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# UNCONDITIONALLY STABLE SCHEMES FOR EQUATIONS OF THIN FILM EPITAXY

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Abstract. We present unconditionally stable and convergent numerical schemes for gradient flows with energy of the form $\int_\Omega \left( F(\nabla\phi(\mathbf{x})) + \frac{\epsilon^2}{2}|\Delta\phi(\mathbf{x})|^2 \right) \mathrm{d}\mathbf{x}$. The construction of the schemes involves an appropriate extension of Eyre's idea of convex-concave decomposition of the energy functional. As an application, we derive unconditionally stable and convergent schemes for epitaxial film growth models with slope selection ($F(\mathbf{y}) = \frac{1}{4}(|\mathbf{y}|^2 - 1)^2$) and without slope selection ($F(\mathbf{y}) = -\frac{1}{2}\ln(1 + |\mathbf{y}|^2)$). We conclude the paper with some preliminary computations that employ the proposed schemes.

1. **Introduction.** Two commonly used phenomenological models for epitaxial thin film growth are the gradient flows of the following "energy" functionals

$$E_1(\phi) \;:=\; \int_\Omega \left( -\frac{1}{2}\ln\left(1 + |\nabla\phi|^2\right) + \frac{\epsilon^2}{2}|\Delta\phi|^2 \right) \mathrm{d}\mathbf{x} \,, \tag{1}$$

$$E_2(\phi) \;:=\; \int_\Omega \left( \frac{1}{4}\left(|\nabla\phi|^2 - 1\right)^2 + \frac{\epsilon^2}{2}|\Delta\phi|^2 \right) \mathrm{d}\mathbf{x} \,, \tag{2}$$

where $\Omega = [0, L_x] \times [0, L_y]$, with $L_x = L_y = 2\pi$ for simplicity, $\phi : \Omega \to \mathcal{R}$ is a periodic height function with average zero, and $\epsilon$ is a constant. The second energy may be viewed as an approximation of the first energy under the assumption that the gradient of the height is small [15].

There are significant differences between the two models with the second (simplified) model having a slope selection mechanism ($|\nabla\phi| = 1$ is preferred) that is

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absent in the first model. This leads to differences in energy minimizers and long-time coarsening processes [12, 13, 15]. Both energy functionals take the form of

$$E(\phi) = \int_\Omega \left( F\left(\nabla\phi(\mathbf{x})\right) + \frac{\epsilon^2}{2}|\Delta\phi(\mathbf{x})|^2 \right) \mathrm{d}\mathbf{x} \ , \tag{3}$$

where $F(\mathbf{y})$ is a smooth function of its argument $\mathbf{y}$. The first term,

$$E_{ES}(\phi) = \int_\Omega F\left(\nabla\phi(\mathbf{x})\right) \mathrm{d}\mathbf{x} \ , \tag{4}$$

represents the Ehrlich-Schwoebel effect — *i.e.*, adatoms (absorbed atoms) must overcome a higher energy barrier to stick to a step from an upper rather than from a lower terrace [6, 15, 19] — while the second term,

$$E_{SD}(\phi) = \int_\Omega \frac{\epsilon^2}{2}|\Delta\phi(\mathbf{x})|^2 \,\mathrm{d}\mathbf{x} \ , \tag{5}$$

represents the surface diffusion effect [15].

The variational derivatives of these functionals, which may be interpreted as chemical potentials, can be calculated formally as

$$\mu := \frac{\delta E(\phi)}{\delta\phi} = -\nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{y}} F(\nabla_{\mathbf{x}}\phi) + \epsilon^2\Delta^2\phi \ . \tag{6}$$

The gradient flow then takes the form

$$\frac{\partial\phi}{\partial t} = -\mu = \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{y}} F(\nabla_{\mathbf{x}}\phi) - \epsilon^2\Delta^2\phi \ , \tag{7}$$

where the boundary conditions for $\phi$ are taken to be periodic in both spatial directions. The physically interesting coarsening process for spatially large systems (small $\epsilon$) occurs on a very long time scale. For instance, for the model with slope selection, the minimal energy is of the order of $\epsilon$ [12]. Assuming the widely believed $t^{-\frac{1}{3}}$ scaling for the energy [13, 15, 16], it requires about $\frac{1}{\epsilon^3}$ time for the system to reach saturation from an initially order one profile. Therefore, numerical simulations for the coarsening process of large systems require long-time accuracy and stability.

In the case of Allen-Cahn or Cahn-Hilliard flow, where, for example, the energy is of the form

$$E(\phi) = \int_\Omega \left( \frac{1}{4}\left(\phi^2 - 1\right)^2 + \frac{\epsilon^2}{2}|\nabla\phi|^2 \right) \mathrm{d}\mathbf{x} \ , \tag{8}$$

Eyre [8] (see also [1, 21]) proposed to decompose the free energy into convex and concave parts and utilize implicit time discretization in the convex part and explicit time stepping in the concave part. (Note that Eyre employed spatial discretization of the energy first.) Eyre's convex-splitting scheme for the Cahn-Hilliard equation can be interpreted as

$$\phi^{n+1} - \phi^n = k\Delta\mu^{n+1} \ , \quad \mu^{n+1} = \left(\phi^{n+1}\right)^3 - \phi^n - \epsilon^2\Delta\phi^{n+1} \ , \tag{9}$$

where $k > 0$ is the time step size. The scheme is first-order accurate in time, unconditionally uniquely solvable, and unconditionally energy stable in the sense that the energy is monotonically non-increasing in (discrete) time, regardless of the time step size. Such unconditionally stable schemes are highly desirable with regard to long time numerical simulation, especially for coarsening processes that require increasingly larger time step sizes to simulate efficiently. Du and Nicolades [3] proposed a different scheme for the Cahn-Hilliard equation. Spacial discretization in [3] was effected by a finite element method, though they also discussed a finite difference version, which was subsequently analyzed by Furihata [9] for one space dimension. In any case, the space continuous version of the scheme in strong form is

$$\phi^{n+1}-\phi^{n}=k\Delta\mu^{n+1/2}\;,\quad \mu^{n+1/2}=\frac{G\left(\phi^{n+1}\right)-G\left(\phi^{n}\right)}{\phi^{n+1}-\phi^{n}}-\frac{\epsilon^2}{2}\Delta\left(\phi^{n+1}+\phi^{n}\right)\;,\quad(10)$$

where $G(\phi):=\frac{1}{4}\left(\phi^2-1\right)^2$. The scheme is second-order in time and energy stable if it is solvable. In the fully discrete setting both Du and Nicolades and Furihata show that if $k/h^2\le C$, where $h>0$ is the uniform space step size and $C>0$ is a constant, then the scheme does indeed possess a unique solution. However, Du and Nicolades point out in a footnote to a theorem [3, Thm. 3.1], that the fully discrete scheme may in fact be solvable, though perhaps not uniquely, for much larger time steps. The issue of solvability for the time-discrete, space-continuous scheme is a more delicate question.

The main purpose of this manuscript is to generalize Eyre's idea to the case of equations for thin film epitaxy, where the total "free energy" takes the form of $\int_\Omega\left(F(\nabla\phi)+\frac{\epsilon^2}{2}|\Delta\phi|^2\right)\mathrm{d}\mathbf{x}$, where $F\left(\mathbf{y}\right)=-\frac{1}{2}\ln\left(1+\left|\mathbf{y}\right|^2\right)$ in the case of no slope selection and $F\left(\mathbf{y}\right)=\frac{1}{4}\left(\left|\mathbf{y}\right|^2-1\right)^2$ in the case with slope selection. Application of a scheme like that proposed by Du and Nicolades would pose significant difficulties for our analysis because of the solvability question. Eyre's original approach emphasized time discretization with spatially discretized energies (*e.g.*, via finite differences) [8, 21]. Herein we emphasize semi-discretization, specifically time discretization, since the stability in time is the central issue. In particular, our time stepping scheme can be combined with any spatial discretization (*e.g.*, Fourier spectral, or continuous Galerkin), provided that the spatial discretization preserves the energy stability features. Although the theory herein is presented for energy functionals suitable for thin film epitaxy, it is easily generalized to a wider class of gradient flow equations, such as Swift-Hohenberg and phase field crystal (PFC) equations [23] (see also [2]). Higher-order (in particular, second-order) convex-splitting schemes can be developed as well [11] that preserve the unconditional energy stability and unconditional solvability aspects of the first-order convex splitting schemes.

