INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 14, Number 2, Pages 283–305

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

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

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

1. Introduction

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

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

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

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

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

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

Received by the editors on December 7, 2016 and in revised form on January 15, 2017.
2000 *Mathematics Subject Classification.* 35K30, 65M06, 65M12, 65T40.

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

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

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

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

On the other hand, the authors observe that, there have been a few works on the improved convergence constant for the Cahn-Hilliard flow. In particular, Feng and Prohl [21] proved – for a first-order-in-time backward Euler scheme coupled with a mixed finite element spatial discretization scheme – that the convergence constant is of order $\exp(C_0T)\,\varepsilon^{-m_0}$, for some positive integer m_0 and a constant C_0 independent of ε. In other words, the exponential dependence on ε^{-1} may be replaced by a polynomial dependence. Two more recent works of Feng, Li and Xing [19, 20] applied a similar technique to analyze the first-order-in-time, discontinuous Galerkin schemes for the Allen-Cahn and Cahn-Hilliard equations. Both the backward Euler and convex splitting temporal discretizations were included in their recent works. Such an elegant improvement was based on a subtle spectrum analysis for the linearized Cahn-Hilliard operator (with certain given structure assumptions of the solution), provided in earlier PDE analyses [1, 2, 11, 12, 13].

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

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