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CONVERGENCE TO EQUILIBRIUM OF A DC ALGORITHM FOR AN EPITAXIAL GROWTH MODEL

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Abstract. A linear numerical scheme for an epitaxial growth model is analyzed in this work. The considered scheme is already established in the literature using a convexity splitting argument. We show that it can be naturally derived from an optimization viewpoint using a DC (difference of convex functions) programming framework. Moreover, we prove the convergence of the scheme towards equilibrium by means of the Lojasiewicz-Simon inequality. The fully discrete version, based on a Fourier collocation method, is also analyzed. Finally, numerical simulations are carried out to accommodate our analyzis.

Key words. Thin film epitaxy, DC programming, coarsening dynamics, Lojasiewicz-Simon inequality, epitaxial growth, model without slope selection, Fourier spectral method, convergence to equilibrium, pattern formation.

1. Introduction

We are concerned in this paper with the dynamics of the following model of thin film epitaxial growth:

$$\frac{\partial h}{\partial t} = -\nabla \cdot \left(\frac{\nabla h}{1 + |\nabla h|^2} \right) - \delta \Delta^2 h \tag{1}$$

where $h : \Omega \times [0, \infty) \to \mathbb{R}$, is a height function of a thin film in a co-moving frame, $\Omega = (0, L)^d$ for $d = 1, 2$ and δ is a nonnegative constant.

The nonlinear term on the right-hand side, the Ehrlich-Schwoebel barrier defined in [19, 17], is the destabilizing surface which was first proposed phenomenologically in the field of molecular beam epitaxy in [8]. The effect of this last term is counterbalanced by the classical linear Mullin regularising term. This last term describes relaxation through surface diffusion. Even though equation (1) describes a physical process far from equilibrium, it happens to be associated with a gradient flow with respect to the L^2 inner product of the free energy functional:

$$\mathcal{J}(h) = \int_\Omega \frac{1}{2} \left(\delta |\Delta h|^2 - \ln \left(1 + |\nabla h|^2 \right) \right). \tag{2}$$

The energy above is known to behave badly, this was mentioned in many references [3, 11], due to the presence of the negative logarithmic term and in fact it is poorly understood mathematically. This model takes its name from the fact that the energy has no relative minima, which implies that there is no energetically favourable value for $|\nabla h|$. Hence the naming without slope selection model.

Fourth order partial differential equations (PDEs) present in general many theoretical and numerical challenges. In the context of molecular beam epitaxy, the considered model attracted the attention of many researchers. In fact, an analytical approach has been carried out in [4] and later on by Guedda *et al.* in [6] in

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order to understand the predicted pyramidal structures characterized by the absence of a preferred slope. The authors show the existence of similarity solutions which predict the typical coarsening process in the limit of larger slope. The results obtained confirm that the typical mound lateral size and the interfacial width grow with time like $t^{\frac{1}{2}}$ and $t^{\frac{1}{4}}$ respectively. In [13], authors studied the free energy in order to understand the interfacial dynamics using energetic arguments and in order to justify rigorously the scaling laws predicted by the model. The authors show that for any $\delta > 0$, $\mathcal{J}$ admits global minimizers h_δ among the class of smooth and periodic height profiles having a null mean value. Li and Liu showed the well posedness and regularity of the solution to the problem (1). Moreover, they prove bounds and error estimates for Galerkin spectral approximation [12].

Numerical investigations of the model without slope selection are extensively studied in the literature. This is due to computational complexity and the long simulation time needed to predict the scaling laws. Moreover, these laws are expected to break down the closer one gets to equilibrium. Many attempt to design linear numerical schemes were made in order to overcome this difficulty. We cite here the reference [3] and the work in [18] where a second-order linearised three-level backward Euler scheme was proposed. Long time simulations for the coarsening process were performed and physically interesting quantities namely the surface roughness, the mound width, saturation time and the energy were computed in order to recover the scaling laws. However this come at the expense of a high computational cost. It could be interesting to focus on second order schemes in the spirit of the recent work [11] where a second order operator splitting Fourier method to tackle the numerical integration of Equation (1). Although linear, such schemes require three step integrations which increase complexity and therefore are neglected at the present time. Cheng and co-authors [1] proposed the first order linear scheme we are considering in this paper. They proved the unconditional stability and solvability of the fully discrete scheme and showed numerical simulations using a collocation-type Fourier spectral differentiation. Related schemes were proposed in [2, 9].

Our aim in this paper is to prove and numerically analyze the convergence to an equilibrium of the time semidiscrete linear scheme established in [1]. Convergence to a single equilibrium is not obvious because there is typically a continuum of critical points for the functional $\mathcal{J}$, due to the periodic boundary conditions. For the continuous-in-time equation (1), it has been proved by Grasselli *et al.* [5] by means of a Lojasiewicz-Simon inequality. Our proof is similar to the approach in [15, 16], but the novelty is that the scheme here is *linearly* implicit and not fully implicit. We will also consider the fully discrete scheme, where the space discretization is the Fourier spectral collocation method from [1].

The layout of the paper is organized as follows: we start our manuscript by stating the problem and recovering the expression of the linear scheme using a DC programming framework (Section 2). In Section 3, we show the convergence of the algorithm towards a critical value of the functional (2) by using a Lojasiewicz-Simon inequality. We prove a similar result for the fully discrete scheme in Section 4. Numerical simulations accommodated with some interpretations are presented in Section 5. Finally, a summary and conclusion are drawn in the last section.