Artificial Regularization Parameter Analysis for the No-Slope-Selection Epitaxial Thin Film Model

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Abstract. In this paper we study the effect of the artificial regularization term for the second order accurate (in time) numerical schemes for the no-slope-selection (NSS) equation of the epitaxial thin film growth model. In particular, we propose and analyze an alternate second order backward differentiation formula (BDF) scheme, with Fourier pseudo-spectral spatial discretization. The surface diffusion term is treated implicitly, while the nonlinear chemical potential is approximated by a second order explicit extrapolation formula. A second order accurate Douglas-Dupont regularization term, in the form of $-A\Delta t\Delta_N^2(u^{n+1}-u^n)$, is added in the numerical scheme to justify the energy stability at a theoretical level. Due to an alternate expression of the nonlinear chemical potential terms, such a numerical scheme requires a minimum value of the artificial regularization parameter as $A = \frac{289}{1024}$, much smaller than the other reported artificial parameter values in the existing literature. Such an optimization of the artificial parameter value is expected to reduce the numerical diffusion, and henceforth improve the long time numerical accuracy. Moreover, the optimal rate convergence analysis and error estimate are derived in details, in the $\ell^{\infty}(0,T;\ell^2) \cap \ell^2(0,T;H_k^2)$ norm, with the help of a linearized estimate for the nonlinear error terms. Some numerical simulation results are presented to demonstrate the efficiency and accuracy of the alternate second order numerical scheme. The long time simulation results for $\varepsilon = 0.02$ (up to $T = 3 \times 10^5$) have indicated a logarithm law for the energy decay, as well as the power laws for growth of the surface roughness and the mound width.

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1 Introduction

The no-slope-selection (NSS) epitaxial thin film growth equation is the L^2 gradient flow associated with the following energy functional

$$E(u) := \int_{\Omega} \left(-\frac{1}{2} \ln(1 + |\nabla u|^2) + \frac{\varepsilon^2}{2} |\Delta u|^2 \right) d\mathbf{x},$$
(1.1)

in which $\Omega = (0, L_x) \times (0, L_y)$, $u : \Omega \to \mathbb{R}$ is a periodic height function, and ε is a constant parameter of transition layer width. In fact, the first non-quadratic term represents the Ehrlich-Schwoebel (ES) effect, which means that an atom has to overcome a higher energy barrier to stick to a step from an upper rather than from a lower terrace [11,21–23,33]. This results in an uphill atom current in the dynamics and the steepening of mounds in the film. The second higher order quadratic term represents the isotropic surface diffusion effect [22,27]. In turn, the chemical potential becomes the following variational derivative of the energy

$$\mu := \delta_u E = \nabla \cdot \left(\frac{\nabla u}{1 + |\nabla u|^2} \right) + \varepsilon^2 \Delta^2 u, \tag{1.2}$$

and the dynamical equation stands for the L^2 gradient flow

$$\partial_t u = -\mu = -\nabla \cdot \left(\frac{\nabla u}{1 + |\nabla u|^2}\right) - \varepsilon^2 \Delta^2 u. \tag{1.3}$$

On the other hand, under a small-slope assumption that $|\nabla u|^2 \ll 1$, (1.3) may be approximated as

$$\partial_t u = \nabla \cdot \left(|\nabla u|^2 \nabla u \right) - \Delta u - \varepsilon^2 \Delta^2 u, \tag{1.4}$$

with the energy functional given by a polynomial approximation

$$E(u) = \int_{\Omega} \left(\frac{1}{4} (|\nabla u|^2 - 1)^2 + \frac{\varepsilon^2}{2} |\Delta u|^2 \right) d\mathbf{x}.$$
 (1.5)

This model is referred to as the slope-selection (SS) equation [19,20,22,27]. A solution to (1.4) exhibits pyramidal structures, where the faces of the pyramids have slopes $|\nabla u| \approx 1$; meanwhile, the no-slope-selection equation (1.3) exhibits mound-like structures, and the slopes of which (on an infinite domain) may grow unbounded [22, 35]. Both solutions have up-down symmetry in the sense that there is no way to distinguish a hill from a valley. This can be altered by adding adsorption/desorption or other dynamics.

Energy stable numerical algorithms for the thin film epitaxy have attracted a great deal of attentions in recent years, due to the long time nature of the gradient flow coarsening process. There have been many such efforts for both the SS and NSS equations; see the related references [5–7,9,18,25,29–32,34–37,39], etc. Among the energy stable ones, the linear schemes have demonstrated great advantages over the nonlinear algorithms; since the nonlinear chemical potential terms are explicitly updated in the linear schemes, the computational cost is expected to be greatly reduced. In the pioneering work [3] of linear energy stable schemes for thin film epitaxy, an alternate convex-concave decomposition for the Ehrlich-Schwoebel energy is proposed. In more details, such a nonlinear functional is non-convex, non-concave, while its combination with $-\frac{\kappa_0}{2} \|\nabla u\|^2$ becomes concave. In turn, a linear convex splitting scheme is proposed and analyzed, in which only a constant-coefficient linear system needs to be solved at each time step. The theoretical analysis reveals that the energy stability could be justified for $\kappa_0 \geq 1$, and this estimate has been sharpened to $\kappa_0 \ge \frac{1}{8}$ in a later work [18]. However, such a linear convex splitting idea could not be directly extended to derive the second order energy stable method, because of the challenge associated with a nonlinear concave term. To overcome this difficulty, a second order BDF (BDF2)-type scheme is proposed and analyzed in [26], with the energy stability established. The standard BDF2 temporal approximation is applied in this approach, combined with a second order explicit extrapolation formula for the nonlinear term. Meanwhile, such an explicit treatment would not be able to ensure the energy stability at the theoretical level. In fact, a second order Douglas-Dupont regularization term, namely in the form of $-A\Delta t\Delta^2(u^{n+1}-u^n)$, has to be added to stabilize the numerical scheme. A careful energy estimate reveals that a theoretical justification of the energy is available for $A \ge \frac{25}{16}$, under the nonlinear form given by the scheme. In an alternate exponential time differencing (ETD) based approach reported in [4], a similar artificial regularization term, in the form of $-A\Delta t^2 \partial_t \Delta^2 u$, is added in the numerical scheme, and its modified energy stability is theoretically established for the regularization parameter $A \ge \frac{2+\sqrt{3}}{6}$.

In this article, we propose and analyze an alternate BDF2-type numerical scheme for the NSS equation (1.3), so that the artificial regularization parameter A could have an optimized value. The numerical design follows similar idea as the one given by [26], while we take an alternate approximation to the nonlinear chemical potential term at time step t^{n+1} . In more details, the nonlinear term takes a form of $g(2u^n - u^{n-1})$ (with g(u) the nonlinear gradient term), as a second order approximation to g(u) at time step t^{n+1} . In the proposed scheme, we use an alternate second order approximation, in the form of $2g(u^n) - g(u^{n-1})$. Again, an artificial Douglas-Dupont regularization term, in the form of $-A\Delta t\Delta^2(u^{n+1}-u^n)$, has to be included in the numerical scheme for the sake of stability. With such an alternate approximation, a careful estimate reveals that, a modified energy stability could be theoretically justified for any $A \ge \frac{289}{1024}$. In fact, such an improved artificial parameter constant estimate is based on the convexity analysis for the nonlinear chemical potential (as reported in [18]), combined with certain nonlinear inequalities. As a result, the alternate approximation to the nonlinear chemical potential term leads to an optimized value of artificial regularization parameter, in comparison with the existing ones in [4,26]. Again, the subtle fact that all the nonlinear terms have automatically bounded higher order derivative will play an important role in the highly complicated nonlinear analysis. The Fourier pseudo-spectral method is chosen as the spatial approximation, and the discrete summation by parts property will facilitate the corresponding analysis for the fully discrete scheme. In addition to the energy stability analysis, we provide a theoretical analysis of an $\mathcal{O}(\Delta t^2 + h^m)$ rate convergence estimate for the proposed alternate BDF2-type scheme, in the $\ell^{\infty}(0,T;\ell^2) \cap \ell^2(0,T;H_h^2)$ norm.

The rest of the article is organized as follows. In Section 2 we present the numerical scheme. We begin with the notations of Fourier pseudo-spectral spatial approximation, as well as a review of existing energy stable linear numerical methods. Afterward, the alternate BDF2-type scheme is proposed, and a modified energy stability is established. Subsequently, the $\ell^{\infty}(0,T;\ell^2) \cap \ell^2(0,T;H_h^2)$ convergence estimate is provided in Section 3. In Section 4 we present the numerical results, including the accuracy test and the long time simulation for the coarsening process, which indicates a logarithm law for the energy decay, as well as the power laws for growth of the surface roughness and the mound width. Finally, the concluding remarks are given in Section 5.

