

A Comparison of Fourier Spectral Iterative Perturbation Method and Finite Element Method in Solving Phase-Field Equilibrium Equations

Pengcheng Song^{1,2,3,†}, Tiannan Yang^{3,†}, Yanzhou Ji³, Zhuo Wang⁴,
Zhigang Yang², Longqing Chen³ and Lei Chen^{4,*}

¹ *Science and Technology on Reactor Fuel and Materials Laboratory, Nuclear Power Institute of China, Chengdu 610041, China.*

² *Key Laboratory for Advanced Materials of Ministry of Education, Department of Materials Science and Engineering, Tsinghua University, Beijing 100084, China.*

³ *Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802, USA.*

⁴ *Department of Mechanical Engineering, Mississippi State University, MS 39762, USA.*

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Abstract. This paper systematically compares the numerical implementation and computational cost between the Fourier spectral iterative perturbation method (FSIPM) and the finite element method (FEM) in solving partial differential equilibrium equations with inhomogeneous material coefficients and eigen-fields (e.g., stress-free strain and spontaneous electric polarization) involved in phase-field models. Four benchmark numerical examples, including inhomogeneous elastic, electrostatic, and steady-state heat conduction problems demonstrate that (1) the FSIPM rigorously requires uniform hexahedral (3D) and quadrilateral (2D) mesh and periodic boundary conditions for numerical implementation while the FEM permits arbitrary mesh and boundary conditions; (2) the FSIPM solutions are comparable to their FEM counterparts, and both of them agree with the analytic solutions, (3) the FSIPM is much faster in solving equilibrium equations than the FEM to achieve the accurate solutions, thus exhibiting a greater potential for large-scale 3D computations.

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[†]The authors contribute equally.

*Corresponding author. *Email addresses:* chen@me.msstate.edu (L. Chen), 15828622005@163.com (P. C. Song), tuy123@psu.edu (T. N. Yang), yxj135@psu.edu (Y. Z. Ji), zw352@msstate.edu (Z. Wang), zgyang@tsinghua.edu.cn (Z. G. Yang), lqc3@psu.edu (L. Q. Chen)

1 Introduction

The phase-field method, as a powerful computational approach, has been widely applied to model and predict microstructure evolution during various material processes [10], for instance, martensitic phase transformations [1, 13, 29], electromigration [2, 21], grain growth [11, 15], solidification [19, 22], and so forth. In the phase-field method, the mesoscale morphology and microstructure in materials are described by a set of continuous phase-field variables, including the conserved field variables $\{c_1, c_2, \dots, c_n\}$ and non-conserved field variables $\{\eta_1, \eta_2, \dots, \eta_m\}$ that represent the compositional and structural differences in the microstructure, respectively. The corresponding total free energy is given by:

$$F = \int \left[f(c_1, c_2, \dots, c_n, \eta_1, \eta_2, \dots, \eta_m) + \sum_{i=1}^n \alpha_i (\nabla c_i)^2 + \sum_{i=1}^3 \sum_{j=1}^3 \sum_{k=1}^p \beta_{ij} \nabla_i \eta_k \nabla_j \eta_k \right] d^3 \mathbf{r} + \int \int \mathbf{G}(\mathbf{r} - \mathbf{r}') d^3 \mathbf{r} d^3 \mathbf{r}'. \quad (1.1)$$

The first volume integral in Eq. (1.1) represents the local contribution from short-range interactions to the free energy, including the bulk free energy f , as well as the gradient energy terms, $\sum_{i=1}^n \alpha_i (\nabla c_i)^2 + \sum_{i=1}^3 \sum_{j=1}^3 \sum_{k=1}^p \beta_{ij} \nabla_i \eta_k \nabla_j \eta_k$ that describe the inhomogeneity at interfaces. α_i and β_{ij} are the gradient energy coefficients. The second volume integral in Eq. (1.1) represents the energy contribution from long-range interactions, such as elastic interactions and electrostatic interactions, which are represented by $\mathbf{G}(\mathbf{r} - \mathbf{r}')$. The evolution of the microstructure is governed by the Cahn-Hilliard diffusion equation [4] (Eq. (1.2)), and/or the Allen-Cahn relaxation equation [5] (Eq. (1.3)) with a given total free energy F from Eq. (1.1):

$$\frac{\partial c_i(\mathbf{r}, t)}{\partial t} = \nabla \cdot M_{ij} \nabla \frac{\delta F}{\delta c_j(\mathbf{r}, t)}, \quad (1.2)$$

$$\frac{\partial \eta_k(\mathbf{r}, t)}{\partial t} = -L_{kl} \frac{\delta F}{\delta \eta_l(\mathbf{r}, t)}. \quad (1.3)$$

M_{ij} and L_{kl} are the kinetic coefficients related to atomic and interfacial mobility, respectively.

The formulation of the free energy densities in Eq. (1.1) is the key to the construction of phase-field models. The short-range chemical interactions (the first volume integral in Eq. (1.1)), once formulated, are explicit with respect to field variables and their driving forces (the variational derivatives with respect to field variables) can be directly obtained. The long-range interactions, however, are implicit with respect to field variables; additional constraints for long-range interactions, *i.e.*, long-range equilibria, are required. Typically, the microstructure inhomogeneity imposes a "source term", as a function of field variables, to the long-range interaction fields, and correspondingly, the long-range interaction fields respond to this "source term" to establish the long-range