The rest of the manuscript is organized as follows. In section 2 we motivate the convex-concave splitting of the Ehrlich-Schwoebel energy, derive the convex-splitting scheme, and prove some properties of the scheme. Specifically, in section 2.1 we prove a lemma that will facilitate a convex-concave decomposition of the energy; in section 2.2 we define the semi-discrete convexity splitting scheme; in section 2.3 we show the unconditional stability and well-posedness of the scheme; in section 2.4 we prove an error estimate that demonstrates the local-in-time convergence of the scheme; and in section 2.5 we prove another desirable property of the scheme, *i.e.*, all solutions to the scheme converge to critical points of the original energy functional as time approaches infinity. In section 3 we apply the general convex-concave splitting scheme to the thin film epitaxy equations by verifying that the two classical energies (1) and (2) satisfy the assumptions imposed in section 2. We also show some preliminary computations using the proposed schemes. We offer our concluding remarks in section 4.

2. **The general numerical scheme and its properties.** It is quite clear that the linear fourth order surface diffusion term must be treated implicitly in the discretization in order for any scheme to enjoy unconditional stability. One of the interesting features with the models we examine here is that a fully implicit scheme may not provide the answer to the stability question. Specifically the energy functional may not be monotonically decreasing at each time step. Moreover, fully implicit time stepping could suffer from non-uniqueness of solutions at each time step due to non-convexity. The question then is the treatment of the nonlinear second order Ehrlich-Schwoebel terms. The key observation is that the energy increment is proportional to the variational derivative acted on the increment in the phase field plus a second order correction term. Hence whether the energy is convex or concave plays a central role in the sign of the correction term. We will explore this below.

2.1. **Convex-concave decomposition of the energy.** Consider a general differentiable Ehrlich-Schwoebel type energy functional $E_{ES}$ given by (4), associated with a (smooth) function $F : \mathcal{R}^2 \to \mathcal{R}$. Now for any two admissible functions $\phi$, $\psi$, we define the scalar function $f(\lambda)$, $\lambda \in \mathcal{R}$ as

$$f(\lambda) = E_{ES}(\phi + \lambda(\psi - \phi)) \; . \tag{11}$$

It is easy to see that $f(0) = E_{ES}(\phi)$ and $f(1) = E_{ES}(\psi)$. Therefore

$$E_{ES}(\psi) - E_{ES}(\phi) = f(1) - f(0) = f'(0) + \int_0^1 \int_0^s f^{''}(\tau)\, \mathrm{d}\tau \mathrm{d}s \; . \tag{12}$$

Notice that

$$\begin{aligned} f'(\lambda) &= \int_\Omega \sum_{j=1}^2 \frac{\partial F}{\partial y_j}(\nabla(\phi + \lambda(\psi - \phi)))\frac{\partial}{\partial x_j}(\psi - \phi)\, \mathrm{d}\mathbf{x} \\ &= -\int_\Omega \sum_{j=1}^2 \frac{\partial}{\partial x_j}\frac{\partial F}{\partial y_j}(\nabla(\phi + \lambda(\psi - \phi)))(\psi - \phi)\, \mathrm{d}\mathbf{x} \\ &= \int_\Omega \left.\frac{\delta E_{ES}}{\delta \phi}\right|_{\phi + \lambda(\psi - \phi)} (\psi - \phi)\, \mathrm{d}\mathbf{x} \; , \qquad (13) \\ f^{''}(\lambda) &= \int_\Omega \sum_{j=1}^2 \sum_{k=1}^2 \frac{\partial^2 F}{\partial y_j \partial y_k}(\nabla(\phi + \lambda(\psi - \phi)))\frac{\partial(\psi - \phi)}{\partial x_j}\frac{\partial(\psi - \phi)}{\partial x_k}\, \mathrm{d}\mathbf{x} \; , \qquad (14) \end{aligned}$$

where $\frac{\delta E}{\delta \phi}$ denotes the functional (variational) derivative of $E$. Hence we have

$$\begin{aligned} &E_{ES}(\psi) - E_{ES}(\phi) \\ &\quad = \int_\Omega \left.\frac{\delta E_{ES}}{\delta \phi}\right|_{\phi} (\psi - \phi)\, \mathrm{d}\mathbf{x} \\ &\qquad + \int_0^1 \int_0^s \int_\Omega \nabla(\psi - \phi) \cdot D^2_{\mathbf{y}} F(\nabla \phi + \tau \nabla(\psi - \phi)) \nabla(\psi - \phi)\, \mathrm{d}\mathbf{x}\mathrm{d}\tau\mathrm{d}s \; , \qquad (15) \end{aligned}$$

where $D^2_{\mathbf{y}} F = \left(\frac{\partial^2 F}{\partial y_i \partial y_j}\right)$ denotes the Hessian matrix of the function $F$. Therefore we have the following simple calculus lemma.

**Lemma 2.1.** *For the energy functional $E_{ES}$ given in (4), we have the following inequalities:*

$$E_{ES}(\psi) - E_{ES}(\phi) \geq \int_\Omega \left.\frac{\delta E_{ES}}{\delta\phi}\right|_\phi (\psi-\phi)\,\mathrm{d}\mathbf{x}\ ,\ \text{if } D^2_{\mathbf{y}}F(\nabla\phi)\geq 0,\ \forall\phi\in H^2_{per}\ , \tag{16}$$

$$E_{ES}(\psi) - E_{ES}(\phi) \leq \int_\Omega \left.\frac{\delta E_{ES}}{\delta\phi}\right|_\phi (\psi-\phi)\,\mathrm{d}\mathbf{x}\ ,\ \text{if } D^2_{\mathbf{y}}F(\nabla\phi)\leq 0,\ \forall\phi\in H^2_{per}\ , \tag{17}$$

*where $D^2_{\mathbf{y}}F(\nabla\phi)\geq 0$ ($D^2_{\mathbf{y}}F(\nabla\phi)\leq 0$) indicates positive (negative) semi-definiteness of the Hessian matrix.*

2.2. **A semi-implicit convex-splitting scheme.** We now consider the case of an abstract total "free energy" functional $E$ which takes the form of (3).

Let $C^\infty_{per}(\Omega)$ denote the set of all $\Omega-$periodic $C^\infty$ functions, and let $\dot{C}^\infty_{per}(\Omega)$ denote the subset of $C^\infty_{per}(\Omega)$ whose functions have zero average on $\Omega$. The natural function space for our problem is

$$\dot{H}^2_{per}(\Omega) := \{\text{closure of } \dot{C}^\infty_{per} \text{ in } H^2(\Omega)\}\ . \tag{18}$$

$E_{ES}$ (and hence $E$) is assumed to be well-defined on this space. This is guaranteed by a Sobolev embedding in two dimensions provided the growth rate of $F(\mathbf{y})$ is at most polynomial.

Suppose that $F$ can be decomposed into convex $(+)$ and concave $(-)$ terms in the sense that [1]

$$F(\mathbf{y}) = F_+(\mathbf{y}) + F_-(\mathbf{y})\,, \tag{19}$$

$$D^2_{\mathbf{y}}F_+ \geq 0,\quad E_+(\phi) := \int_\Omega F_+(\nabla_{\mathbf{x}}\phi)\,\mathrm{d}\mathbf{x}\ , \tag{20}$$

$$D^2_{\mathbf{y}}F_- \leq 0,\quad E_-(\phi) := \int_\Omega F_-(\nabla_{\mathbf{x}}\phi)\,\mathrm{d}\mathbf{x}\ . \tag{21}$$

The associated gradient flow is given by

$$\frac{\partial\phi}{\partial t} = -\frac{\delta E_{ES}}{\delta\phi} - \epsilon^2\Delta^2\phi = -\frac{\delta E_+}{\delta\phi} - \frac{\delta E_-}{\delta\phi} - \epsilon^2\Delta^2\phi\ . \tag{22}$$

As will be clear later, Lemma 2.1 suggests we treat the "convex" part implicitly and the "concave" part explicitly. Therefore, we propose the following **general one step scheme** for the gradient flow (22) with time step size $k>0$:

$$\begin{aligned}\frac{\phi^{n+1}-\phi^n}{k} &= -\left.\frac{\delta E_+}{\delta\phi}\right|_{\phi=\phi^{n+1}} - \left.\frac{\delta E_-}{\delta\phi}\right|_{\phi=\phi^n} - \epsilon^2\Delta^2\phi^{n+1}\\ &= \nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{y}}F_+\left(\nabla_{\mathbf{x}}\phi^{n+1}\right) + \nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{y}}F_-\left(\nabla_{\mathbf{x}}\phi^n\right) - \epsilon^2\Delta^2\phi^{n+1}\ .\end{aligned} \tag{23}$$

Notice that there could exist many such schemes since the convex-concave splitting is not unique in general.