2 The numerical scheme

2.1 Review of the Fourier pseudo-spectral approximation

For simplicity of presentation, we assume that the domain is given by $\Omega = (0,L)^2$, $N_x = N_y = N$ and $N \cdot h = L$. A more general domain could be treated in a similar manner. Furthermore, to facilitate the pseudo-spectral analysis in later sections, we set N = 2K+1. All the variables are evaluated at the regular numerical grid (x_i, y_j) , with $x_i = ih$, $y_j = jh$, $0 \le i, j \le 2K+1$.

Without loss of generality, we assume that L = 1. For a periodic function f over the given 2-D numerical grid, set its discrete Fourier expansion as

$$f_{i,j} = \sum_{k,\ell=-K}^{K} \hat{f}_{k,\ell} \exp\left(2\pi i(kx_i + \ell y_j)\right),$$
(2.1)

its collocation Fourier spectral approximations to first and second order partial derivatives in the *x*-direction become

$$(\mathcal{D}_{Nx}f)_{i,j} = \sum_{k,\ell=-K}^{K} (2k\pi i) \, \hat{f}_{k,\ell} \exp\left(2\pi i (kx_i + \ell y_j)\right), \tag{2.2}$$

$$\left(\mathcal{D}_{Nx}^{2}f\right)_{i,j} = \sum_{k,\ell=-K}^{K} \left(-4\pi^{2}k^{2}\right) \hat{f}_{k,\ell} \exp\left(2\pi i(kx_{i}+\ell y_{j})\right).$$
(2.3)

The differentiation operators in the *y* direction, namely, \mathcal{D}_{Ny} and \mathcal{D}_{Ny}^2 , could be defined in the same fashion. In turn, the discrete Laplacian, gradient and divergence become

$$\Delta_N f = \left(\mathcal{D}_{Nx}^2 + \mathcal{D}_{Ny}^2 \right) f,$$

$$\nabla_N f = \left(\begin{array}{c} \mathcal{D}_{Nx} f \\ \mathcal{D}_{Ny} f \end{array} \right), \quad \nabla_N \cdot \left(\begin{array}{c} f_1 \\ f_2 \end{array} \right) = \mathcal{D}_{Nx} f_1 + \mathcal{D}_{Ny} f_2, \qquad (2.4)$$

at the point-wise level. See the derivations in the related references [1,2,14,17], etc.

Given any periodic grid functions f and g (over the 2-D numerical grid), the spectral approximations to the L^2 inner product and L^2 norm are introduced as

$$||f||_2 = \sqrt{\langle f, f \rangle}, \quad \text{with} \quad \langle f, g \rangle = h^2 \sum_{i,j=0}^{N-1} f_{i,j} g_{i,j}.$$
(2.5)

A careful calculation yields the following formulas of summation by parts at the discrete level (see the related discussions [3,6,15,16]):

$$\langle f, \Delta_N g \rangle = - \langle \nabla_N f, \nabla_N g \rangle, \quad \langle f, \Delta_N^2 g \rangle = \langle \Delta_N f, \Delta_N g \rangle.$$
 (2.6)

Similarly, for any grid function f with $\overline{f} = 0$, the operator $(-\Delta_N)^{-1}$ and the discrete $\|\cdot\|_{-1}$ norm are defined as

$$\left((-\Delta_N)^{-1} f \right)_{i,j} = \sum_{k,\ell \neq \mathbf{0}} \frac{1}{\lambda_{k,\ell}} \hat{f}_{k,\ell} \exp\left(2\pi i (kx_i + \ell y_j) \right), \quad \lambda_{k,\ell} = (2k\pi)^2 + (2\ell\pi)^2, \tag{2.7}$$

$$\|f\|_{-1} = \sqrt{\langle f, (-\Delta_N)^{-1}f \rangle}.$$
(2.8)

In addition to the standard ℓ^2 norm, we also introduce the ℓ^p and discrete maximum norms for a grid function f, to facilitate the analysis in later sections:

$$||f||_{\infty} := \max_{i,j} |f_{i,j}|, \qquad ||f||_{p} := \left(\sum_{i,j=0}^{N-1} |f_{i,j}|^{p}\right)^{\frac{1}{p}}, \quad 1 \le p < \infty.$$
(2.9)

Moreover, for any numerical solution ϕ , the discrete energy is defined as

$$E_{N}(\phi) = E_{c,1,N}(\phi) + \frac{\varepsilon^{2}}{2} \|\Delta_{N}\phi\|_{2}^{2}, \quad E_{c,1,N}(\phi) = h^{2} \sum_{i,j=0}^{N-1} \left(-\frac{1}{2} \ln \left(1 + |\nabla_{N}\phi|^{2} \right)_{i,j} \right).$$
(2.10)

2.2 A review of existing energy stable linear schemes for (1.3)

In the pioneering work [3], the following convex-concave decomposition for the nonlinear energy functional is presented:

$$E_{ES}(u) := \int_{\Omega} -\frac{1}{2} \ln(1 + |\nabla u|^2) d\mathbf{x} = E_{ES,c}(u) - E_{ES,e}(u), \qquad (2.11)$$

with
$$E_{ES,c}(u) := \int_{\Omega} \frac{\kappa_0}{2} |\nabla u|^2 d\mathbf{x}, \quad E_{ES,e}(u) := \int_{\Omega} \left(\frac{\kappa_0}{2} |\nabla u|^2 + \frac{1}{2} \ln(1 + |\nabla u|^2) \right) d\mathbf{x}, \quad (2.12)$$

so that both $E_{ES,c}(u)$ and $E_{ES,e}(u)$ are convex in terms of u. In turn, the following first order accurate, linear splitting scheme is proposed and analyzed in [3]:

$$\frac{u^{n+1}-u^n}{\Delta t} = -\nabla \cdot \left(\frac{\nabla u^n}{1+|\nabla u^n|^2}\right) + \kappa_0 \Delta (u^{n+1}-u^n) - \varepsilon^2 \Delta^2 u^{n+1}.$$
(2.13)

The energy stability, $E(u^{n+1}) \leq E(u^n)$, is proved under the constraint that $\kappa_0 \geq 1$.

In a more recent work [18], such a constraint has been improved to $\kappa_0 \ge \frac{1}{8}$.

Meanwhile, it is observed that a direct linear splitting method (2.13) is only first order accurate (in time). To obtain a second order temporal accuracy while preserving the energy stability, a BDF2-type scheme is proposed and analyzed in [26], which turns out to be the mixed finite element version of the following algorithm:

$$\frac{\frac{3}{2}u^{n+1} - 2u^n + \frac{1}{2}u^{n-1}}{\Delta t} + \varepsilon^2 \Delta^2 u^{n+1} + \nabla \cdot \left(\frac{\nabla \hat{u}^{n+1}}{1 + |\nabla_N \hat{u}^{n+1}|^2}\right) + A \Delta t \Delta^2 (u^{n+1} - u^n) = 0,$$

with $\hat{u}^{n+1} = 2u^n - u^{n-1}.$ (2.14)

In other words, with the nonlinear chemical potential term denoted as $g(u) = \nabla \cdot \left(\frac{\nabla u}{1+|\nabla u|^2}\right)$, a second order approximation to $g(u^{n+1})$ is taken as an explicit extrapolation $g(2u^n - u^{n-1})$. With such an approximation, a modified energy stability was proved in [26] under a constraint for the artificial regularization parameter: $A \ge \frac{25}{16}$.

Other than the BDF2-type approach, exponential time differencing (ETD) based approach has also been extensively studied in recent years. A direct application of the ETD-based multi-step method was reported in [18], while a stability proof in terms of the original energy functional has not been available. To overcome this theoretical difficulty, a stabilized version is proposed and analyzed in [4], in which the numerical solution u^{n+1} is given by the following solution of linear PDE,

$$\partial_t u_s = -Lu_s - f_L(s, u^n, u^{n-1}) - A\Delta t^2 \partial_t \Delta^2 u_s, \quad u_s(t^n) = u^n, \quad u^{n+1} = u_s(t^{n+1}),$$
(2.15)

with
$$Lu = (\varepsilon^2 \Delta^2 - \kappa_0 \Delta)u$$
, $f_L(s, u^n, u^{n-1}) = g(u^n) + \frac{s}{\Delta t} (g(u^n) - g(u^{n-1}))$. (2.16)

In more details, the artificial regularization is given by the form of $-A\Delta t^2 \partial_t \Delta^2 u_s$, which shares a similar idea as the BDF2-type scheme. For such a stabilized ETD-based scheme, a theoretical analysis provides a modified energy stability under a similar constraint for the artificial regularization parameter: $A \ge \frac{2+\sqrt{3}}{6}$.

