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A BDF2-SSAV Numerical Scheme with Fourier-Spectral Method for a Droplet Thin Film Coarsening Model

Juan Zhang[1], Lixiu Dong[2,*] and Zhengru Zhang[3]

[1] *School of Sciences, Lanzhou University of Technology, Lanzhou 730050, P.R. China*
[2] *Department of Mathematics, Faculty of Arts and Sciences, Beijing Normal University, Zhuhai 519087, P.R. China*
[3] *School of Mathematical Sciences, Laboratory of Mathematics and Complex Systems, Beijing Normal University, Beijing 100875, P.R. China*

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Abstract. A linear and second order numerical scheme is proposed and analyzed for a droplet thin film coarsening model, with a singular Leonard-Jones energy potential involved. This numerical scheme with unconditional energy stability is based on the backward differentiation formular (BDF) method in time derivation combining with the stabilized scalar auxiliary variable approach in time and the Fourier spectral method in space. A second order accurate artificial regularization term, in the form of $S\Delta(\phi^{n+1}-2\phi^n+\phi^{n-1})$, is added in the numerical scheme to make better stability of the numerical scheme. Moreover, we present the detail proof for unconditional energy stability property of the numerical scheme, without any restriction for the time step size. In addition, an $\mathcal{O}(\Delta t^2+h^m)$ rate convergence estimate in the $\ell^\infty(0,T;\ell^2)$ norm are derived in details with the help of a priori assumption for the error at the previous time step. Some numerical simulation results are presented to demonstrate the efficiency and accuracy of the second-order numerical scheme.

AMS subject classifications: 35K35, 35K55, 49J40, 65M06, 65M12

Key words: Droplet coarsening model, scalar auxiliary variable, Fourier-spectral method, energy stability, optimal rate convergence analysis.

1. Introduction

Certain liquids on a solid, chemo-attractive substrate spontaneously form a droplet structure connected by a very thin precursor (or wetting) layer. After the droplets ap-

*Corresponding author. *Email addresses:* jzhang@lut.edu.cn (J. Zhang), lxdong@bnu.edu.cn (L. Dong), zrzhang@bnu.edu.cn (Z. Zhang)

pear, coarsening will occur, whereby smaller droplets will shrink and larger droplets will grow. The coarsening behavior, especially the rate of coarsening, of droplets has been of great scientific interest [62]. The average droplet size increases with the decrease of the number of droplets and the increase of the characteristic distance. The droplet coarsening model with a singular Lennard-Jones energy potential involved mainly describes the coarsening phenomenon of droplets. Some liquids on the solid substrate form a droplet structure connected by a precursor layer, then a series of phenomena including coarsening will occur due to two mechanisms: collapse or collision. The related content of liquid thin film coarsening phenomenon and some numerical simulation results can be found in [15, 19, 21, 35, 42, 45, 46, 51, 52, 56].

In this paper, we consider a well-known Lennard-Jones-type potential [25], which is expressed as $\mathcal{U}(\phi) = \phi^{-8}/3 - 4\phi^{-2}/3$. Considering the gradient flow associated with the following energy functional:

$$E(\phi) = \int_\Omega \left(\frac{1}{3}\phi^{-8} - \frac{4}{3}\phi^{-2} + \frac{\xi^2}{2}|\nabla\phi|^2 \right) \mathrm{d}\mathbf{x}, \tag{1.1}$$

where $\phi : \Omega \to \mathbb{R}$ is a periodic height function and $\xi > 0$ is the surface diffusion coefficient. In turn, the chemical potential becomes the following variational derivative of the energy

$$\mu := \delta_\phi E = -\frac{8}{3}\left(\phi^{-9} - \phi^{-3}\right) - \xi^2\Delta\phi.$$

And the dynamical equation stands for the H^{-1} gradient flow

$$\phi_t = \Delta\mu = \Delta\left(-\frac{8}{3}\left(\phi^{-9} - \phi^{-3}\right) - \xi^2\Delta\phi \right). \tag{1.2}$$

We assume periodic boundary conditions hold for the height function ϕ over the rectangular domain Ω. Given the highly nonlinear and highly singular nature of the Leonard-Jones potential, the numerical analysis for this model has been very limited. To obtain the solution of the droplet liquid film coarsening equation, we need to solve a fourth-order nonlinear parabolic partial differential equation.

Many physical problems can be modeled by partial differential equations (PDEs) taking form of gradient flows [3, 5, 11, 32, 34, 59]. There are various different time marching strategies for the Cahn-Hilliard equation, such as fully implicit method, (i.e. Backward Euler scheme) [18, 43]. The unconditional nonlinear energy stable scheme with time step sufficient small to have a unique solution. So it usually requires solving a large nonlinear system of equations. Convex splitting method was introduced in [16, 17]. In this method the free energy functional is represented as the difference of two convex functionals. One can easily show that the convex splitting scheme satisfies the unconditional energy dissipation. However, the nonlinear equations also have to be solved at each time step size, usually, the implicit term is nonlinear [10, 12, 22, 53, 62]. Exponential time differencing (ETD) approach have been proposed in [5, 14, 28–31, 55, 66], the linear scheme results in additional accuracy issues and