Other numerical schemes have been proposed for the models under consideration, most notably the slope-selection model. The scheme proposed by Li and Liu [15] is

[1]Such a decomposition always exists provided that the "energy density" $F$ is convex for large enough $\mathbf{y}$. In this case the convex part will be given by $F(\mathbf{y})+\beta|\mathbf{y}|^2$ with $\beta>0$ sufficiently large.

essentially

$$\frac{\phi^{n+1}-\phi^n}{k} = \frac{3}{2}\nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{y}}F\left(\nabla_{\mathbf{x}}\phi^n\right) - \frac{1}{2}\nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{y}}F\left(\nabla_{\mathbf{x}}\phi^{n-1}\right) - \frac{\epsilon^2}{2}\left(\Delta^2\phi^{n+1}+\Delta^2\phi^n\right) , \tag{24}$$

which is second-order and unconditionally uniquely solvable. Li and Liu [15] did not analyze the stability of the scheme, though it is not expected to be unconditionally stable. Xu and Tang [24] proposed the first-order linear scheme

$$\frac{\phi^{n+1}-\phi^n}{k} = A\left(\Delta\phi^{n+1}-\Delta\phi^n\right) + \nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{y}}F\left(\nabla_{\mathbf{x}}\phi^n\right) - \epsilon^2\Delta^2\phi^{n+1} , \tag{25}$$

where $A$ is a linear splitting parameter. Xu and Tang prove that, for the slope selection case, the scheme is energy stable, provided $A$ is sufficiently large. However, they show that the appropriate $A$ depends on the unknown $\phi^{n+1}$, and thus the scheme is not unconditionally stable. The convex-splitting scheme has no such restriction, as we show presently.

2.3. **Unconditional solvability and stability of the scheme.** We claim that our convex splitting scheme (23) is well-posed and unconditionally "gradient" stable, *i.e.*, stable in the sense that the energy is a non-increasing function in (discrete) time regardless of the time step size $k$.

**Theorem 2.2** (Solvability and energy stability)**.** *Assume that the energy functional $E$ defined in (3) is twice functionally differentiable on $\dot{H}^2_{per}(\Omega)$, and $F(\mathbf{y})$, $\nabla_{\mathbf{y}}F(\mathbf{y})$ grow at most like a polynomial in $\mathbf{y}$. Then the scheme given by (23) for the gradient system (22) satisfying the decomposition (19) is well-posed with the solution given by the unique minimizer of the following modified energy functional:*

$$E_{scheme}(\phi) := \frac{\epsilon^2}{2}\left\|\Delta\phi\right\|^2 + E_+(\phi) + \frac{1}{2k}\left\|\phi\right\|^2 + \int_\Omega\left(\left.\frac{\delta E_-}{\delta\phi}\right|_{\phi=\phi^n} - \frac{1}{k}\phi^n\right)\phi\, \mathrm{d}\mathbf{x} . \tag{26}$$

*Moreover, the energy is a non-increasing function of time,* i.e.*, we have*

$$E(\phi^{n+1}) \le E(\phi^n) - \frac{1}{k}\left\|\phi^{n+1}-\phi^n\right\|^2 - \frac{\epsilon^2}{2}\left\|\Delta\left(\phi^{n+1}-\phi^n\right)\right\|^2 ,\ \forall\ k>0 . \tag{27}$$

*Proof.* Here and in the sequel let us denote by $\|\cdot\|$ the $L^2$ norm on $\Omega$. The proof of the decay of the energy is a straightforward application of the Lemma 2.1 above. Indeed, multiplying the gradient system (23) by $-\left(\phi^{n+1}-\phi^n\right)$; integrating over $\Omega$; and utilizing the lemma, the decomposition (19), and the identity $a(a-b) = \frac{1}{2}(a^2-b^2+(a-b)^2)$, we have

$$\begin{aligned}
-\frac{1}{k}\left\|\phi^{n+1}-\phi^n\right\|^2 \quad &= \quad \int_\Omega \left.\frac{\delta E_+}{\delta\phi}\right|_{\phi=\phi^{n+1}}\left(\phi^{n+1}-\phi^n\right)\,\mathrm{d}\mathbf{x} \\
&\quad + \int_\Omega \left.\frac{\delta E_-}{\delta\phi}\right|_{\phi=\phi^n}\left(\phi^{n+1}-\phi^n\right)\,\mathrm{d}\mathbf{x} \\
&\quad + \frac{\epsilon^2}{2}\left(\left\|\Delta\phi^{n+1}\right\|^2 - \left\|\Delta\phi^n\right\|^2 + \left\|\Delta\left(\phi^{n+1}-\phi^n\right)\right\|^2\right) \\
&\ge \quad E_+\left(\phi^{n+1}\right) - E_+\left(\phi^n\right) + E_-\left(\phi^{n+1}\right) - E_-\left(\phi^n\right) \\
&\quad + \frac{\epsilon^2}{2}\left(\left\|\Delta\phi^{n+1}\right\|^2 - \left\|\Delta\phi^n\right\|^2 + \left\|\Delta\left(\phi^{n+1}-\phi^n\right)\right\|^2\right) \\
&= \quad E\left(\phi^{n+1}\right) - E\left(\phi^n\right) + \frac{\epsilon^2}{2}\left\|\Delta\left(\phi^{n+1}-\phi^n\right)\right\|^2 .
\end{aligned} \tag{28}$$

For the convex part $(+)$ in the last calculation we have utilized Lemma 2.1 with $\phi = \phi^{n+1}$ and $\psi = \phi^n$ and for the concave part $(-)$ we have $\phi = \phi^n$ and $\psi = \phi^{n+1}$.

The uniqueness of the solution to the scheme (23) is also straightforward. Let $\phi$ and $\tilde{\phi}$ be two solutions of the scheme with given $\phi^n$. Then $\psi = \phi - \tilde{\phi}$ satisfies the following equation

$$\frac{\psi}{k} = - \left.\frac{\delta E_+}{\delta \phi}\right|_{\phi=\phi} + \left.\frac{\delta E_+}{\delta \phi}\right|_{\phi=\tilde{\phi}} - \epsilon^2 \Delta^2 \psi \ .$$

Multiplying this equation by $\psi$, integrating over the domain and utilizing the lemma we have

$$\frac{1}{2k} \|\psi\|^2 \leq -\frac{\epsilon^2}{2} \|\Delta \psi\|^2 \ ,$$

which implies that $\psi \equiv 0$.

As for the existence, we notice that the scheme (23) is the Euler-Lagrange equation of the modified energy functional (26). The convexity of $E_+$ implies the convexity and coercivity (when combined with the diffusion term) of $E_{scheme}$ in (26). The convexity in fact implies sequential lower semi-continuity, which in turn leads to the existence of an absolute minimizer $\phi^{n+1}$ of (26) [7]. This minimizer must satisfy the Euler-Lagrange equation, *i.e.*, (23), under the assumed differentiability and growth condition [4, 7, 10]. This ends the proof of the theorem. ☐

**Remark 1.** Although for (23) a nonlinear problem needs to be solved at each time step, the problem is a strictly convex one, and, hence, most classical methods would work very efficiently here [8, 21].

**Remark 2.** The energy non-increasing property for the convex splitting of a general gradient system was recently proven in [23], based on the functional splitting inequality given by [23, Thm. 1.1]. For the energy functional taking the special form of (3), this article gives a slightly more detailed estimate (27), which will be utilized in the numerical analysis of the long-time behavior as can be seen in later sections.

Before our discussion of the convergence analysis, we establish the $L^\infty(0,T;H^2)$ stability of the numerical method. That in turn gives the $L^\infty$ and $L^\infty(0,T;W^{1,p})$ bounds of the numerical solution by a Sobolev embedding in the 2D case. As in Thm. 2.2, a polynomial growth bound for $F(\mathbf{y})$, $\nabla_{\mathbf{y}} F(\mathbf{y})$, and $D^2_{\mathbf{y}} F(\mathbf{y})$ (the Hessian matrix of $F$) needs to be imposed, for technical reasons. We will see later that both thin film models examined here (one with and one without slope selection) satisfy this assumption.