2.3 The proposed alternate BDF2 numerical scheme

As usual, we denote u^k as the numerical approximation to the PDE solution at time step $t^k := k\Delta t$, with any integer *n*. Given u^n , u^{n-1} , u^{n-2} , we propose a second order BDF-type

scheme for the NSS equation (1.3):

$$\frac{\frac{3}{2}u^{n+1} - 2u^n + \frac{1}{2}u^{n-1}}{\Delta t} + \varepsilon^2 \Delta_N^2 u^{n+1} + \nabla_N \cdot \left(2\frac{\nabla_N u^n}{1 + |\nabla_N u^n|^2} - \frac{\nabla_N u^{n-1}}{1 + |\nabla_N u^{n-1}|^2}\right) + A\Delta t \Delta_N^2 (u^{n+1} - u^n) = 0.$$
(2.17)

In particular, we notice that a second order approximation to the nonlinear chemical potential at time step t^{n+1} is taken as $2g(u^n) - g(u^{n-1})$, in comparison with $g(2u^n - u^{n-1})$ in [26]. Such alternate treatment of the nonlinear term has also been reported to have better stability for Cahn-Hilliard equation in [24].

Remark 2.1. As be well-known, a second-order accurate multi-step scheme requires two initial values. In general, the two other initial values are obtained by using a sufficiently accurate Runge-Kutta method, the known initial data. And here, without loss of generality, we give the three exact initial values directly.

For the proposed scheme (2.17), the mass-conservative property is always valid: $\overline{u^{n+1}} = \overline{u^n} = \overline{u^0} := \beta_0$, which comes from the following obvious identities:

$$\overline{\nabla_N \cdot f} = 0, \quad \overline{\Delta_N g} = 0. \tag{2.18}$$

2.4 The energy stability analysis

The following two preliminary estimates in [18] will be useful in the energy stability analysis.

Lemma 2.1. [18] Denote a mapping $\beta: \mathbb{R}^2 \to \mathbb{R}^2$: $\beta(v) = \frac{v}{1+|v|^2}$. Then we have

$$|\boldsymbol{\beta}(\boldsymbol{v}) - \boldsymbol{\beta}(\boldsymbol{w})| \le |\boldsymbol{v} - \boldsymbol{w}|, \quad \forall \boldsymbol{v}, \boldsymbol{w} \in \mathbb{R}^2.$$
(2.19)

Lemma 2.2. [18] *Define* $H(a,b) = \frac{1}{2}\ln(1+a^2+b^2) + \frac{\kappa_0}{2}(a^2+b^2)$. Then H(a,b) is convex in \mathbb{R}^2 if and only if $\kappa_0 \ge \frac{1}{8}$.

As a result of these convexity result, we are able to obtain the following energy estimate.

Lemma 2.3. For the numerical solutions u^{n+1} and u^n with $\overline{u^{n+1}} = \overline{u^n}$, we have

$$\left\langle \nabla_{N} \cdot \left(\frac{\nabla_{N} u^{n}}{1 + |\nabla_{N} u^{n}|^{2}} \right), u^{n+1} - u^{n} \right\rangle$$

$$\geq E_{c,1,N}(u^{n+1}) - E_{c,1,N}(u^{n}) - \frac{\kappa_{0}}{2} \|\nabla_{N}(u^{n+1} - u^{n})\|_{2}^{2}, \qquad (2.20)$$

with the nonlinear energy functional $E_{c,1,N}(\phi)$ defined in (2.10).

Proof. For simplicity of presentation, we denote

$$f_N^{(0)}(u) = \nabla_N \cdot \left(\frac{\nabla_N u}{1 + |\nabla_N u|^2}\right) + \kappa_0 \Delta_N u.$$
(2.21)

By Lemma 2.2, $f_N^{(0)}(u)$ corresponds to a concave energy functional, so that the following convexity inequality is valid:

$$\langle f_N^{(0)}(u^n), u^{n+1} - u^n \rangle \ge H_N(u^{n+1}) - H_N(u^n),$$
with $H_N(\phi) = E_{c,1,N}(\phi) - \frac{\kappa_0}{2} \|\nabla_N \phi\|_2^2,$
(2.22)

which is equivalent to (2.20). This finishes the proof of Lemma 2.3.

The energy stability of the proposed second order BDF-type scheme (2.17) is stated in the following theorem, in a modified version.

Theorem 2.1. The numerical solution produced by the proposed BDF-type scheme (2.17) satisfies

$$\tilde{E}_{N}(u^{n+1},u^{n}) \leq \tilde{E}_{N}(u^{n},u^{n-1}),$$
with $\tilde{E}_{N}(u^{n+1},u^{n}) = E_{N}(u^{n+1}) + \frac{1}{4\Delta t} ||u^{n+1} - u^{n}||_{2}^{2} + \frac{1}{2} ||\nabla_{N}(u^{n+1} - u^{n})||_{2}^{2},$
(2.23)

for any $\Delta t > 0$, provided that $A \ge \frac{289}{1024}$.

Proof. The numerical scheme (2.17) could be rewritten as

$$\nabla_{N} \cdot \left(\frac{\nabla_{N}u^{n}}{1+|\nabla_{N}u^{n}|^{2}}\right) = -\frac{\frac{3}{2}u^{n+1}-2u^{n}+\frac{1}{2}u^{n-1}}{\Delta t} -\varepsilon^{2}\Delta_{N}^{2}u^{n+1} - A\Delta t\Delta_{N}^{2}(u^{n+1}-u^{n}) -\nabla_{N} \cdot \left(\frac{\nabla_{N}u^{n}}{1+|\nabla_{N}u^{n}|^{2}} - \frac{\nabla_{N}u^{n-1}}{1+|\nabla_{N}u^{n-1}|^{2}}\right).$$
(2.24)

Taking a discrete ℓ^2 inner product with (2.24) by $u^{n+1} - u^n$ yields

$$\left\langle \nabla_{N} \cdot \left(\frac{\nabla_{N} u^{n}}{1 + |\nabla_{N} u^{n}|^{2}} \right), u^{n+1} - u^{n} \right\rangle + \frac{1}{\Delta t} \left\langle \frac{3}{2} u^{n+1} - 2u^{n} + \frac{1}{2} u^{n-1}, u^{n+1} - u^{n} \right\rangle$$

$$+ \varepsilon^{2} \left\langle \Delta_{N}^{2} u^{n+1}, u^{n+1} - u^{n} \right\rangle + A \Delta t \left\langle \Delta_{N}^{2} (u^{n+1} - u^{n}), u^{n+1} - u^{n} \right\rangle$$

$$+ \left\langle \nabla_{N} \cdot \left(\frac{\nabla_{N} u^{n}}{1 + |\nabla_{N} u^{n}|^{2}} - \frac{\nabla_{N} u^{n-1}}{1 + |\nabla_{N} u^{n-1}|^{2}} \right), u^{n+1} - u^{n} \right\rangle = 0.$$

$$(2.25)$$

The temporal stencil term could be analyzed as follows:

$$\left\langle \frac{3}{2}u^{n+1} - 2u^n + \frac{1}{2}u^{n-1}, u^{n+1} - u^n \right\rangle$$

$$= \left\langle \frac{3}{2}(u^{n+1} - u^n) - \frac{1}{2}(u^n - u^{n-1}), u^{n+1} - u^n \right\rangle$$

$$\ge \frac{3}{2} \|u^{n+1} - u^n\|_2^2 - \frac{1}{4}(\|u^n - u^{n-1}\|_2^2 + \|u^{n+1} - u^n\|_2^2)$$

$$= \|u^{n+1} - u^n\|_2^2 + \frac{1}{4}(\|u^{n+1} - u^n\|_2^2 - \|u^n - u^{n-1}\|_2^2).$$

$$(2.26)$$

448

For the nonlinear increment term, the following estimate could be derived:

$$-\left\langle \frac{\nabla_{N}u^{n}}{1+|\nabla_{N}u^{n}|^{2}} - \frac{\nabla_{N}u^{n-1}}{1+|\nabla_{N}u^{n-1}|^{2}}, \nabla_{N}(u^{n+1}-u^{n})\right\rangle$$

$$\leq \|\nabla_{N}(u^{n}-u^{n-1})\|_{2} \cdot \|\nabla_{N}(u^{n+1}-u^{n})\|_{2}$$

$$\leq \frac{1}{2}(\|\nabla_{N}(u^{n+1}-u^{n})\|_{2}^{2} + \|\nabla_{N}(u^{n}-u^{n-1})\|_{2}^{2}), \qquad (2.27)$$

in which the point-wise inequality (2.19) (in Lemma 2.1) has been applied. For the surface diffusion term, the following identity is available:

$$\langle \Delta_N^2 u^{n+1}, u^{n+1} - u^n \rangle = \frac{1}{2} (\|\Delta_N u^{n+1}\|_2^2 - \|\Delta_N u^n\|_2^2 + \|\Delta_N (u^{n+1} - u^n)\|_2^2).$$
(2.28)

