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An Adaptive Block Bregman Proximal Gradient Method for Computing Stationary States of Multicomponent Phase-Field Crystal Model

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Abstract. In this paper, we compute the stationary states of the multicomponent phase-field crystal model by formulating it as a block constrained minimization problem. The original infinite-dimensional non-convex minimization problem is approximated by a finite-dimensional constrained non-convex minimization problem after an appropriate spatial discretization. To efficiently solve the above optimization problem, we propose a so-called adaptive block Bregman proximal gradient (AB-BPG) algorithm that fully exploits the problem's block structure. The proposed method updates each order parameter alternatively, and the update order of blocks can be chosen in a deterministic or random manner. Besides, we choose the step size by developing a practical linear search approach such that the generated sequence either keeps energy dissipation or has a controllable subsequence with energy dissipation. The convergence property of the proposed method is established without the requirement of global Lipschitz continuity of the derivative of the bulk energy part by using the Bregman divergence. The numerical results on computing stationary ordered structures in binary, ternary, and quinary component coupled-mode Swift-Hohenberg models have shown a significant acceleration over many existing methods.

AMS subject classifications: 54C40, 14E20

Key words: Multicomponent coupled-mode Swift-Hohenberg model, stationary states, adaptive block Bregman proximal gradient algorithm, convergence analysis, adaptive step size.

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1 Introduction

Multicomponent systems, such as alloys, soft matters, are an important class of materials, particularly for technical applications and processes. The microstructures of materials play a central role for a broad range of industrial application, such as the mechanical property of the quality and the durability, optical device, high-capacity data storage devices [23,37–39,48]. Advances in modeling and computation have significantly improved the understanding of the fundamental nature of microstructure and phase selection processes. Notable contributions have been made through using the phase-field methodology [20,21], which has been successful at examining mesoscale microstructure evolution over diffusive time scales. Recently, phase field crystal (PFC) models have been proposed to efficiently simulate eutectic solidification, elastic anisotropy, solute drag, quasicrystal formation, solute clustering and precipitation mechanisms [14, 38, 46]. Besides, binary and ternary component phase field models have attracted many research interests from the computation perspective [2,3,5,11,15,43,54].

The PFC model for a general class of multicomponent systems is formulated consisting s components in d dimensional space. The concentrations of the components are described by s vector-valued functions $\{\phi_i(\boldsymbol{r})\}_{i=1}^s=(\phi_1(\boldsymbol{r}),\cdots,\phi_s(\boldsymbol{r}))$. The variable $\phi_\alpha(\boldsymbol{r})$, so-called order parameter, denotes the local fraction of phase α. The free energy functional of PFC model of a s-component system can be described by two contributions, a bulk free energy $F[\{\phi_i(\boldsymbol{r})\}_{i=1}^s]$ and an interaction potential $G[\{\phi_i(\boldsymbol{r})\}_{i=1}^s]$, which drive the density fields to become ordered by creating minimal in the free energy for these states. Formally, we can write the free energy functional of the multicomponent system as

$$E[\{\phi_i(\boldsymbol{r})\}_{i=1}^s;\Theta]=G[\{\phi_i(\boldsymbol{r})\}_{i=1}^s;\Theta]+F[\{\phi_i(\boldsymbol{r})\}_{i=1}^s;\Theta], \tag{1.1}$$

where Θ are relevant physical parameters. F has polynomial or logarithmic formulation [12, 16, 47] and G is the interaction potential, such as high-order differential terms or convolution terms [12, 42]. Usually, some constraints are imposed on the PFC model, such as the mass conservation or incompressibility which means the order parameter $\{\phi_i(\boldsymbol{r})\}_{i=1}^s$ belong to a feasible space.

To understand the fundamental nature of multicomponent systems, it often involves finding stationary states corresponding to ordered structures. Denote V_i $(i=1,2,\cdots,s)$ to be a feasible space of the i-th order parameter, the above problem is transformed into solving the minimization problem

$$\min \quad E[\{\phi_i(\boldsymbol{r})\}_{i=1}^s;\Theta], \quad \text{s.t.} \quad \phi_i(\boldsymbol{r})\in V_i \ (i=1,2,\cdots,s), \tag{1.2}$$

with different physical parameters Θ, which brings a tremendous computational burden.

Different methods have been proposed for computing the stationary states of multicomponent models and can be classified into two categories through different formulations and numerical techniques. One is to solve the steady nonlinear Euler-Lagrangian system of (1.2) through different spatial discretization approaches. The other class of