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Numerical Approximations of Phase Field Models using a General Class of Linear Time-Integration Schemes

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Abstract. In this paper, we develop a new class of linear time-integration schemes for phase-field models. The newly proposed schemes extend the recently developed energy quadratization technique by introducing extra free parameters to further stabilize the schemes and improve their accuracy. The freshly proposed schemes have several advantages. First of all, they are rather generic such that they apply to most existing phase-field models in the literature. The resulted schemes are also linear in time, which means only a linear system needs to be solved during each time marching step. Thus, it significantly reduces the computational cost. Besides, they are unconditionally energy stable such that a larger time step size is practical. What is more, the solution existence and uniqueness in each time step are guaranteed without any dependence on the time step size. To demonstrate the generality of the proposed schemes, we apply them to several typical examples, including the widely-used molecular beam epitaxy (MBE) model, the Cahn-Hilliard equation, and the diblock copolymer model. Numerical tests reveal that the proposed schemes are accurate and efficient. This new family of linear and unconditionally energy stable schemes provides insights in developing numerical approximations for general phase field models.

AMS subject classifications: 65M06, 65M12, 65M70

Key words: Phase field, linear scheme, energy stable, Cahn-Hilliard, diblock copolymer, molecular beam epitaxy growth.

1 Introduction

As an approach to solve interfacial problems, the phase field model has witnessed its popularity in the past decade. It has been widely applied to various fields, including vesicle dynamics, crystal growth, microstructure evolution, brittle fracture, and many

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others in material science and engineering. In general, the phase field models are driven by dissipative mechanisms, where the free energy is decreasing in time for isothermal systems. When the temperature changes can't be ignored, entropy is usually considered instead. These could be better explained by embracing the generalized Onsager principle [37,38,53,59].

Generically, the dynamics of the phase field variable Φ, which may be a vector, takes the form of

$$\partial_t \Phi = -\mathcal{G}\frac{\delta E}{\delta \Phi}, \tag{1.1}$$

where E is the effective free energy in the system that could be a functional of the phase variable Φ and its high-order gradient terms. Here $\mathcal{G}$ is a semi positive-definite operator, known as the mobility operator. In other words, the triplet $(\Phi,\mathcal{G},E)$ uniquely determines a thermodynamically consistent phase field model. When there is no flux contribution from the boundary, the dynamics of the phase field model (1.1) satisfies the following energy dissipation law

$$\frac{dE}{dt} = \Big(\frac{\delta E}{\delta \Phi},\frac{\delta \Phi}{\delta t}\Big) = -\Big(\mathcal{G}\frac{\delta E}{\delta \Phi},\frac{\delta E}{\delta \Phi}\Big) \leq 0. \tag{1.2}$$

Here the inner product is defined by

$$(\mathbf{f},\mathbf{g}) = \sum_i \int_\Omega f_i g_i d\Omega.$$

In the literature, many existing thermodynamically consistent phase field models could be reformulated into the general form in (1.1), including the Allen-Cahn model, Cahn-Hilliard model, phase-field crystal model, molecular beam epitaxy growth model, surfactant model, diblock copolymer model, and many others [2,3,15,16,46].

Due to the extensive applications of phase field models in various fields, many novel approaches of developing numerical approximations for the phase field PDE models are introduced in the literature. However, most numerical schemes are tailed specifically for a particular model, making their applications restricted. Among the existing numerical schemes published in the literature, if the numerical algorithms preserving the energy dissipation property of (1.2) in the discrete or semi-discrete level, they are known as energy stable algorithms. Furthermore, if such energy-stable property does not depend on the choice of the time-step size, they are usually named unconditionally energy stable. Such unconditionally energy stable schemes are always desirable and sometimes mandatory for solving the phase field models numerically. The energy stability properties guarantee the numerical solution's stability in certain norms. Theoretically, the solution's existence and uniqueness can usually be derived based on the discrete energy dissipation law. Meanwhile, since the energy dissipation of (1.2) is an intrinsic physical property for phase field models, unconditionally energy stable schemes usually guarantee long time stability with large time marching steps, though we shall point out unconditionally energy stable schemes do not necessarily guarantee solution accuracy [50]. Thus high-order energy stable schemes are more desired than first-order ones.