Similarly, the following identity is straightforward to the artificial Douglas-Dupont regularization term:

$$A\Delta t \langle \Delta_N^2 (u^{n+1} - u^n), u^{n+1} - u^n \rangle = A\Delta t \| \Delta_N (u^{n+1} - u^n) \|_2^2.$$
(2.29)

As a consequence, a substitution of (2.20) and (2.25)-(2.29) into (2.24) results in

$$E_{N}(u^{n+1}) - E_{N}(u^{n}) + \left(\frac{\varepsilon^{2}}{2} + A\Delta t\right) \|\Delta_{N}(u^{n+1} - u^{n})\|_{2}^{2} + \frac{1}{\Delta t} \|u^{n+1} - u^{n}\|_{2}^{2} + \frac{1}{4\Delta t} (\|u^{n+1} - u^{n}\|_{2}^{2} - \|u^{n} - u^{n-1}\|_{2}^{2})$$

$$(2.30)$$

$$\leq \frac{9}{16} \|\nabla_N (u^{n+1} - u^n)\|_2^2 + \frac{1}{2} \|\nabla_N (u^n - u^{n-1})\|_2^2, \tag{2.31}$$

with the optimal value of $\kappa_0 = \frac{1}{8}$ taken. To control the right hand side of (2.30), we have the following observation

$$A\Delta t \|\Delta_N(u^{n+1}-u^n)\|_2^2 + \frac{1}{\Delta t} \|u^{n+1}-u^n\|_2^2$$

$$\geq 2A^{1/2} \|\Delta_N(u^{n+1}-u^n)\|_2 \cdot \|u^{n+1}-u^n\|_2 \geq 2A^{1/2} \|\nabla_N(u^{n+1}-u^n)\|_2^2, \qquad (2.32)$$

in which the summation by parts formula has been applied in the last step. Under the constraint that

$$2A^{1/2} \ge \frac{17}{16}$$
, i.e. $A \ge \frac{289}{1024}$, (2.33)

the following inequality is valid:

$$E_{N}(u^{n+1}) - E_{N}(u^{n}) + \frac{17}{16} \|\nabla_{N}(u^{n+1} - u^{n})\|_{2}^{2} + \frac{1}{4\Delta t} (\|u^{n+1} - u^{n}\|_{2}^{2} - \|u^{n} - u^{n-1}\|_{2}^{2})$$

$$\leq \frac{9}{16} \|\nabla_{N}(u^{n+1} - u^{n})\|_{2}^{2} + \frac{1}{2} \|\nabla_{N}(u^{n} - u^{n-1})\|_{2}^{2}.$$
(2.34)

In fact, (2.34) is equivalent to

$$\tilde{E}_N(u^{n+1}, u^n) - \tilde{E}_N(u^n, u^{n-1}) \le 0.$$
(2.35)

This completes the proof of Theorem 2.1.

Corollary 2.1. For the numerical solution (2.17), we have

$$E_N(u^k) \le E_N(u^0) + \frac{1}{4\Delta t} \|u^0 - u^{-1}\|_2^2 + \frac{1}{2} \|\nabla_N(u^0 - u^{-1})\|_2^2 := \tilde{C}_0, \quad \forall k \ge 0,$$
(2.36)

provided that (2.33) is satisfied.

Proof. By the modified energy inequality (2.23), the following induction analysis could be performed:

$$E_N(u^k) \le \tilde{E}_N(u^k, u^{k-1}) \le \dots \le \tilde{E}_N(u^0, u^{-1}) := \tilde{C}_0, \quad \forall k \ge 0.$$
(2.37)

This completes the proof.

Remark 2.2. In the proposed BDF2-type scheme, an alternate second order approximation to the nonlinear chemical potential at time step t^{n+1} is taken as $2g(u^n) - g(u^{n-1})$, instead of $g(2u^n - u^{n-1})$ reported in [26]. Such an alternate approximation leads to a much improved regularization parameter constraint: $A \ge \frac{289}{1024}$, to justify a modified energy stability, in comparison with $A \ge \frac{25}{16}$ reported in [26]. In fact, such an improved estimate is based on the convexity analysis for the nonlinear chemical potential (given by Lemma 2.2), combined with certain nonlinear inequalities. In fact, this estimate turns out to be an optimized value of artificial regularization parameter for the second order accurate, energy stable schemes for the NSS equation (1.3), in comparison with the existing ones in [4, 26].

Remark 2.3. There have been a few recent works of the BDF2-type schemes for certain gradient flow models, such as Cahn-Hilliard [8, 38], slope-selection thin film equation [12], square phase field crystal [10], in which the energy stability was theoretically established. Similarly, a Douglas-Dupont type regularization has to be included in the numerical scheme, while a careful analysis reveals its energy stability at a modified level. Such a BDF2-type approach turns out to be a very robust numerical tool in the study of gradient flows.

Remark 2.4. In one recent work [28], a similar BDF2-type scheme is proposed for the NSS equation (1.3), as the mixed finite element version of the following semi-discrete algorithm:

$$\frac{\frac{3}{2}u^{n+1} - 2u^n + \frac{1}{2}u^{n-1}}{\Delta t} + \varepsilon^2 \Delta^2 u^{n+1} + \nabla \cdot \left(2\frac{\nabla u^n}{1 + |\nabla u^n|^2} - \frac{\nabla u^{n-1}}{1 + |\nabla u^{n-1}|^2}\right) + A\Delta t \Delta^2 \left(\frac{3}{2}u^{n+1} - 2u^n + \frac{1}{2}u^{n-1}\right) = 0, \quad (2.38)$$

450

and a modified energy stability is proved under a constraint $A \ge 1$. In more details, the standard regularization term $A\Delta t\Delta^2(u^{n+1}-u^n)$ is applied in our proposed numerical method (2.17), in comparison with $A\Delta t\Delta^2(\frac{3}{2}u^{n+1}-2u^n+\frac{1}{2}u^{n-1})$ in (2.38). This brings more convenience in the numerical implementation. In addition, an optimal coefficient estimate has been derived in our work: $A \ge \frac{289}{1024}$ for (2.17), in comparison with $A \ge 1$ for (2.38).

3 The convergence analysis for the alternate BDF2 scheme

The global existence of weak solution, strong solution and smooth solution for the NSS equation (1.3) has been established in [22]. In more details, a global in time estimate of $L^{\infty}(0,T;H^m) \cap L^2(0,T;H^{m+2})$ for the phase variable was proved, assuming initial data in H^m , for any $m \ge 2$. Therefore, with an initial data with sufficient regularity, we could assume that the exact solution has regularity of class \mathcal{R} :

$$u_e \in \mathcal{R} := H^4(0,T;C^0) \cap H^1(0,T;H^4) \cap H^3(0,T;H^{m+2}) \cap L^{\infty}(0,T;H^{m+4}).$$
(3.1)

Define $U_N(\cdot,t) := \mathcal{P}_N u_e(\cdot,t)$, the (spatial) Fourier projection of the exact solution into \mathcal{B}^N , the space of trigonometric polynomials of degree to and including *N*. The following projection approximation is standard: if $u_e \in L^{\infty}(0,T;H_{\text{per}}^{\ell}(\Omega))$, for some $\ell \in \mathbb{N}$,

$$\|U_N - u_e\|_{L^{\infty}(0,T;H^m)} \le Ch^{\ell-k} \|u_e\|_{L^{\infty}(0,T;H^{\ell})}, \quad \forall \ 0 \le k \le \ell.$$
(3.2)

By U_N^n we denote $U_N(\cdot, t^n)$, with $t^n = n \cdot \Delta t$. Since $U_N \in \mathcal{B}^N$, the mass conservative property is available at the discrete level:

$$\overline{U_N^n} = \frac{1}{|\Omega|} \int_{\Omega} U_N(\cdot, t_n) d\mathbf{x} = \frac{1}{|\Omega|} \int_{\Omega} U_N(\cdot, t_{n-1}) d\mathbf{x} = \overline{U_N^{n-1}}, \quad \forall \ n \in \mathbb{N}.$$
(3.3)

On the other hand, the solution of the numerical scheme (2.17) is also mass conservative at the discrete level:

$$\overline{u^n} = \overline{u^{n-1}}, \quad \forall \ n \in \mathbb{N}.$$
(3.4)

Meanwhile, we denote U^n as the interpolation values of U_N at discrete grid points at time instant t^n : $U_{i,j}^n := U_N(x_i, y_j, t^n)$. As indicated before, we use the mass conservative projection for the initial data:

$$u_{i,j}^{0} = U_{i,j}^{0} := U_N(x_i, y_j, t = 0).$$
(3.5)

The error grid function is defined as

$$e^{n} := U^{n} - u^{n}, \quad \forall \ n \in \{0, 1, 2, 3, \cdots\}.$$
 (3.6)

Therefore, it follows that $\overline{e^n} = 0$, for any $n \in \{0, 1, 2, 3, \dots\}$.