**Theorem 2.3** ($H^2$ stability)**.** *Consider the convex splitting scheme (23) for the gradient flow (22). Under the additional technical assumption on the lower bound of $F$,* i.e.*, that for any $\beta > 0$, there exists a $C_\beta > 0$ such that*

$$F(\mathbf{y}) \geq -\beta |\mathbf{y}|^2 - C_\beta \ , \tag{29}$$

*we have*

$$\|\phi\|_{L^\infty(0,T;H^2)} \leq C_4, \ \|\phi\|_{L^\infty} \leq C_4 C_5, \ \|\phi\|_{L^\infty(0,T;W^{1,p})} \leq C_4 C_p \ , \tag{30}$$

*for any $p : 2 < p < +\infty$. $C_4$ depends on the initial $H^2$ data, $L_x$ and $L_y$ (both of which equal $2\pi$ here), and $\epsilon$, but is independent of final time $T$. $C_5$ and $C_p$ are positive Sobolev embedding constants.*

*Proof.* The energy stability (27) for the numerical scheme shows that

$$E\left(\phi^n\right) \le E\left(\phi^0\right) := C_0 \ , \quad \forall\ n \ ,$$

or, equivalently,

$$\int_\Omega F\left(\nabla \phi^n\right)\, \mathrm{d}\mathbf{x} + \frac{\epsilon^2}{2} \left\|\Delta \phi^n\right\|^2 \le C_0 \ , \quad \forall\ n \ . \tag{31}$$

Meanwhile, by the technical assumption (29), we take $\beta = \frac{\epsilon^2}{4C_1}$ and observe the following inequality

$$F\left(\nabla \phi\right) \ge -\frac{1}{4C_1}\epsilon^2 \left|\nabla \phi\right|^2 - C_\beta \ , \tag{32}$$

where $C_1$ corresponds to the constant in the Poincaré inequality:

$$\left\|\nabla \phi\right\|^2 \le C_1 \left\|\Delta \phi\right\|^2 \ . \tag{33}$$

In turn, a substitution of (32) into the total physical energy gives

$$\begin{aligned} E(\phi) &= \int_\Omega F\left(\nabla \phi\right)\, \mathrm{d}\mathbf{x} + \frac{\epsilon^2}{2}\left\|\Delta\phi\right\|^2 \\ &\ge -\frac{1}{4C_1}\epsilon^2 \left\|\nabla \phi\right\|^2 - C_\beta L_x L_y + \frac{\epsilon^2}{2}\left\|\Delta\phi\right\|^2 \\ &\ge -\frac{1}{4}\epsilon^2 \left\|\Delta \phi\right\|^2 - C_\beta L_x L_y + \frac{\epsilon^2}{2}\left\|\Delta\phi\right\|^2 \\ &\ge \frac{\epsilon^2}{4}\left\|\Delta\phi\right\|^2 - C_\beta L_x L_y \ . \end{aligned} \tag{34}$$

Subsequently, a combination of (31) and (34) leads to

$$\left\|\Delta \phi^n\right\|^2 \le \frac{4}{\epsilon^2}\left(C_0 + C_\beta L_x L_y\right), \quad \forall\ n \ . \tag{35}$$

As a direct consequence, we arrive at

$$\left\|\phi^n\right\|_{H^2} \le C_3 \left\|\Delta\phi^n\right\| \le \frac{2C_3}{\epsilon}\sqrt{C_0 + C_\beta L_x L_y} := C_4 \ , \quad \forall\ n \ , \tag{36}$$

where the constant $C_3 > 0$ comes from elliptic regularity with the assumption $\int_\Omega \phi^n\, \mathrm{d}\mathbf{x} = 0$. The first part of the theorem is proven. The second and third parts come directly from the following Sobolev inequalities:

$$\left\|\phi\right\|_{L^\infty} \le C_5 \left\|\phi\right\|_{H^2} \ , \quad \left\|\phi\right\|_{W^{1,p}} \le C_p \left\|\phi\right\|_{H^2} \ , \quad \forall\ p:\ 2 < p < +\infty \ . \tag{37}$$

□

### 2.4. **Local-in-time convergence.**

**Theorem 2.4** (Error estimate)**.** *Given smooth, periodic initial data $\phi_0(x,y)$, suppose the unique, smooth solution for the gradient flow (22) is given by $\phi_e(x,y,t)$ on $\Omega$ for $t \in [0,T]$, for some $T < \infty$. We also assume that $D^2_{\mathbf{y}} F\left(\mathbf{y}\right)$ (the Hessian matrix of $F$) grows at most like a polynomial in* $\mathbf{y}$, i.e.*, there exists a positive integer $m$ and a constant $C$ such that*

$$\left\|D^2_{\mathbf{y}} F_+\left(\mathbf{y}\right)\right\| + \left\|D^2_{\mathbf{y}} F_-\left(\mathbf{y}\right)\right\| \le C\left(1 + \left|\mathbf{y}\right|^m\right). \tag{38}$$

*Define $\phi_e^n := \phi_e(\,\cdot\,, nk)$, and $\tilde{\phi}^n := \phi_e^n - \phi^n$, where $\phi^n$ is the numerical solution of (23) with $\phi^0 := \phi_e^0$. Then*

$$\left\|\tilde{\phi}^n\right\| \le Ck \ , \quad \forall\ n:\ n \le \left\lfloor \frac{T}{k} \right\rfloor \ , \tag{39}$$

*provided $k$ is sufficiently small, for some $C > 0$ that is independent of $k$.*

*Proof.* The exact solution $\phi_e$ solves the numerical scheme

$$\frac{\phi_e^{n+1} - \phi_e^n}{k} = \nabla \cdot \left(\nabla_{\mathbf{y}} F_+ \left(\nabla \phi_e^{n+1}\right) + \nabla_{\mathbf{y}} F_- \left(\nabla \phi_e^n\right)\right) - \epsilon^2 \Delta^2 \phi_e^{n+1} + \tau^{n+1}, \tag{40}$$

where $\tau^{n+1}$ is the local truncation error, which satisfies

$$\left|\tau^{n+1}\right| \leq M_1 k, \tag{41}$$

for some $M_1 \geq 0$ that depends only on $T$, $L_x$, and $L_y$. In particular, we have

$$M_1 \leq C \left( \|\phi_e\|_{C^2(0,T;C^0(\Omega))} + \|\phi_e\|_{C^1(0,T;C^{m+2}(\Omega))} \right). \tag{42}$$

The regularity of the exact solution to the epitaxial equations can be found in [15], for instance. The unconditional stability and the well-posedness for the semi-discrete in time scheme (23) can be used to show the well-posedness of the underlying gradient system (22) just as the case for the Navier-Stokes equation [20].

Subtracting (23) from (40) yields

$$\begin{aligned} \frac{\tilde{\phi}^{n+1} - \tilde{\phi}^n}{k} &= \nabla \cdot \left(\nabla_{\mathbf{y}} F_+(\nabla \phi_e^{n+1}) - \nabla_{\mathbf{y}} F_+(\nabla \phi^{n+1})\right) \\ &\quad + \nabla \cdot \left(\nabla_{\mathbf{y}} F_-(\nabla \phi_e^n) - \nabla_{\mathbf{y}} F_-(\nabla \phi^n)\right) - \epsilon^2 \Delta^2 \tilde{\phi}^{n+1} + \tau^{n+1}. \end{aligned} \tag{43}$$

Taking inner product with $2k\tilde{\phi}^{n+1}$ and applying integration by parts shows that

$$\begin{aligned} &\left\|\tilde{\phi}^{n+1}\right\|^2 - \left\|\tilde{\phi}^n\right\|^2 + \left\|\tilde{\phi}^{n+1} - \tilde{\phi}^n\right\|^2 + 2\epsilon^2 k \left\|\Delta \tilde{\phi}^{n+1}\right\|^2 - 2k\left(\tilde{\phi}^{n+1}, \tau^{n+1}\right) \\ &\quad = -2k\left(\nabla \tilde{\phi}^{n+1}, \left(\nabla_{\mathbf{y}} F_+(\nabla \phi_e^{n+1}) - \nabla_{\mathbf{y}} F_+(\nabla \phi^{n+1})\right)\right) \\ &\qquad -2k\left(\nabla \tilde{\phi}^{n+1}, \left(\nabla_{\mathbf{y}} F_-(\nabla \phi_e^n) - \nabla_{\mathbf{y}} F_-(\nabla \phi^n)\right)\right). \end{aligned} \tag{44}$$

The local truncation error term can be directly controlled by the Cauchy inequality:

$$2\left(\tilde{\phi}^{n+1}, \tau^{n+1}\right) \leq \left\|\tilde{\phi}^{n+1}\right\|^2 + \left\|\tau^{n+1}\right\|^2 \leq \left\|\tilde{\phi}^{n+1}\right\|^2 + M_1^2 k^2 L_x L_y . \tag{45}$$

For the term related to the convex part of $F$, we see that the technical assumption (38) implies that

$$\begin{aligned} \left|\nabla_{\mathbf{y}} F_+(\mathbf{y}_1) - \nabla_{\mathbf{y}} F_+(\mathbf{y}_2)\right| &\leq \max_{t \in [0,1]} \left\|D_{\mathbf{y}}^2 F_+(\mathbf{y}_2 + t(\mathbf{y}_1 - \mathbf{y}_2))\right\| \left|\mathbf{y}_1 - \mathbf{y}_2\right| \\ &\leq C\left(|\mathbf{y}_1|^m + |\mathbf{y}_2|^m + 1\right)\left|\mathbf{y}_1 - \mathbf{y}_2\right| , \end{aligned} \tag{46}$$

in which a vector form of the mean value theorem was utilized in the first step. By substituting $\mathbf{y}_1 = \nabla \phi_e^{n+1}$, $\mathbf{y}_2 = \nabla \phi^{n+1}$, we get

$$\left|\nabla_{\mathbf{y}} F_+(\nabla \phi_e^{n+1}) - \nabla_{\mathbf{y}} F_+(\nabla \phi^{n+1})\right| \leq C\left(\left|\nabla \phi_e^{n+1}\right|^m + \left|\nabla \phi^{n+1}\right|^m + 1\right)\left|\nabla \tilde{\phi}^{n+1}\right| . \tag{47}$$

