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On Linear and Unconditionally Energy Stable Algorithms for Variable Mobility Cahn-Hilliard Type Equation with Logarithmic Flory-Huggins Potential

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Abstract. In this paper, we consider numerical approximations for the fourth-order Cahn-Hilliard equation with the concentration-dependent mobility and the logarithmic Flory-Huggins bulk potential. One numerical challenge in solving such system is how to develop proper temporal discretization for nonlinear terms in order to preserve its energy stability at the time-discrete level. We overcome it by developing a set of first and second order time marching schemes based on a newly developed "Invariant Energy Quadratization" approach. Its novelty is producing linear schemes, by discretizing all nonlinear terms semi-explicitly. We further rigorously prove all proposed schemes are unconditionally energy stable. Various 2D and 3D numerical simulations are presented to demonstrate the stability, accuracy, and efficiency of the proposed schemes thereafter.

AMS subject classifications: 65N12, 65P40, 65Z05

Key words: Phase-field, linear, Cahn-Hilliard, stability, variable mobility, Flory-Huggins.

1 Introduction

In this paper, we consider the numerical approximations for the fourth order Cahn-Hilliard equation with the variable concentration-dependent mobility and the logarithmic Flory-Huggins (F-H) bulk potential. The Cahn-Hilliard equation is one of the two typical equations of the phase field method. This method has now become a well-known efficient modeling and a numerical tool to resolve the motion of free interfaces between

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multiple material components. About the most recent advances in modeling, algorithms or computational technologies, we refer to [2,21] and the references therein.

There exist many advantages in the phase field modeling approaches from the mathematical point of view. In particular, the developed model is usually energy stable and well-posed due to the energy-based variational approach. Therefore, it is possible to carry out effective mathematical/numerical analysis and perform reliable computer simulations. For algorithms design, a significant goal is to verify the energy stable property at the discrete level irrespectively of the coarseness of the discretizations. In what follows, those algorithms will be called unconditionally energy stable. A scheme with this property is especially preferred for solving diffusive systems since the dynamics of coarse-graining (macroscopic) process may undergo rapid changes near the interface, the non-compliance of energy dissipation laws may lead to spurious numerical solutions if the mesh or time step size is not carefully controlled. Thus the unconditional energy stability is not only critical for the numerical scheme to capture the correct long-time dynamics of the system, but also provides sufficient flexibility for dealing with the stiffness issue. We also emphasize that the 'unconditional energy stability' there means the schemes have no constraints for the time step only from the energy stability concern. It does not mean that any arbitrarily large time step can be chosen for computations since larger time step size will inevitably induce larger numerical errors in practice. Undoubtedly, higher order time marching schemes are preferable to lower order schemes if the adopted time step is expected to be as large as possible under certain accuracy requests. This fact motivates us to develop higher order schemes, e.g., the second order time marching schemes while preserving the unconditional energy stability in this paper.

We must notice that it is very challenging to develop unconditionally energy stable schemes to resolve the stiffness issue induced by the thin interface since the traditional fully-implicit or explicit discretization for the nonlinear term will cause severe time step constraint (called conditionally energy stable) on the interfacial width [26,27]. Many efforts have been done in order to remove this constraint and two commonly used techniques were developed. The first method is the so-called *convex splitting approach* [10, 14, 48, 49], where the convex part of the potential is treated implicitly and the concave part is treated explicitly. The convex splitting approach is unconditionally energy stable, however, it usually produces the nonlinear scheme, thus the implementation is complicated and the computational cost might be high. It is remarkable that, in [10,32], the authors propose some linear schemes using the convex splitting approach. The scheme presupposes the range of numerical solution is inside the domain $[-1,1]$ (maximum principle). However, this assumption is not provably correct.

The second method is the so-called *stabilized explicit approach* [5, 11, 15, 22, 24–26, 28–31,33,35,44,46], where the nonlinear term is simply treated explicitly. In order to remove the time step constraint dependence on the interfacial width, a linear stabilizing term has to be added, and the magnitude of that term usually depends on the upper bound of the second order derivative of the nonlinear potential. Such a scheme is efficient and very easy to implement since it is purely linear. But, similar to the linear convex splitting