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# Error Analysis of SAV Finite Element Method to Phase Field Crystal Model

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**Abstract.** In this paper, we construct and analyze an energy stable scheme by combining the latest developed scalar auxiliary variable (SAV) approach and linear finite element method (FEM) for phase field crystal (PFC) model, and show rigorously that the scheme is first-order in time and second-order in space for the $L^2$ and $H^{-1}$ gradient flow equations. To reduce efficiently computational cost and capture accurately the phase interface, we give a simple adaptive strategy, equipped with a posteriori gradient estimator, i.e., $L^2$ norm of the recovered gradient. Extensive numerical experiments are presented to verify our theoretical results and to demonstrate the effectiveness and accuracy of our proposed method.

**AMS subject classifications**: 65M12, 65M50, 65M60, 35Q56

**Key words**: Linear finite element method, scalar auxiliary variable approach, phase field crystal model, error analysis, energy stability, adaptive method.

## 1. Introduction

The phase field crystal (PFC) model [1,2] was proposed as an approach to simulate crystals at the atomic scale but on a coarse-grained diffusive time scale [4]. Many physical processes, such as the formation of ordered structures, phase separation of polynary systems, can be described using this model. The PFC model can also explain elastic and plastic deformations of the lattice, dislocations, grain boundaries, multiple crystal orientations and many other observable phenomena [4, 6].

There are several kinds of PFC models. In general, they can be classified into two classes according to characteristic length scale: one-length-scale and multi-length-scale. One-length-scale PFC models can be used to describe the phase behavior of

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periodic structures [7–9]. Accordingly, multi-length-scale PFC models can be employed to explain the formation of quasicrystals [10, 11]. In this work, we focus on the development of numerical methods of one-length-scale PFC model. In particular, the classic Landau-Brazovskii (LB) model [7, 12, 13] will be used to demonstrate our proposed method. The LB model was built to investigate the character of phase transition. It has been discovered in many scientific fields. For example, the LB model can be derived from more complicated self-consistent field theory of diblock copolymers [14]. Compared with the typical Swift-Hohenberg (SH) model with double-well bulk energy [8], LB energy functional includes a cubic term which can be used to study the first-order phase transition.

The $L^2$ (Allen-Cahn) or $H^{-1}$ (Cahn-Hilliard) gradient flow equation is usually adopted to describe the dynamic behavior of the phase-field or PFC model. These dynamic equations are time-dependent nonlinear partial differential equations (PDEs). It is hard to find non-trivial analytical solutions. Therefore, numerically solving these nonlinear PDEs is an efficient approach. To guarantee convergence, numerical schemes of these equations are required to satisfy the energy dissipation property. Meanwhile, an accurate and efficient approach should be designed to deal with nonlinear terms. In terms of time discretization, there have been several effective methods which can preserve energy dissipation law, including the convex splitting method [4, 15–21], stabilized approach [22–25], invariant energy quadratization (IEQ) method [19, 26] and recently developed scalar auxiliary variable (SAV) approach [29]. By introduing a scale auxiliary variable to the nonlinear part of energy functional, the SAV approach has a modified energy dissipation property for a large class of gradient flows. The convergent and error analysis of semi-discrete SAV scheme has been given by Shen and Xu [41]. The analysis of energy stability and convergence of fully discretized SAV block-centered finite difference method has been established for gradient flows [40]. More studies about the PFC problem can be found in recent literature [16, 17, 43–45].

In the study to the PFC model, finite difference methods [2–5, 46] or spectral methods [27–29] are limited to regular regions, such as two-dimensional square region or three-dimensional cube region. For complex geometries, finite element method (FEM) [30, 42, 55] is a better choice. Furthermore, the FEM can be further combined with adaptive technologies, which are well suitable for the phase behavior of PFC models, such as the formation of ordered structures, phase transition processes, and coarse-grained processes. The adaptive method can effectively decrease the cost of computing and accurately capture the phase interface.

In this work, we will combine SAV time discretization and FEM spatial discretization to solve the gradient flow equation of LB model. Based on the energy dissipation and the SAV scheme, the derivation process of $H^2$ bounds of the solution is shown in detail. For our fully discrete scheme, we demonstrate its energy stability, and carry out error estimate. Applying our method, we can effectively simulate the mesoscale self-assembly of the diblock copolymer system in two-dimensional convex geometries. In addition, we will consider an adaptive FEM for the PFC model. There are many adaptive finite element methods for phase field equation [49–53]. To reduce computational cost, we