For the proposed second order BDF-type scheme (2.17), the convergence result is stated below.

Theorem 3.1. Given initial data U_N^0 , $U_N^{-1} \in C_{per}^{m+4}(\overline{\Omega})$, with periodic boundary conditions, suppose the unique solution for the NSS equation (1.3) is of regularity class \mathcal{R} . Then, provided Δt and h are sufficiently small, for all positive integers ℓ , such that $\Delta t \cdot \ell \leq T$, we have

$$\|e^{\ell}\|_{2} + \left(\varepsilon^{2}\Delta t \sum_{k=1}^{\ell} \|\Delta_{N}e^{k}\|_{2}^{2}\right)^{1/2} \le C(\Delta t^{2} + h^{m}),$$
(3.7)

where C > 0 is independent of Δt and h.

3.1 The error evolutionary equation

For the Fourier projection solution U_N and its interpolation U, a careful consistency analysis implies that

$$\frac{\frac{3}{2}U^{n+1} - 2U^n + \frac{1}{2}U^{n-1}}{\Delta t} + \varepsilon^2 \Delta_N^2 U^{n+1} + A \Delta t \Delta_N^2 (U^{n+1} - U^n)$$

= $-\nabla_N \cdot \left(2 \frac{\nabla_N U^n}{1 + |\nabla_N U^n|^2} - \frac{\nabla_N U^{n-1}}{1 + |\nabla_N U^{n-1}|^2} \right) + \tau^n,$ (3.8)

with $\|\tau^n\|_2 \leq C(\Delta t^2 + h^m)$. In turn, subtracting the numerical scheme (2.17) from the consistency estimate (3.8) yields

$$\frac{\frac{3}{2}e^{n+1}-2e^{n}+\frac{1}{2}e^{n-1}}{\Delta t}+\varepsilon^{2}\Delta_{N}^{2}e^{n+1}+A\Delta t\Delta_{N}^{2}(e^{n+1}-e^{n})$$

$$=-\nabla_{N}\cdot\left(2\frac{\nabla_{N}U^{n}}{1+|\nabla_{N}U^{n}|^{2}}-2\frac{\nabla_{N}u^{n}}{1+|\nabla_{N}u^{n}|^{2}}-\frac{\nabla_{N}U^{n-1}}{1+|\nabla_{N}U^{n-1}|^{2}}+\frac{\nabla_{N}u^{n-1}}{1+|\nabla_{N}u^{n-1}|^{2}}\right)+\tau^{n}.$$
(3.9)

3.2 The $\ell^{\infty}(0,T;\ell^2) \cap \ell^2(0,T;H_h^2)$ error estimate

Taking a discrete ℓ^2 inner product with (3.9) by e^{n+1} gives

$$\frac{1}{\Delta t} \left\langle \frac{3}{2} e^{n+1} - 2e^n + \frac{1}{2} e^{n-1}, e^{n+1} \right\rangle + \varepsilon^2 \|\Delta_N e^{n+1}\|_2^2 + A\Delta t \left\langle \Delta_N (e^{n+1} - e^n), \Delta_N e^{n+1} \right\rangle \\
= \sum_{j=0}^1 \gamma^{(j)} \left\langle \frac{\nabla_N U^{n-j}}{1 + |\nabla_N U^{n-j}|^2} - \frac{\nabla_N u^{n-j}}{1 + |\nabla_N u^{n-j}|^2}, \nabla_N e^{n+1} \right\rangle + \left\langle \tau^n, e^{n+1} \right\rangle,$$
(3.10)

with $\gamma^{(0)} = 2$, $\gamma^{(1)} = -1$. Notice that the summation by parts formula has been repeatedly applied in the derivation. The temporal stencil term could be analyzed in a standard way:

$$\left\langle \frac{3}{2}e^{n+1} - 2e^n + \frac{1}{2}e^{n-1}, e^{n+1} \right\rangle$$

= $\frac{1}{4} \left(\|e^{n+1}\|_2^2 - \|e^n\|_2^2 + \|2e^{n+1} - e^n\|_2^2 - \|2e^n - e^{n-1}\|_2^2 + \|e^{n+1} - 2e^n + e^{n-1}\|_2^2 \right).$ (3.11)

X. Meng et al. / CSIAM Trans. Appl. Math., 1 (2020), pp. 441-462

The local truncation error term could also be bounded in a straightforward way:

$$\langle \tau^n, e^{n+1} \rangle \leq \frac{1}{2} (\|\tau^n\|_2^2 + \|e^{n+1}\|_2^2).$$
 (3.12)

The Douglas-Dupont regularization term could be analyzed as follows:

$$\langle \Delta_N(e^{n+1}-e^n), \Delta_N e^{n+1} \rangle = \frac{1}{2} (\|\Delta_N e^{n+1}\|_2^2 - \|\Delta_N e^n\|_2^2 + \|\Delta_N(e^{n+1}-e^n)\|_2^2).$$
(3.13)

For the nonlinear error term on the right hand side of (3.10), we focus on the time instant t^n . By making use of inequality (2.19) (in Lemma 2.1), we see that

$$\left|\frac{\nabla_N U^n}{1+|\nabla_N U^n|^2} - \frac{\nabla_N u^n}{1+|\nabla_N u^n|^2}\right| \le |\nabla_N e^n|, \quad \text{at a point-wise level.}$$
(3.14)

This in turn leads to

$$\gamma^{(0)} \Big\langle \frac{\nabla_N U^n}{1 + |\nabla_N U^n|^2} - \frac{\nabla_N u^n}{1 + |\nabla_N u^n|^2}, \nabla_N e^{n+1} \Big\rangle \le 2 \|\nabla_N e^n\|_2 \cdot \|\nabla_N e^{n+1}\|_2.$$
(3.15)

Similarly, the following inequality is available:

$$\gamma^{(1)} \left\langle \frac{\nabla_N U^{n-1}}{1 + |\nabla_N U^{n-1}|^2} - \frac{\nabla_N u^{n-1}}{1 + |\nabla_N u^{n-1}|^2}, \nabla_N e^{n+1} \right\rangle \le \|\nabla_N e^{n-1}\|_2 \cdot \|\nabla_N e^{n+1}\|_2.$$
(3.16)

Then we arrive at

$$\sum_{j=0}^{1} \gamma^{(j)} \left\langle \frac{\nabla_{N} U^{n-j}}{1+|\nabla_{N} U^{n-j}|^{2}} - \frac{\nabla_{N} u^{n-j}}{1+|\nabla_{N} u^{n-j}|^{2}}, \nabla_{N} e^{n+1} \right\rangle$$

$$\leq (2\|\nabla_{N} e^{n}\|_{2} + \|\nabla_{N} e^{n-1}\|_{2}) \cdot \|\nabla_{N} e^{n+1}\|_{2} \leq \frac{3}{2} \|\nabla_{N} e^{n+1}\|_{2}^{2} + \|\nabla_{N} e^{n}\|_{2}^{2} + \frac{1}{2} \|\nabla_{N} e^{n-1}\|_{2}^{2},$$
(3.17)

with repeated application of Cauchy inequality at the last step.