Consequently, a direct application of the Hölder inequality to the above estimate implies that

$$\begin{aligned} &\left\|\nabla_{\mathbf{y}} F_+(\nabla \phi_e^{n+1}) - \nabla_{\mathbf{y}} F_+(\nabla \phi^{n+1})\right\| \\ &\quad \leq C\left\|\left(\left|\nabla \phi_e^{n+1}\right|^m + \left|\nabla \phi^{n+1}\right|^m + 1\right)\right\|_{L^4} \cdot \left\|\nabla \tilde{\phi}^{n+1}\right\|_{L^4} \\ &\quad \leq C\left(\left\|\nabla \phi_e^{n+1}\right\|_{L^{4m}}^m + \left\|\nabla \phi^{n+1}\right\|_{L^{4m}}^m + 1\right) \cdot \left\|\nabla \tilde{\phi}^{n+1}\right\|_{L^4} . \end{aligned} \tag{48}$$

For the exact solution $\phi_e^{n+1}$, we use $C^*$ to denote the bound of its norms (up to $W^{2,\infty}$ in our case) so that

$$\left\|\nabla \phi_e^{n+1}\right\|_{L^{4m}} \leq C^*, \quad \forall\, n: \; n \leq \left\lfloor \frac{T}{k} \right\rfloor. \tag{49}$$

For the numerical solution $\phi^{n+1}$, we recall from Thm. 2.3 (with $p = 4m$):

$$\left\|\nabla \phi^{n+1}\right\|_{L^{4m}} \leq C_4 C_p \;. \tag{50}$$

As a result, a substitution of (49) and (50) into (48) shows that

$$\left\|\nabla_{\mathbf{y}} F_+(\nabla \phi_e^{n+1}) - \nabla_{\mathbf{y}} F_+(\nabla \phi^{n+1})\right\| \leq C \left\|\nabla \tilde{\phi}^{n+1}\right\|_{L^4} \;. \tag{51}$$

Similarly, for the concave part of $F$, we have

$$\left\|\nabla_{\mathbf{y}} F_-(\nabla \phi_e^{n}) - \nabla_{\mathbf{y}} F_-(\nabla \phi^{n})\right\| \leq C \left\|\nabla \tilde{\phi}^{n}\right\|_{L^4} \;. \tag{52}$$

Consequently, the above two estimates indicate that

$$\begin{aligned}
&- 2\left(\nabla \tilde{\phi}^{n+1}, \left(\nabla_{\mathbf{y}} F_+(\nabla \phi_e^{n+1}) - \nabla_{\mathbf{y}} F_+(\nabla \phi^{n+1})\right)\right) \\
&\qquad \leq 2\left\|\nabla \tilde{\phi}^{n+1}\right\| \cdot \left\|\nabla_{\mathbf{y}} F_+(\nabla \phi_e^{n+1}) - \nabla_{\mathbf{y}} F_+(\nabla \phi^{n+1})\right\| \\
&\qquad \leq 2C\left\|\nabla \tilde{\phi}^{n+1}\right\| \cdot \left\|\nabla \tilde{\phi}^{n+1}\right\|_{L^4},
\end{aligned} \tag{53}$$

$$\begin{aligned}
&2\left(\nabla \tilde{\phi}^{n+1}, \left(\nabla_{\mathbf{y}} F_-(\nabla \phi_e^{n}) - \nabla_{\mathbf{y}} F_-(\nabla \phi^{n})\right)\right) \\
&\qquad \leq 2\left\|\nabla \tilde{\phi}^{n+1}\right\| \cdot \left\|\nabla_{\mathbf{y}} F_-(\nabla \phi_e^{n}) - \nabla_{\mathbf{y}} F_-(\nabla \phi^{n})\right\| \\
&\qquad \leq 2C\left\|\nabla \tilde{\phi}^{n+1}\right\| \cdot \left\|\nabla \tilde{\phi}^{n}\right\|_{L^4} \;.
\end{aligned} \tag{54}$$

Recall that standard interpolation inequalities imply

$$\left\|\nabla \tilde{\phi}^{n+1}\right\| \leq C \left\|\tilde{\phi}^{n+1}\right\|^{1/2} \cdot \left\|\Delta \tilde{\phi}^{n+1}\right\|^{1/2}, \tag{55}$$

$$\left\|\nabla \tilde{\phi}^{n+1}\right\|_{L^4} \leq C \left\|\tilde{\phi}^{n+1}\right\|^{1/4} \cdot \left\|\Delta \tilde{\phi}^{n+1}\right\|^{3/4}, \tag{56}$$

$$\left\|\nabla \tilde{\phi}^{n}\right\|_{L^4} \leq C \left\|\tilde{\phi}^{n}\right\|^{1/4} \cdot \left\|\Delta \tilde{\phi}^{n}\right\|^{3/4} \;. \tag{57}$$

Therefore, a combination of (55), (56) and (57) gives

$$\begin{aligned}
\left\|\nabla \tilde{\phi}^{n+1}\right\| \cdot \left\|\nabla \tilde{\phi}^{n+1}\right\|_{L^4} &\leq C \left\|\tilde{\phi}^{n+1}\right\|^{3/4} \cdot \left\|\Delta \tilde{\phi}^{n+1}\right\|^{5/4} \\
&\leq C \left\|\tilde{\phi}^{n+1}\right\|^{2} + \frac{\epsilon^2}{4}\left\|\Delta \tilde{\phi}^{n+1}\right\|^{2}.
\end{aligned} \tag{58}$$

Similarly, we have

$$\begin{aligned}
\left\|\nabla \tilde{\phi}^{n+1}\right\| \cdot \left\|\nabla \tilde{\phi}^{n}\right\|_{L^4} &\leq C \left\|\tilde{\phi}^{n+1}\right\|^{1/2} \cdot \left\|\tilde{\phi}^{n}\right\|^{1/4} \cdot \left\|\Delta \tilde{\phi}^{n+1}\right\|^{1/2} \cdot \left\|\Delta \tilde{\phi}^{n}\right\|^{3/4} \\
&\leq C\left(\left\|\tilde{\phi}^{n+1}\right\|^{2} + \left\|\tilde{\phi}^{n}\right\|^{2}\right) \\
&\quad + \frac{\epsilon^2}{8}\left(\left\|\Delta \tilde{\phi}^{n+1}\right\|^{2} + \left\|\Delta \tilde{\phi}^{n}\right\|^{2}\right).
\end{aligned} \tag{59}$$

Consequently, a substitution of the above two inequalities into (53) and (54) results in an estimate of the inner product related to $F$:

$$\begin{aligned}
&-2\left(\nabla\tilde{\phi}^{n+1},\left(\nabla_{\mathbf{y}}F_+(\nabla\phi_e^{n+1})-\nabla_{\mathbf{y}}F_+(\nabla\phi^{n+1})\right)\right)\\
&\quad-2\left(\nabla\tilde{\phi}^{n+1},\left(\nabla_{\mathbf{y}}F_-(\nabla\phi_e^{n})-\nabla_{\mathbf{y}}F_-(\nabla\phi^{n})\right)\right)\\
&\qquad\le C\left(\left\|\tilde{\phi}^{n+1}\right\|^2+\left\|\tilde{\phi}^{n}\right\|^2\right)+\frac{3}{8}\epsilon^2\left\|\Delta\tilde{\phi}^{n+1}\right\|^2+\frac{1}{8}\epsilon^2\left\|\Delta\tilde{\phi}^{n}\right\|^2\ . \qquad (60)
\end{aligned}$$

Finally, a substitution of (45), and (60) into (44) leads to

$$\begin{aligned}
&\left\|\tilde{\phi}^{n+1}\right\|^2-\left\|\tilde{\phi}^{n}\right\|^2+\left\|\tilde{\phi}^{n+1}-\tilde{\phi}^{n}\right\|^2+\epsilon^2k\left\|\Delta\tilde{\phi}^{n+1}\right\|^2\\
&\qquad\le k\,(1+C)\left(\left\|\tilde{\phi}^{n+1}\right\|^2+\left\|\tilde{\phi}^{n}\right\|^2\right)+M_1^2k^3L_xL_y\ . \qquad (61)
\end{aligned}$$

