applied in the last step.

On the other hand, we have to estimate the difference between $(\mathbf{g}_1 \cdot \mathbf{g}_2, \mathbf{g}_3 \cdot \mathbf{g}_4)$ and $(\partial_x \mathbf{f}_1 \cdot \partial_x \mathbf{f}_2, \partial_x \mathbf{f}_3 \cdot \partial_x \mathbf{f}_4)$:

$$
\begin{aligned}
(\mathbf{g}_1 \cdot \mathbf{g}_2, \mathbf{g}_3 \cdot \mathbf{g}_4) - & \ (\partial_x \mathbf{f}_1 \cdot \partial_x \mathbf{f}_2, \partial_x \mathbf{f}_3 \cdot \partial_x \mathbf{f}_4) \\
= & \ (\mathbf{g}_1 \cdot \mathbf{g}_2 - \partial_x \mathbf{f}_1 \cdot \partial_x \mathbf{f}_2, \mathbf{g}_3 \cdot \mathbf{g}_4) \\
& + (\partial_x \mathbf{f}_1 \cdot \partial_x \mathbf{f}_2, \partial_x \mathbf{f}_1 \cdot \partial_x \mathbf{f}_2 - \partial_x \mathbf{f}_3 \cdot \partial_x \mathbf{f}_4) \\
= & \ (\mathbf{g}_1 - \partial_x \mathbf{f}_1, \partial_x \mathbf{f}_2 \cdot \mathbf{g}_3 \cdot \mathbf{g}_4) + (\mathbf{g}_2 - \partial_x \mathbf{f}_2, \mathbf{g}_1 \cdot \mathbf{g}_3 \cdot \mathbf{g}_4) \\
& + (\mathbf{g}_3 - \partial_x \mathbf{f}_3, \partial_x \mathbf{f}_4 \cdot \partial_x \mathbf{f}_1 \cdot \partial_x \mathbf{f}_2) + (\mathbf{g}_4 - \partial_x \mathbf{f}_4, \mathbf{g}_3 \partial_x \mathbf{f}_1 \cdot \partial_x \mathbf{f}_2) \, .
\end{aligned} \tag{153}
$$

The following preliminary estimates are available, for $1 \le j \le 4$:

$$
\|\mathbf{g}_j - \partial_x \mathbf{f}_j\| \le C h^2 \|\mathbf{f}_j\|_{H^3}, \quad \text{(by taking } k = 0 \text{ in (150))}, \tag{154}
$$

$$
\|\partial_x \mathbf{f}_j\|_{L^\infty} \le C \|\mathbf{f}_j\|_{H^2}, \quad \|\mathbf{g}_j\|_{L^\infty} \le C \|\mathbf{g}_j\|_{H^1} \le C \|\mathbf{f}_j\|_{H^2}, \tag{155}
$$

with Sobolev inequalities applied in (155). In turn, the first term in (153) could be bounded as follows:

$$
\begin{aligned}
|(\mathbf{g}_1 - \partial_x \mathbf{f}_1, \partial_x \mathbf{f}_2 \mathbf{g}_3 \cdot \mathbf{g}_4)| & \le \|\mathbf{g}_1 - \partial_x \mathbf{f}_1\| \cdot \|\partial_x \mathbf{f}_2\|_{L^\infty} \cdot \|\mathbf{g}_3\|_{L^\infty} \cdot \|\mathbf{g}_4\|_{L^\infty} \\
& \le C h^2 \|\mathbf{f}_1\|_{H^3} \cdot \|\mathbf{f}_2\|_{H^2} \cdot \|\mathbf{f}_3\|_{H^2} \cdot \|\mathbf{f}_4\|_{H^2} \\
& \le C h^2 (\|\mathbf{f}_1\|_{H^3}^2 + \|\mathbf{f}_2\|_{H^3}^2)(\|\mathbf{f}_3\|_{H^3}^2 + \|\mathbf{f}_4\|_{H^3}^2).
\end{aligned} \tag{156}
$$

The three other terms in (153) could be analyzed in the same way. Then we arrive at

$$
\begin{aligned}
& \Big| (\mathbf{g}_1 \cdot \mathbf{g}_2, \mathbf{g}_3 \cdot \mathbf{g}_4) - (\partial_x \mathbf{f}_1 \cdot \partial_x \mathbf{f}_2, \partial_x \mathbf{f}_3 \cdot \partial_x \mathbf{f}_4) \Big| \\
& \qquad \le C h^2 (\|\mathbf{f}_1\|_{H^3}^2 + \|\mathbf{f}_2\|_{H^3}^2)(\|\mathbf{f}_3\|_{H^3}^2 + \|\mathbf{f}_4\|_{H^3}^2).
\end{aligned} \tag{157}
$$

Finally, a combination of (152) and (157) yields (37). This finishes the proof of Lemma 2.4. □

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