Therefore, a substitution of (3.11), (3.12)-(3.13) and (3.17) into (3.10) leads to

$$\frac{1}{\Delta t}(F^{n+1}-F^n) + \varepsilon^2 \|\Delta_N e^{n+1}\|_2^2 + \frac{A}{2}\Delta t(\|\Delta_N e^{n+1}\|_2^2 - \|\Delta_N e^n\|_2^2)$$

$$\leq \frac{3}{2} \|\nabla_N e^{n+1}\|_2^2 + \|\nabla_N e^n\|_2^2 + \frac{1}{2} \|\nabla_N e^{n-1}\|_2^2 + \frac{1}{2} (\|\tau^n\|_2^2 + \|e^{n+1}\|_2^2), \qquad (3.18)$$

with

$$F^{n+1} = \frac{1}{4} (\|e^{n+1}\|_2^2 + \|2e^{n+1} - e^n\|_2^2).$$
(3.19)

Meanwhile, for the error gradient term $\|\nabla_N e^{n+1}\|_2^2$, the following estimate could be derived:

$$\frac{3}{2} \|\nabla_{N} e^{n+1}\|_{2}^{2} = -\frac{3}{2} \langle e^{n+1}, \Delta_{N} e^{n+1} \rangle \leq \frac{3}{2} \|e^{n+1}\|_{2} \cdot \|\Delta_{N} e^{n+1}\|_{2}$$
$$\leq \frac{27}{8} \varepsilon^{-2} \|e^{n+1}\|_{2}^{2} + \frac{\varepsilon^{2}}{6} \|\Delta_{N} e^{n+1}\|_{2}^{2}.$$
(3.20)

The error gradient terms at the other time step instants could be bounded in a similar way:

$$\|\nabla_N e^n\|_2^2 \le \frac{3}{2}\varepsilon^{-2} \|e^n\|_2^2 + \frac{\varepsilon^2}{6} \|\Delta_N e^n\|_2^2, \tag{3.21}$$

$$\frac{1}{2} \|\nabla_N e^{n-1}\|_2^2 \le \frac{3}{8} \varepsilon^{-2} \|e^{n-1}\|_2^2 + \frac{\varepsilon^2}{6} \|\Delta_N e^{n-1}\|_2^2.$$
(3.22)

Going back (3.18), we arrive at

$$\frac{1}{\Delta t}(F^{n+1}-F^n) + \frac{5}{6}\varepsilon^2 \|\Delta_N e^{n+1}\|_2^2 + \frac{A}{2}\Delta t(\|\Delta_N e^{n+1}\|_2^2 - \|\Delta_N e^n\|_2^2) \\
\leq \left(\frac{27}{8}\varepsilon^{-2} + \frac{1}{2}\right) \|e^{n+1}\|_2^2 + \frac{3}{2}\varepsilon^{-2}\|e^n\|_2^2 + \frac{3}{8}\varepsilon^{-2}\|e^{n-1}\|_2^2 \\
+ \frac{\varepsilon^2}{6}(\|\Delta_N e^n\|_2^2 + \|\Delta_N e^{n-1}\|_2^2) + \frac{1}{2}\|\tau^n\|_2^2.$$
(3.23)

By introducing a modified quantity

$$\widetilde{F}^{n+1} := F^{n+1} + \frac{A}{2} \Delta t^2 \|\Delta_N e^{n+1}\|_{2^{\prime}}^2,$$
(3.24)

and making use of the following obvious fact:

$$\|e^k\|_2^2 \le 4\widetilde{F}^k, \quad \forall k \ge 0, \tag{3.25}$$

we obtain the following estimate

$$\frac{1}{\Delta t} (\widetilde{F}^{n+1} - \widetilde{F}^n) + \frac{5}{6} \varepsilon^2 \|\Delta_N e^{n+1}\|_2^2 - \frac{\varepsilon^2}{6} (\|\Delta_N e^n\|_2^2 + \|\Delta_N e^{n-1}\|_2^2)$$

$$\leq 4 \left(\frac{27}{8} \varepsilon^{-2} + \frac{1}{2}\right) (\widetilde{F}^{n+1} + \widetilde{F}^n + \widetilde{F}^{n-1}) + \frac{1}{2} \|\tau^n\|_2^2.$$
(3.26)

In turn, an application of discrete Gronwall inequality results in the convergence estimate:

$$F^{n+1} + \frac{1}{2} \varepsilon^2 \Delta t \sum_{k=1}^{n+1} \|\Delta_N e^k\|_2^2 \le \hat{C} (\Delta t^2 + h^m)^2.$$
(3.27)

Furthermore, its combination with definition (3.19) (for F^{n+1}) indicates the desired result (3.7). This completes the proof of Theorem 3.1.

454

4 Numerical results

4.1 Convergence test for the numerical scheme

We perform a numerical accuracy check for the proposed alternate BDF2-type scheme (2.17). The computational domain is set to be $\Omega = (0,1)^2$, and the exact profile for the phase variable is set to be

$$U(x,y,t) = \sin(2\pi x)\cos(2\pi y)\cos(t). \tag{4.1}$$

To make *U* satisfy the original PDE (1.3), we have to add an artificial, time-dependent forcing term. In turn, the BDF-type scheme (2.17) can be implemented to solve for (1.3). To demonstrate the accuracy in time, the spatial numerical error has to be negligible. We fix the spatial resolution as N = 192 (so that $h = \frac{1}{192}$), and set the final time T = 1. The surface diffusion parameter is taken as $\varepsilon = 0.05$, and we set the artificial regularization parameter as $A = \frac{289}{1024}$. Naturally, a sequence of time step sizes are taken as $\Delta t = \frac{T}{N_T}$, with $N_T = 100:100:1000$. The expected temporal numerical accuracy assumption $e = C\Delta t^k$ indicates that $\ln|e| = \ln(CT^k) - k \ln N_T$, so that we plot $\ln|e|$ vs. $\ln N_T$ to demonstrate the temporal convergence order. The fitted line displayed in Fig. 1 shows an approximate slope of -2, which in turn verifies a nice second order temporal convergence order, in both the discrete ℓ^2 and ℓ^{∞} norms.



Figure 1: The discrete ℓ^2 and ℓ^{∞} numerical errors vs. temporal resolution N_T for $N_T = 100:100:1000$, with a spatial resolution N = 192. The surface diffusion parameter is taken to be $\varepsilon = 0.05$. The data lie roughly on curves CN_T^{-2} , for appropriate choices of *C*, confirming the full second-order accuracy of the scheme.

4.2 Long time simulation results of the coarsening process

With the assumption that $\varepsilon \ll \min \{L_x, L_y\}$, the temporal evolution of the solution to (1.3) has always been of great interests. The physically interesting quantities include (i) the

energy E(t); (ii) the characteristic (average) height (the surface roughness) h(t); and (iii) the characteristic (average) slope m(t). These quantities are precisely defined as

$$h(t) = \sqrt{\frac{1}{|\Omega|} \int_{\Omega} \left| u(\mathbf{x}, t) - \bar{u}(t) \right|^2} d\mathbf{x}, \quad \text{with} \quad \bar{u}(t) := \frac{1}{|\Omega|} \int_{\Omega} u(\mathbf{x}, t) d\mathbf{x}, \tag{4.2}$$

$$m(t) = \sqrt{\frac{1}{|\Omega|} \int_{\Omega} |\nabla u(\mathbf{x}, t)|^2} \,\mathrm{d}\mathbf{x}.$$
(4.3)

For the no-slope-selection equation (1.3), asymptotic scaling law could be formally derived as $h \sim \mathcal{O}(t^{1/2})$, $m(t) \sim \mathcal{O}(t^{1/4})$, and $E \sim \mathcal{O}(-\ln(t))$ as $t \to \infty$; see [13, 22, 23] and other related references. This in turn implies that the characteristic (average) length $\ell(t):=h(t)/m(t)\sim \mathcal{O}(t^{1/4})$ as $t\to\infty$. In other words, the average length and average slope scale the same with increasing time. We also observe that the average mound height h(t) grows faster than the average length $\ell(t)$, which is expected because there is no preferred slope of the height function u.

At a theoretical level, as described in [19,20,23], one can at best obtain lower bounds for the energy dissipation and, conversely, upper bounds for the average height. However, the rates quoted as the upper or lower bounds are typically observed for the averaged values of the quantities of interest. It is quite challenging to numerically predict these scaling laws, since very long time scale simulations are needed. To capture the full range of coarsening behaviors, numerical simulations for the coarsening process require short-time and long-time accuracy and stability, in addition to high spatial accuracy for small values of ε .

In this section we display the numerical simulation results obtained from the alternate BDF2-type algorithm (2.17) for the no-slope-selection equation (1.3), and compare the computed solutions against the predicted coarsening rates. Similar results have also been reported in the existing literature, such as the ones given by [3, 18, 35], etc. The surface diffusion coefficient parameter is taken to be $\varepsilon = 0.02$ in this article, and the domain is set as $L = L_x = L_y = 12.8$. The uniform spatial resolution is given by h = L/N, N = 512, which is adequate to resolve the small structures in the solution with such a value of ε . The artificial regularization parameter is taken as A = 0.1 in our simulation.