An application of a discrete Grownwall inequality implies that

$$\left\|\tilde{\phi}^{n}\right\|\le Ce^{CT}M_1(L_xL_y)^{1/2}k\ ,\quad \forall\ n:\ n\le\left\lfloor\frac{T}{k}\right\rfloor\ . \qquad (62)$$

This completes the proof of the theorem. □

**Remark 3.** In fact, the additional growth condition on the Hessian of the convex part is not necessary here since we have

$$\begin{aligned}
&(\nabla_{\mathbf{y}}F_+(\mathbf{y}_1)-\nabla_{\mathbf{y}}F_+(\mathbf{y}_2))\cdot(\mathbf{y}_1-\mathbf{y}_2)\\
&\qquad=(\mathbf{y}_1-\mathbf{y}_2)\cdot\left(\int_0^1 D^2_{\mathbf{y}}F_+(\mathbf{y}_2+t(\mathbf{y}_1-\mathbf{y}_2))\,\mathrm{d}t\right)(\mathbf{y}_1-\mathbf{y}_2)\\
&\qquad\ge 0\ .
\end{aligned}$$

2.5. **Long time behavior of the scheme.** Besides the unconditional stability and the convergence of the scheme (23), we can also show that the scheme shares another property with the gradient system (22) that it is approximating, namely, solutions to the numerical scheme (23) must converge to critical points of the energy functional (3) (no convergence to energy minimizer is guaranteed).

Thanks to the estimates (27, 34), we have

$$\|\Delta\phi^n\|\le C,\quad \sum_{n=0}^{\infty}\left\|\Delta\phi^{n+1}-\Delta\phi^n\right\|^2<\infty. \qquad (63)$$

Therefore $\{\phi^n\}$ must have weakly convergent subsequence in $H^2$. Let $\{\phi^{n_j}\}$ be a weakly convergent subsequence of $\{\phi^n\}$ in $H^2$ with the limit being $\phi^\infty$. Thanks to (63), we see that $\{\phi^{n_j+1}\}$ also converges to $\phi^\infty$ in $H^2$. We restrict the scheme to these special subsequences and we have

$$\frac{\phi^{n_j+1}-\phi^{n_j}}{k}=\nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{y}}F_+(\nabla_{\mathbf{x}}\phi^{n_j+1})+\nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{y}}F_-(\nabla_{\mathbf{x}}\phi^{n_j})-\epsilon^2\Delta^2\phi^{n_j+1}\ . \qquad (64)$$

Taking the limit as $j$ approaches infinity in the weak sense, we have that $\phi^\infty$ satisfies the Euler-Lagrange equation of the energy functional (3) since both $\{\phi^{n_j}\}$ and $\{\phi^{n_j+1}\}$ converges to $\phi^\infty$. Indeed, for $\psi\in\dot{H}^2_{per}$ and $F=F_+$ or $F=F_-$, we have

$$
\begin{aligned}
&|(\nabla_{\mathbf{y}} F(\nabla_{\mathbf{x}}\phi^n) - \nabla_{\mathbf{y}} F(\nabla_{\mathbf{x}}\phi^\infty), \nabla\psi)| \\
&\qquad \le \left| \left( \max_{t\in[0,1]} \left\| D^2_{\mathbf{y}} F(\phi^\infty + t(\phi^n - \phi^\infty)) \right\| \, |\nabla(\phi^n - \phi^\infty)| \, , \nabla\psi \right) \right| \\
&\qquad \le C \left| \left( (1 + |\nabla\phi^n|^m + |\nabla\phi^\infty|^m) \; |\nabla(\phi^n - \phi^\infty)| \, , \nabla\psi \right) \right| \\
&\qquad \le C(1 + \|\nabla\phi^n\|^m_{L^{3m}} + \|\nabla\phi^\infty\|^m_{L^{3m}}) \, \|\nabla(\phi^n - \phi^\infty)\|_{L^3} \, \|\nabla\psi\|_{L^3} \\
&\qquad \to 0 \; ,
\end{aligned}
$$

where in the last step we have applied the Rellich compactness theorem. Hence

$$
\begin{aligned}
0 &= \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{y}} F_+(\nabla_{\mathbf{x}}\phi^\infty) + \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{y}} F_-(\nabla_{\mathbf{x}}\phi^\infty) - \epsilon^2 \Delta^2 \phi^\infty \\
&= \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{y}} F(\nabla_{\mathbf{x}}\phi^\infty) - \epsilon^2 \Delta^2 \phi^\infty. \qquad (65)
\end{aligned}
$$

This proves that $\phi^\infty$ must be a critical point of the energy functional (3). Therefore we have

**Theorem 2.5.** *All solutions of the numerical scheme (23) must converge to critical points of the energy functional (3) as time approaches infinity provided that the convexity decomposition assumption (19) and the growth assumptions (29, 38) are satisfied.*

This result indicates that the scheme viewed as a discrete dynamical system shares exactly the same very important long-time behavior of the continuous dynamical system associated with the gradient flows (22) in the sense that they converge to exactly the same set of critical points. These critical points are not necessarily minimizers of the energy functional (3), since an arbitrary critical point of the energy (3) is a steady state of the numerical scheme (23) as well.

We could talk about the stationary statistical properties of the scheme (23) and the gradient system (22) just as in [22]. However, we will refrain from doing so here since it is not the extremely long-time behavior (described by the critical points of the energy functional and their connecting orbits) that are of importance for thin film epitaxial growth systems. It is the behavior on the intermediate time scale (up to the order of $\frac{1}{\epsilon^3}$, see the introduction) that is of physical relevance here.

## 3. Application of the schemes to thin film epitaxy equations.

**3.1. Solvability, stability, and convergence.** For application to thin film epitaxy, we naturally decompose the Ehrlich-Schwoebel energy into a "convex" and "concave" part as in the theorem. For the energy with slope selection, it is easy to see that we have the following decomposition

$$
E_2(\phi) = \int_\Omega \frac{1}{4}\left(|\nabla\phi|^4 + 1\right) \mathrm{d}\mathbf{x} + \int_\Omega \left(-\frac{1}{2}|\nabla\phi|^2\right) \mathrm{d}\mathbf{x} + \int_\Omega \frac{\epsilon^2}{2} |\Delta\phi(\mathbf{x})|^2 \, \mathrm{d}\mathbf{x} \; , \qquad (66)
$$

with the first integral on the right hand side being "convex" and the second integral being "concave." Hence, we propose the following scheme for this case with slope selection:

$$
\frac{\phi_2^{n+1} - \phi_2^n}{k} = \nabla \cdot \left( \nabla\phi_2^{n+1} \left| \nabla\phi_2^{n+1} \right|^2 \right) - \Delta\phi_2^n - \epsilon^2 \Delta^2 \phi_2^{n+1} \; . \qquad (67)
$$

In the case without slope selection, we have

$$E_1(\phi) = \int_\Omega \frac{1}{2}\left(|\nabla\phi|^2 - \ln\left(1+|\nabla\phi|^2\right)\right)\,\mathrm{d}\mathbf{x} + \int_\Omega \left(-\frac{1}{2}|\nabla\phi|^2\right)\,\mathrm{d}\mathbf{x} + \int_\Omega \frac{\epsilon^2}{2}|\Delta\phi(\mathbf{x})|^2\,\mathrm{d}\mathbf{x}\,, \tag{68}$$

with the first integral "convex," the second one "concave," and, hence, we propose the following scheme for the equation without slope selection:

$$\frac{\phi_1^{n+1}-\phi_1^n}{k} = \nabla\cdot\left(\frac{\nabla\phi_1^{n+1}\left|\nabla\phi_1^{n+1}\right|^2}{1+\left|\nabla\phi_1^{n+1}\right|^2}\right) - \Delta\phi_1^n - \epsilon^2\Delta^2\phi_1^{n+1}\,. \tag{69}$$

The *gradient stability* for both schemes is then a corollary of Thm. 2.2:

**Corollary 1.** *The schemes (67, 69) are well-posed and stable in the sense that the following hold:*

$$E_i\left(\phi_i^{n+1}\right) \le E_i\left(\phi_i^n\right) - \frac{1}{k}\left\|\phi_i^{n+1}-\phi_i^n\right\|^2 - \frac{\epsilon^2}{2}\left\|\Delta\left(\phi_i^{n+1}-\phi_i^n\right)\right\|^2\,, \tag{70}$$

*for $i = 1, 2$. Moreover, the numerical solutions converge to the exact solution as $k \searrow 0$ on any finite time interval $[0, T]$, and the solution of the schemes converge to critical points of the corresponding energy functionals as time approaches infinity.*

*Proof.* The well-posedness of the schemes and their unconditional stability as well as the monotonic decay of the energies follows from the stability theorem (Thm. 2.2) directly with the convex-concave decomposition given above. As for the local in time convergence and the long-time behavior, we need to to verify the growth assumptions (29, 38). Since (38) is obvious, we simply check (29).

