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STABILIZED INVARIANT ENERGY QUADRATIZATION (S-IEQ) METHOD FOR THE MOLECULAR BEAM EPITAXIAL MODEL WITHOUT SLOPE SECTION

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Abstract. The design of numerical approaches for the molecular beam epitaxy models has always been a hot issue in numerical analysis, in which one of the main challenges for algorithm design is how to establish a high-order time-accurate numerical method with unconditional energy stability. The numerical method developed in this paper is based on the "stabilized-Invariant Energy Quadratization" (S-IEQ) approach. Its novelty is that by adding a very simple linear stabilization term, the difficulty that the original energy potential for the no-slope selection case is not bounded from below can be easily overcome. Then by using the standard format of the IEQ method, we can easily obtain a linear, unconditionally energy stable, and second-order time accurate scheme for solving the system. We further implement various numerical examples to demonstrate the stability and accuracy of the proposed scheme.

Key words. Molecular beam epitaxy, linear, second-order, unconditional energy stability.

1. Introduction

Molecular Beam Epitaxy (MBE) model refers to a continuum model to describe the growth of crystalline layer deposited on a substrate. By using a scalar variable to represent the height of the crystalline layer, the model is derived by using the gradient flow approach in L^2 space. The postulated energy of the system is composed of a linear entropy and a nonlinear potential where the nonlinear potential can take two forms, one is the fourth-order Ginzburg-Landau double-well potential and the model built on that is called the slope selection model, and the other is the logarithmic potential and the model built on it is called the no-slope selection model. Since the algorithm development for the double-well potential of the slope selection model has been extensively studied, see [11,15,17,20,21,30], in this paper, we consider the numerical approximations of the no-slope selection model, i.e., the time marching scheme for the logarithmic potential. Formally, the governing system of the MBE model with no-slope selection is not complicated where only two terms (a linear term and a nonlinear term) are involved. However, it is still very challenging to develop an effective numerical scheme due to the complexity of the logarithmic format of the nonlinear term.

Here, we briefly introduce the available numerical schemes for the MBE no-slope selection model here. According to the discretization method of the nonlinear potential, the available approaches can be categorized to the following two types, explicit type and semi-implicit type. The explicit type methods includes the operator splitting approach [10], explicit method [11], stabilized-explicit method [8,13], convex-splitting method [17], and ETD approaches [3–5,9], etc. The semi-implicit approach includes the quadratization approach, including the Invariant Energy Quadratization (IEQ) method [30] and its various version of Scalar Auxiliary Variable (SAV) method [7], etc. It is worth noting that almost all available schemes are linear and their implementation are very effective practically (e.g., most schemes

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only need to solve linear systems with variable coefficients or even constant coefficients at each time step). Among so many effective algorithms that can be used to solve the MBE model, considering that the process of constructing and implementing the quadratization type scheme is relatively simpler and easier, in this article we use IEQ method to solve the model.

However, the choice of the IEQ method raises a direct open question. Although the IEQ method developed in [30] enables one to construct linear, second-order, and unconditionally energy stable schemes for a large class of gradient flows, it is problematic whether it is applicable for solving the MBE model without slope selection since the nonlinear logarithmic potential is not obviously bounded from below. To overcome it, in this paper, we modify the IEQ approach to the stabilized version where we modify the total free energy by adding a gradient potential. With the help of it, we can easily show that the boundedness (from below) can be naturally satisfied, and the second-order time marching scheme can be obtained easily. Note that the total free energy of the model has not changed, because while adding that gradient term, we also subtract it and the subtracted item can be further bounded by the higher-order linear potential. In this way, the bounded-from-below property of the total free energy can still be strictly guaranteed. Moreover, the magnitude of the stabilization term can be arbitrarily small as long as it is positive, which implies that the splitting error caused by this term can actually be controlled within the machine precision. We further prove the well-posedness of the developed scheme and also show that the constructed scheme is unconditionally energy stable.

The structure of this article is as follows. In Section 2, the MBE model without slope selection is briefly introduced. The numerical scheme is further constructed in Section 3. The practical implementation process is also given in detail. The unconditional energy stability is proved rigorously. In Section 4, we implement the numerical simulations numerically to demonstrate the stability, accuracy of the developed schemes. In Section 5, we give some concluding remarks.

2. MBE model with no slope selection

We first give a brief introduction on the MBE model with no slope selection. The computed domain is set as $\Omega = [0, L]^d, d = 2$. Suppose $\phi(\boldsymbol{x})$ is a height function and the total phenomenological free energy is postulated as [11]

$$E(\phi) = \int_\Omega \Big(L(\Delta\phi) + F(\nabla\phi) \Big) d\boldsymbol{x}, \tag{1}$$

where the $L(\Delta\phi) = \frac{\epsilon^2}{2}(\Delta\phi)^2$ is the linear entropy that represents the surface diffusion effect, the coefficient ϵ is used to controls the diffusive strength, and $F(\phi)$ is the nonlinear potential that represents a continuum description of the Ehrlich-Schwoebel effect. For the no slope selection case, $F(\nabla\phi)$ reads as

$$F(\nabla\phi) = -\frac{1}{2}\ln(1 + |\nabla\phi|^2). \tag{2}$$

The evolution equation for the height function ϕ is derived by using the gradient flow approach in the L^2 space, that reads as

$$\phi_t = -M\big(\epsilon^2\Delta^2\phi + f(\nabla\phi)\big), \tag{3}$$

where M is the mobility constant, and

$$f(\nabla\phi) = \nabla\cdot\Big(\frac{\nabla\phi}{1 + |\nabla\phi|^2}\Big). \tag{4}$$