East Asian Journal on Applied Mathematics
doi: 10.4208/eajam.2023-159.170324

Vol. **15**, No. 2, pp. 344-372
May 2025

A Relaxed Decoupled Second-Order Energy-Stable Scheme for the Binary Phase-Field Crystal Model

Xin Zhang[1], Junxiang Yang[1] and Zhijun Tan[1,2,*]

[1]*School of Computer Science and Engineering, Sun Yat-sen University, Guangzhou 510275, China.*
[2]*Guangdong Province Key Laboratory of Computational Science, Sun Yat-sen University, Guangzhou 510275, China.*

Received 6 July 2023; Accepted (in revised version) 17 March 2024.

Abstract. In this study, we construct a relaxed second-order time-accurate scheme for the binary phase-field crystal model based on the recent paper [J. Wu, J. Yang and Z. Tan, Eng. Comput. (2023)]. This scheme can significantly improve the consistency between original and modified energies. Using the exponential SAV method, we construct the first- and second-order time-accurate schemes by using the backward Euler formula and the second-order backward difference formula, respectively. Then a new second-order numerical scheme with relaxation is developed. This new numerical scheme satisfies the energy dissipation law. Meanwhile, it is fully decoupled and efficient. Extensive numerical experiments are carried out in 2D and 3D to verify the accuracy and stability of the proposed scheme, as well as its ability to improve the consistency between the original energy and modified energy.

AMS subject classifications: 65M10, 78A48

Key words: Binary phase-field crystal, unconditional energy stability, relaxed technique, second-order scheme.

1. Introduction

There are many methods for studying crystal growth at the atomic length scale. One of them is the phase-field crystal (PFC) model proposed by Elder *et al*. [3, 5]. It has been widely used because of its advantage in capturing the phase transition phenomena. In the PFC model, the time-average density of atoms is described by a phase-field variable ϕ. The governing equations for the PFC model can be obtained by applying a variational method to total free energy with respect to ϕ. The PFC model has been applied to simulate diverse phenomena, such as elastic and plastic deformation, colloidal growth, and crystal growth — cf. [5, 21].

*Corresponding author. *Email addresses:* zhangx399@sysu.edu.cn (X. Zhang), nexusxiang@outlook.com (J. Yang), tzhij@mail.sysu.edu.cn (Z. Tan)

The binary PFC (BPFC) model for binary alloys was developed by Elder *et al*. [4, 6]. Similar to the PFC model, the BPFC model introduces two phase-field variables. Adopting the same derivation method as the PFC model, the governing equations for the BPFC model can be derived, which includes two coupled nonlinear partial differential equations.

There are various numerical studies devoted to energy-stable schemes for PFC models — e.g. invariant energy quadratization (IEQ) approach [35], convex splitting method [10, 28, 32], and scalar auxiliary variable (SAV) approach [22–24]. Two unconditionally energy-stable finite difference schemes for the modified phase-field crystal (MPFC) model have been proposed in [1]. The convergence of a second-order accurate convex splitting scheme of [1] has been discussed in [2]. Shin *et al*. [25] constructed a first-order unconditional gradient-stabilized scheme and a second-order unconditionally weakly energy-stable scheme using new convex splitting. Applied the IEQ method, Yang [37] developed temporal approximation schemes to solve the model for homopolymer blends. Liu and Li [19] presented an improved IEQ method and an improved stable IEQ method. Li *et al*. [16] proposed an unconditionally energy-stable scheme based on the IEQ method for the modified PFC model. Li and Shen [17] developed a fully discrete scheme for the PFC model based on a stable SAV method. Li and Mei [15] considered decoupled second-order accurate linear schemes for the BPFC models for binary colloidal crystals. Wang *et al*. [29] combined the SAV method and the finite element approach to construct an energy stabilization scheme for the PFC model. For other methods for solving PFC models, the reader can consult [7–9, 12, 14, 18, 20, 26, 30, 31, 34].

For the PFC model, the difficulty of constructing energy-stable numerical schemes is the stiffness issue caused by the nonlinear double-well potential. In addition, the two phase-field variables of the BPFC model are nonlinearly coupled, which makes the development of numerical methods more difficult. Therefore, there are only few studies of numerical schemes for BPFC models. Tegze *et al.* [27] presented an efficient, first-order accurate and explicit-type scheme to solve numerically the BPFC model by applying the operator splitting method. However, this scheme does not follow any energy dissipation law. Wu *et al.* [33] developed two energy-stable and decoupled schemes based on an exponential semi-implicit SAV approach to solve the BPFC model, but numerical simulations show that the consistency between the original and modified energy is not good.

As a result, we want to develop an energy-stable and efficient numerical scheme for the BPFC model. Meanwhile, we use a relaxation technique [11, 38] to improve poor consistency between the original and modified energy. Using the exponential SAV method, we expand the original equations and then construct numerical schemes. Thus, adding a relaxation step to the second-order numerical scheme, we obtain a new numerical scheme. All variables are still fully decoupled at each time step, which can be updated easily. Therefore, the relaxed second-order numerical scheme enhances the consistency between two energies while ensuring high efficiency and stability.

The organization of this work is as follows. In Section 2, we introduce the governing equations of the BPFC model. In Section 3, we construct a second-order scheme. In Section 4, we carry out plenty of numerical simulations. Some conclusions are written in Section 5.