For the temporal step size Δt , we use increasing values of Δt , namely, $\Delta t = 0.004$ on the time interval [0,400], $\Delta t = 0.04$ on the time interval [400,6000], $\Delta t = 0.16$ on the time interval $[6000,3 \times 10^5]$. Whenever a new time step size is applied, we initiate the two-step numerical scheme by taking $u^{-1} = u^0$, with the initial data u^0 given by the final time output of the last time period. Fig. 2 displays time snapshots of the film height u with $\varepsilon = 0.02$, with significant coarsening observed in the system. At early times many small hills (red) and valleys (blue) are present. At the final time, t=300000, a one-hill-one-valley structure emerges, and further coarsening is not possible.

The long time characteristics of the solution, especially the energy decay rate, average height growth rate, and the mound width growth rate, are of interest to surface



Figure 2: (Color online) Snapshots of the computed height function u at the indicated times for the parameters L=12.8, $\varepsilon=0.02$. The hills at early times are not as high as time at later times, and similarly with the valley. The average height/depth evolution with time could be seen in Fig. 3.

physics community. The last two quantities can be easily measured experimentally. On the other hand, the discrete energy E_N is defined via (2.10); the space-continuous average height and average slope have been defined in (4.2), (4.3), and the analogous discrete versions are also available. Theoretically speaking, the lower bound for the energy decay rate is of the order of $-\ln(t)$, and the upper bounds for the average height and average slope/average length are of the order of $t^{1/2}$, $t^{1/4}$, respectively, as established for the no-slope-selection equation (1.3) in [23]. Fig. 3 presents the semi-log plots for the energy versus time and log-log plots for the average height versus time, and average slope versus time, respectively, with the given physical parameter ε =0.02, and the artificial regularization parameter A =0.1. The detailed scaling "exponents" are obtained using least squares fits of the computed data up to time t = 400. A clear observation of the $-\ln(t)$, $t^{1/2}$ and $t^{1/4}$ scaling laws can be made, with different coefficients dependent upon ε , or, equivalently, the domain size, L.

Now we recall that a lower bound for the energy (1.1), assuming $\Omega = (0, L)^2$, which has been derived and published in our earlier works [3,6,35]:

$$E(\phi) \ge \frac{L^2}{2} \left(\ln\left(\frac{4\varepsilon^2 \pi^2}{L^2}\right) - \frac{4\varepsilon^2 \pi^2}{L^2} + 1 \right) =: \gamma.$$

$$(4.4)$$

Obviously, since the energy is bounded below it cannot keep decreasing at the rate $-\ln(t)$. This fact manifests itself in the calculated data as the rate of decrease of the energy, for



Figure 3: Time evolution of the physical quantities with $\varepsilon = 0.02$, and the artificial regularization parameter A = 0.1. Left: Semi-log plot of the temporal evolution the energy E_N . The energy decreases like $-\ln(t)$ until saturation. Middle: The log-log plot of the average height (or roughness) of u, denoted as h(t), which grows like $t^{1/2}$. Right: The log-log plot of the average width of u, denoted m(t), which grows like $t^{1/4}$. The dotted lines correspond to the minimum energy reached by the numerical simulation. The red lines represent the energy plot obtained by the simulations, while the straight lines are obtained by least squares approximations to the energy data. The least squares fit is only taken for the linear part of the calculated data, only up to about time t=400. The fitted line for the energy has the form $a_e \ln(t) + b_e$, with $a_e = -39.7488$, $b_e = -152.3815$; the (blue) fitting line for the average height has the form $a_h t^{b_h}$, with $a_h = 0.4017$, $b_h = 0.5002$, and the fitting line for the average width has the form $a_m t^{b_m}$, with $a_m = 4.1488$, $b_m = 0.2543$.

example, begins to wildly deviate from the predicted $-\ln(t)$ curve. Sometimes the rate of decrease increases, and sometimes it slows as the systems "feels" the periodic boundary conditions. Interestedly, regardless of this later-time deviation from the accepted rates, the time at which the system saturates (*i.e.*, the time when the energy abruptly and essentially stops decreasing) is roughly that predicted by extending the blue lines in Fig. 3 to the predicted minimum energy (4.4).

In addition, we perform a numerical test to make a comparison between different artificial regularization parameter values of A, in terms of its impact on the long time simulation. In addition to the numerical results obtained with A = 0.1, we carried out another numerical simulation with exactly the same set-up, the physical parameters, as well as the computational domain, while choosing another regularization parameter value $A = \frac{289}{1024}$, the theoretically critical value given by Theorem 2.1. With this regularization parameter, the overall structures are very similar, the final steady state solutions have the same pattern, while the long time behavior and the scaling law for the physical quantities have minor difference. Fig. 4 displays the semi-log plots for the energy versus time and log-log plots for the average height versus time, and average slope versus time, respectively, with the regularization parameter $A = \frac{289}{1024}$. For instance, the saturation time scale for the numerical results with A = 0.1 is around 3×10^5 , while the one with $A = \frac{289}{1024}$ is around 5×10^5 . By the numerical simulation of a third order accurate ETD-based numerical scheme reported in a recent work [9], we believe that the saturation time scale of 3×10^5 would be more accurate. And also, the detailed numerical data show that long time asymptotic growth rate of the standard deviation given by the regularization pa-



Figure 4: Time evolution of the physical quantities with $\varepsilon = 0.02$, and the artificial regularization parameter $A = \frac{289}{1024}$. The figure set up is the same as in Fig. 3. For this artificial regularization parameter, the saturation time scale is 5×10^5 . The fitted line for the energy has the form $a_e \ln(t) + b_e$, with $a_e = -41.1038$, $b_e = -148.9292$; the (blue) fitting line for the average height has the form $a_h t^{b_h}$, with $a_h = 0.4116$, $b_h = 0.5064$, and the fitting line for the average width has the form $a_m t^{b_m}$, with $a_m = 4.1906$, $b_m = 0.2575$.

rameter A = 0.1 is closer to $t^{1/2}$ than that by the one with $A = \frac{289}{1024}$: $m_r = 0.5002$ for A = 0.1, vs. $m_r = 0.5064$ for $A = \frac{289}{1024}$, as recorded in Figs. 3 and 4, respectively. Similarly, the long time asymptotic growth rate of the mound width given by the results with A = 0.1 is closer to $t^{1/4}$ than that by the one with $A = \frac{289}{1024}$: $b_m = 0.2543$ for A = 0.1 vs. $b_m = 0.2575$ for $A = \frac{289}{1024}$, as recorded in the two figures. This gives more evidence that the artificial regularization parameter really makes impact on the long time simulation of the epitaxial thin film model. In general, the long time accuracy improves with a decreasing value such a regularization parameter.

For the regularization parameter $A \ge \frac{289}{1024}$, the theoretical analysis has ensured an unconditional energy stability, independent on the time step size. For $A \le \frac{289}{1024}$, such as A = 0.1 in this numerical simulation, extensive numerical experiments have also demonstrated energy stability independent on the time step size.

As mentioned at the beginning of this work, the proposed BDF-type scheme (2.17) is a variation of an existing work [26], in which the nonlinear term takes an alternate form, and the regularization coefficient has a constraint $A \ge \frac{25}{16}$. We have performed a few more numerical simulations, with increasing values of A, and these numerical results lead to larger saturation time scale. As a result, we conclude that an optimized regularization coefficient is valuable in the large time computation of no-slope-selection epitaxial thin film equation.

5 Concluding remarks

In this article, the effect of the artificial regularization term for the second order accurate numerical schemes for the no-slope-selection equation (1.3) of the epitaxial thin film growth model is studied. In particular, we propose and analyze an alternate BDF2-type

scheme, combined with Fourier pseudo-spectral spatial discretization. As usual, the surface diffusion term is treated implicitly, while the nonlinear chemical potential is approximated by an explicit extrapolation formula for the sake of solvability. A second order accurate Douglas-Dupont regularization term, in the form of $-A\Delta t\Delta_N^2(u^{n+1}-u^n)$, is added to stabilize the numerical scheme. Instead of the standard approximation to the nonlinear chemical potential at time step t^{n+1} , given by $g(2u^n - u^{n-1})$ in an existing work, we use alternate approximation as $2g(u^n) - g(u^{n-1})$ in the proposed scheme. Such an alternate approximation leads to a much improved regularization parameter constraint: $A \ge \frac{289}{1024}$ to justify a modified energy stability, in comparison with $A \ge \frac{25}{16}$ and $A \ge \frac{2+\sqrt{3}}{6}$ in the existing literature, for the standard stabilized BDF2-type and the stabilized ETD-based schemes, respectively. In addition to the energy stability, the optimal rate convergence analysis and error estimate are derived in details, in the $\ell^{\infty}(0,T;\ell^2) \cap \ell^2(0,T;H_h^2)$ norm, with the help of a linearized estimate for the nonlinear error terms. Some numerical simulation results are presented to demonstrate the robustness and accuracy of the alternate second order numerical scheme. The long time simulation results for the coarsening process have indicated a logarithm law for the energy decay, as well as the power laws for growth of the surface roughness and the mound width. A numerical test is carried out to make a comparison between different artificial regularization parameter values of A, in terms of its impact on the long time simulation. In general, the long time accuracy improves with a decreasing value such a regularization parameter. This gives another evidence that the improvement of the regularization parameter value (as reported in this article) would lead to more accurate scientific computing tools in the large time-scale computations.

