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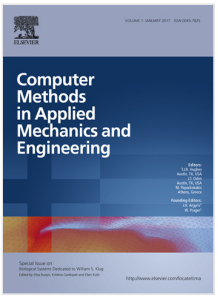


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PII: S0045-7825(16)31775-3
DOI: http://dx.doi.org/10.1016/j.cma.2017.02.022
Reference: CMA 11349

To appear in: *Comput. Methods Appl. Mech. Engrg.*

Received date: 10 December 2016
Revised date: 13 January 2017
Accepted date: 16 February 2017

Please cite this article as: Y. Li, J. Kim, An efficient and stable compact fourth-order finite difference scheme for the phase field crystal equation, *Comput. Methods Appl. Mech. Engrg.* (2017), http://dx.doi.org/10.1016/j.cma.2017.02.022

# An efficient and stable compact fourth-order finite difference scheme for the phase field crystal equation

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**Abstract**

In this paper, we present a high-order accurate compact scheme for the phase field crystal model in two- and three-dimensional spaces. The proposed scheme is derived by combining a fourth-order compact finite difference formula in space and a backward differentiation for the time derivative term, which is second-order accurate in time. Furthermore, a nonlinearly stabilized splitting scheme is used and thus a larger time step can be allowed. Since the equations at the implicit time level are nonlinear, we introduce a Newton-type iterative method and employ a fast and efficient nonlinear multigrid solver to solve the resulting discrete system. In particular, we implement the compact scheme in the adaptive mesh refinement framework. An adaptive time step method for the phase field crystal model is also proposed. Various numerical experiments are presented and confirm the accuracy, stability, and efficiency of our proposed method.

*Keywords:* Phase-field crystal equation; Fourth-order compact scheme; Adaptive mesh refinement; Adaptive time-stepping

## 1. Introduction

The aim of the research presented in this paper is to develop a high-order accurate compact scheme, i.e., second-order accurate in time and fourth-order accurate in space, for the phase field crystal model [1, 2]:

$$\frac{\partial \phi}{\partial t}(\mathbf{x},t) = M\Delta\mu(\mathbf{x},t), \tag{1}$$

$$\mu(\mathbf{x},t) = \phi^3(\mathbf{x},t) + (1-\epsilon)\phi(\mathbf{x},t) + 2\Delta\phi(\mathbf{x},t) + \Delta^2\phi(\mathbf{x},t), \quad \mathbf{x}\in\Omega,\ 0<t\le T, \tag{2}$$

$$\phi(\mathbf{x},t) \text{ is } \Omega-\text{periodic}, \tag{3}$$

$$\phi(\mathbf{x},0) = \phi_0(\mathbf{x}), \tag{4}$$

where the phase field $\phi(\mathbf{x},t)$ approximates the number density of atoms in a binary mixture in the domain $\Omega = \Pi_{i=1}^{d}(0,L_i) \subset \mathbb{R}^d$ ($d = 2$ or 3). $\mu$ is the chemical potential and $\Delta$ is the Laplacian operator. The

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