For the free energy (1) (without slope selection), a direct Taylor expansion for ln gives

$$F_1(\mathbf{y}) = -\frac{1}{2}\ln\left(1+|\mathbf{y}|^2\right) \ge -\beta|\mathbf{y}|^2 - C_\beta\,. \tag{71}$$

For the free energy (2) (with a slope selection), the estimate is more straightforward:

$$F_2(\mathbf{y}) = \frac{1}{4}\left(|\mathbf{y}|^2-1\right)^2 \ge 0\,. \tag{72}$$

□

**Remark 4.** Note that a lower bound for the energy $E_1$ is straightforward to obtain. For simplicity, we take $\Omega = (0, L)\times(0, L)$. Then the (independently) sharp estimates

$$F_1(\mathbf{y}) = -\frac{1}{2}\ln\left(1+|\mathbf{y}|^2\right) \ge -\frac{1}{2}\left(\alpha|\mathbf{y}|^2 - \ln(\alpha) + \alpha - 1\right)\,,\quad \forall\,\alpha\le 1\,, \tag{73}$$

and

$$\|\Delta\phi\|^2 \ge 8\frac{\pi^2}{L^2}\|\nabla\phi\|^2\,,\quad \forall\,\phi\in H^2_{per}(\Omega)\,, \tag{74}$$

are obtained. Thus choosing $\alpha = \frac{8\epsilon^2\pi^2}{L^2}$, we obtain the lower bound

$$E_1(\phi) \ge \frac{L^2}{2}\left(\ln\left(\frac{8\epsilon^2\pi^2}{L^2}\right) - \frac{8\epsilon^2\pi^2}{L^2} + 1\right) =: \gamma\,. \tag{75}$$

This lower bound is not, in general, sharp.

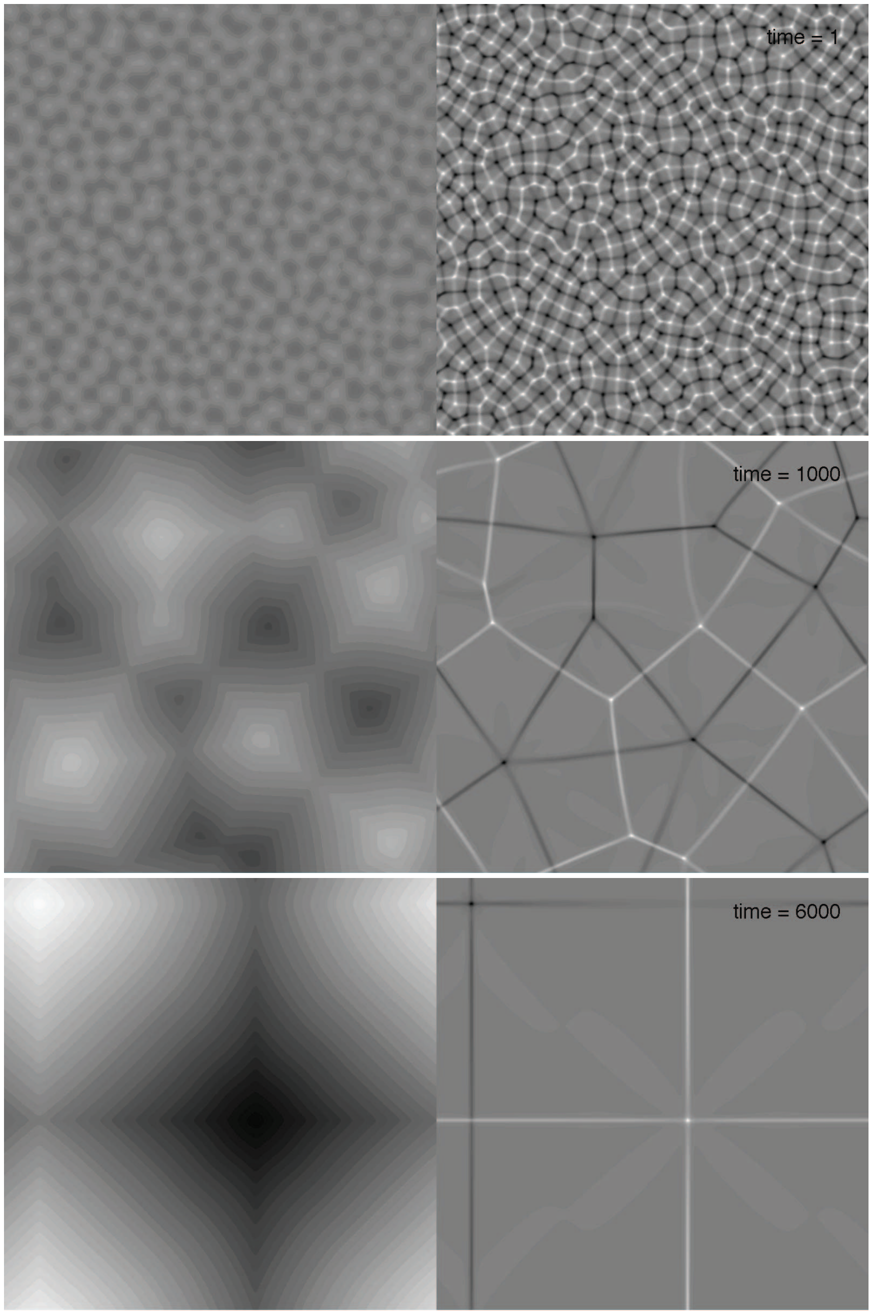


FIGURE 1. Time snapshots of the evolution of the model with slope selection. Parameters are given in the text. The left-hand column shows the filled contour plot of $\phi$; the right-hand column, the filled contour plot of $\Delta\phi$. The latter gives an indication of the curvature of the surface $z = \phi(x, y)$. The pyramid/anti-pyramid shapes of the hills and valleys are evident in the plots, and the system clearly saturates by time 6000.

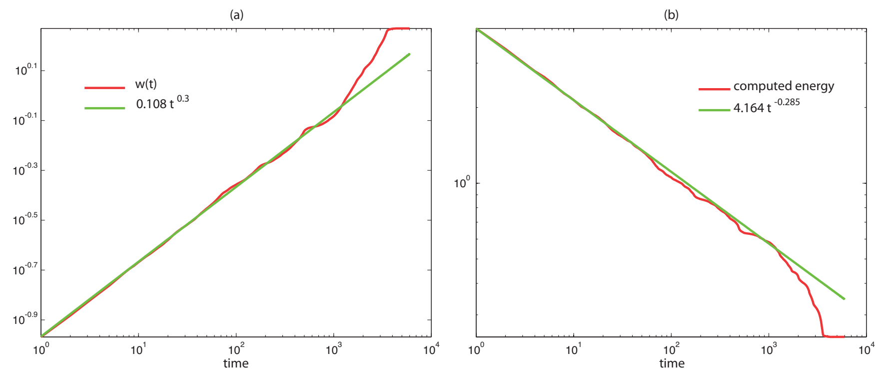


FIGURE 2. Log-log plots of the temporal evolution of (a) the standard deviation of $\phi$, denoted $w(t)$ in the plot and defined in the text, and (b) the energy for the model with slope selection. The standard deviation is a good measure of the feature size scale (the wavelength), because in this model the slopes of the pyramids are nearly fixed. Notice $w(t)$ grows like $t^{1/3}$ until saturation. The energy decreases like $t^{-1/3}$ until saturation.

3.2. **Preliminary computations.** Now we show some preliminary computations using our convexity splitting schemes for models with and without slope selection. Space is discretized using second-order accurate finite differences. This leads to discrete energies that approximate (1) and (2). The schemes, in turn, are constructed so that (discrete) energy stability is preserved. In other words, one still obtains energy estimates like (70) but in terms of the discrete energies and space-discrete norms. Many of the details are similar to those presented in our previous work [11, 23] and will be discussed in a forthcoming paper.

For the simulations we use the parameters $\epsilon = 0.03$, $L_x = L_y = 12.8$, and $h = L_x/512$, where $h$ is the uniform spatial step size. With these numbers, our lower bound on $E_1$ is discovered to be $\gamma \approx -552.43$. For the temporal step size $k$, we use $k = 0.001$ on the time interval $[0, 400]$ and $k = 0.01$ on the time interval $[400, 6000]$. To solve the resulting nonlinear finite-difference equations at the implicit time level, we employ a nonlinear conjugate gradient method, using the Polak Ribiére formula [18] to determine the line search direction.