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References

- [1] J. Boyd. Chebyshev and Fourier Spectral Methods. Dover, New York, NY, 2001.
- [2] C. Canuto and A. Quarteroni. Approximation results for orthogonal polynomials in Sobolev spaces. *Math. Comp.*, 38:67–86, 1982.
- [3] W. Chen, S. Conde, C. Wang, X. Wang, and S.M. Wise. A linear energy stable scheme for a thin film model without slope selection. *J. Sci. Comput.*, 52:546–562, 2012.
- [4] W. Chen, W. Li, Z. Luo, C. Wang, and X. Wang. A stabilized second order exponential time differencing multistep method for thin film growth model without slope selection. *EASIM Math. Model. Numer. Anal.*, 54:727–750, 2020.

- [5] W. Chen, W. Li, C. Wang, S. Wang, and X. Wang. Energy stable higher order linear ETD multi-step methods for gradient flows: application to thin film epitaxy. *Res. Math. Sci.*, 7:13, 2020.
- [6] W. Chen, C. Wang, X. Wang, and S.M. Wise. A linear iteration algorithm for energy stable second order scheme for a thin film model without slope selection. *J. Sci. Comput.*, 59:574– 601, 2014.
- [7] W. Chen and Y. Wang. A mixed finite element method for thin film epitaxy. *Numer. Math.*, 122:771–793, 2012.
- [8] K. Cheng, W. Feng, C. Wang, and S.M. Wise. An energy stable fourth order finite difference scheme for the Cahn-Hilliard equation. J. Comput. Appl. Math., 362:574–595, 2019.
- [9] K. Cheng, Z. Qiao, and C. Wang. A third order exponential time differencing numerical scheme for no-slope-selection epitaxial thin film model with energy stability. J. Sci. Comput., 81(1):154–185, 2019.
- [10] K. Cheng, C. Wang, and S.M. Wise. An energy stable Fourier pseudo-spectral numerical scheme for the square phase field crystal equation. *Commun. Comput. Phys.*, 26:1335–1364, 2019.
- [11] G. Ehrlich and F. G. Hudda. Atomic view of surface diffusion: Tungsten on tungsten. J. Chem. Phys., 44:1036–1099, 1966.
- [12] W. Feng, C. Wang, S.M. Wise, and Z. Zhang. A second-order energy stable Backward Differentiation Formula method for the epitaxial thin film equation with slope selection. *Numer. Methods Partial Differ. Equ.*, 34(6):1975–2007, 2018.
- [13] L. Golubović. Interfacial coarsening in epitaxial growth models without slope selection. *Phys. Rev. Lett*, 78:90–93, 1997.
- [14] D. Gottlieb and S.A. Orszag. Numerical Analysis of Spectral Methods, Theory and Applications. SIAM, Philadelphia, PA, 1977.
- [15] S. Gottlieb, F. Tone, C. Wang, X. Wang, and D. Wirosoetisno. Long time stability of a classical efficient scheme for two dimensional Navier-Stokes equations. *SIAM J. Numer. Anal.*, 50:126– 150, 2012.
- [16] S. Gottlieb and C. Wang. Stability and convergence analysis of fully discrete Fourier collocation spectral method for 3-D viscous Burgers' equation. J. Sci. Comput., 53:102–128, 2012.
- [17] J. Hesthaven, S. Gottlieb, and D. Gottlieb. Spectral Methods for Time-dependent Problems. Cambridge University Press, Cambridge, UK, 2007.
- [18] L. Ju, X. Li, Z. Qiao, and H. Zhang. Energy stability and convergence of exponential time differencing schemes for the epitaxial growth model without slope selection. *Math. Comp.*, 87:1859–1885, 2018.
- [19] R.V. Kohn. Energy-driven pattern formation. Proceedings of the International Congress of Mathematicians, M. Sanz-Sole, J. Soria, J.L. Varona, and J. Verdera, eds., European Mathematical Society Publishing House, Madrid, 1:359–384, 2007.
- [20] R.V. Kohn and X. Yan. Upper bound on the coarsening rate for an epitaxial growth model. *Comm. Pure Appl. Math.*, 56:1549–1564, 2003.
- [21] B. Li. High-order surface relaxation versus the Ehrlich-Schwoebel effect. *Nonlinearity*, 19:2581–2603, 2006.
- [22] B. Li and J.-G. Liu. Thin film epitaxy with or without slope selection. *Eur. J. Appl. Math.*, 14:713–743, 2003.
- [23] B. Li and J.-G. Liu. Epitaxial growth without slope selection: energetics, coarsening, and dynamic scaling. *J. Nonlinear Sci.*, 14:429–451, 2004.
- [24] D. Li and Z. Qiao. On second order semi-implicit Fourier spectral methods for 2D Cahn-

Hilliard equations. J. Sci. Comput., 70:301–341, 2017.

- [25] D. Li, Z. Qiao, and T. Tang. Characterizing the stabilization size for semi-implicit Fourierspectral method to phase field equations. *SIAM J. Numer. Anal.*, 54:1653–1681, 2016.
- [26] W. Li, W. Chen, C. Wang, Y. Yan, and R. He. A second order energy stable linear scheme for a thin film model without slope selection. *J. Sci. Comput.*, 76(3):1905–1937, 2018.
- [27] D. Moldovan and L. Golubovic. Interfacial coarsening dynamics in epitaxial growth with slope selection. *Phys. Rev. E*, 61(6):6190, 2000.
- [28] H. Pan, Z. Luo, and S. Wang. Second order energy stable linear schemes for the molecular beam epitaxy model without slope selection. J. Fudan Univ. (Natural Sci.), 59:137–148, 2020.
- [29] Z. Qiao, Z. Sun, and Z. Zhang. The stability and convergence of two linearized finite difference schemes for the nonlinear epitaxial growth model. *Numer. Methods Partial Differ. Equ.*, 28:1893–1915, 2012.
- [30] Z. Qiao, Z. Sun, and Z. Zhang. Stability and convergence of second-order schemes for the nonlinear epitaxial growth model without slope selection. *Math. Comp.*, 84:653–674, 2015.
- [31] Z. Qiao, C. Wang, S.M. Wise, and Z. Zhang. Error analysis of a finite difference scheme for the epitaxial thin film growth model with slope selection with an improved convergence constant. *Int. J. Numer. Anal. Model.*, 14:283–305, 2017.
- [32] Z. Qiao, Z. Zhang, and T. Tang. An adaptive time-stepping strategy for the molecular beam epitaxy models. *SIAM J. Sci. Comput.*, 33:1395–1414, 2012.
- [33] R. L. Schwoebel. Step motion on crystal surfaces: II. J. Appl. Phys., 40:614–618, 1969.
- [34] J. Shen, C. Wang, X. Wang, and S.M. Wise. Second-order convex splitting schemes for gradient flows with Ehrlich-Schwoebel type energy: Application to thin film epitaxy. *SIAM J. Numer. Anal.*, 50:105–125, 2012.
- [35] C. Wang, X. Wang, and S.M. Wise. Unconditionally stable schemes for equations of thin film epitaxy. *Discrete Contin. Dyn. Syst.*, 28:405–423, 2010.
- [36] S. Wang, W. Chen, H. Pan, and C. Wang. Optimal rate convergence analysis of a second order scheme for a thin film model with slope selection. *J. Comput. Appl. Math.*, 377:112855, 2020.
- [37] C. Xu and T. Tang. Stability analysis of large time-stepping methods for epitaxial growth models. SIAM J. Numer. Anal., 44(4):1759–1779, 2006.
- [38] Y. Yan, W. Chen, C. Wang, and S.M. Wise. A second-order energy stable BDF numerical scheme for the Cahn-Hilliard equation. *Commun. Comput. Phys.*, 23:572–602, 2018.
- [39] X. Yang, J. Zhao, and Q. Wang. Numerical approximations for the molecular beam epitaxial growth model based on the invariant energy quadratization method. *J. Comput. Phys.*, 333:104–127, 2017.