Output for a simulation using the slope-selection model is presented in Figs. 1 and 2. The corresponding simulation results for the model without slope selection are shown Figs. 3 and 4. Figures 1 and 3 show contour plots of $\phi$ (on the left) and $\Delta\phi$ (on the right). Figures 2 and 4 show the time evolution of the discrete standard deviation $w(t)$ of the computed height function $\phi$ (on the left) and discrete energy (on the right). The standard deviation is defined as

$$w(t_n) = \sqrt{\frac{h^2}{L_x L_y} \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \left( \phi_{i,j}^n - \bar{\phi} \right)^2}, \tag{76}$$

where $N_x$ and $N_y$ are the number of grid points in the $x$ and $y$ direction and $\phi$ is the average value of $\phi$ on the uniform grid. The initial data for the simulations is

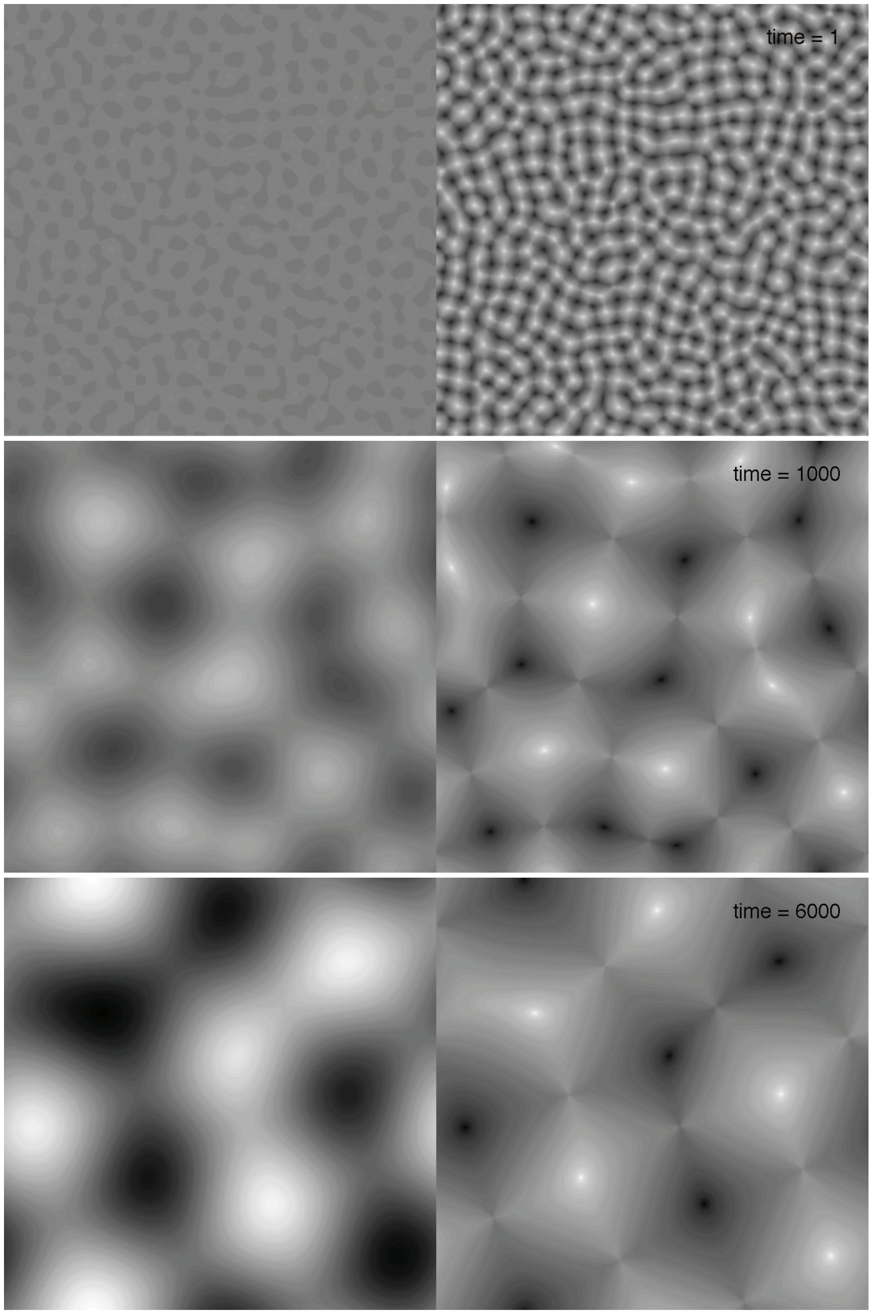


FIGURE 3. Time snapshots of the evolution of the model without slope selection. The plots are as in Fig. 1, with $\phi$ on the left-hand-side and $\Delta\phi$ on the right-hand-side. The system does not saturate by time 6000.

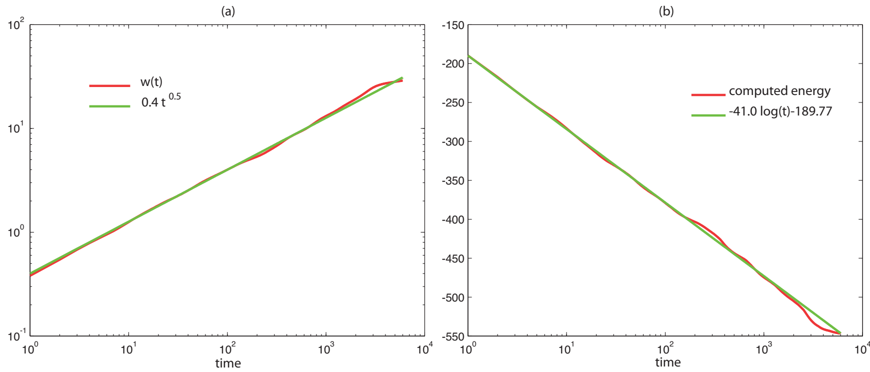


FIGURE 4. (a) The log-log plot of the standard deviation of $\phi$, denoted $w(t)$, and (b) the semi-log plot of the energy for the model without slope selection. Here the standard deviation is not such a good measure of the feature size scale (the wavelength), because in this model the slopes of the pyramids grow in time. Notice $w(t)$ grows like $t^{1/2}$, much faster than the $t^{1/3}$ growth for the model with slope selection. However, the feature size grows more slowly in time. The energy decays like $-\ln(t)$. Such decay cannot persist, since the energy is bounded below. The rate will slow down near saturation.

taken as $\phi^0_{i,j} = \bar{\phi} + r_{i,j}$, where the $r_{i,j}$ are uniformly distributed random numbers in $[-0.05, 0.05]$.

A couple of aspects of the simulations are worth pointing out. First the slope selection mechanism of the model corresponding to energy (2) is evident in Fig. 1. Mounds are observed to have nearly flat sides with slightly rounded edges where the faces meet. Fine length scale structures coarsen over time until the system saturates. The steady state of the system consists of a single pyramid and anti-pyramid configuration. As predicted by Moldovan and Golubovic [17], Kohn and Yan [13], and Li and Liu [15] and as observed in Fig. 2, the standard deviation (or the roughness as Li and Liu refer to it) $w(t)$ grows approximately like $t^{1/3}$ until around the saturation time when the system feels the finite size of the periodic domain. The energy, plotted on the right-hand-side of Fig 2, is observed to decrease approximately like $t^{-1/3}$, which is also expected [13].

Referring now to Figs. 3 and 4, for the model with no slope selection (associated to energy (1)) mounds have curved sides with very steep faces. Unlike the previous case, saturation is not reached by time $t = 6000$. This is because, while the roughness $w(t)$ grows faster then for the slope selection case (like $t^{1/2}$, left-hand-side of Fig. 4), the feature size (not shown) only grows like $t^{1/4}$ [15, 16]. The energy for the system decays rather rapidly, like $-\ln(t)$ before saturation. This is expected from the work in [16]. However, such decay cannot persist, since the energy is bounded below on a periodic domain. It is expect that the rate of energy decay will slow down dramatically near the saturation point.

4. **Summary.** We derived a class of unconditionally uniquely solvable, unconditionally stable schemes for certain phenomenological thin film epitaxial growth

models. The key ingredient is a proper generalization of Eyre's idea of decomposing the energy functional into convex and concave parts, with the convex part treated implicitly and the concave part treated explicitly in the time discretization. We have shown that the derived scheme converges to the gradient flow associated with the energy functional as the time step approaches zero, provided certain natural growth conditions are satisfied by the Ehrlich-Schwoebel energy. We have also demonstrated that the solutions of the scheme converges to exact steady states of the underlying gradient flow as time approaches infinity. We concluded the paper with some preliminary computational results using the proposed schemes.

Although the schemes herein are first order in time, the same ideas can be used to derive higher order unconditionally stable schemes [11]. The examination of higher order schemes together with extensive numerical experiments and the comparison with experimental data will be presented in a subsequent work.

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