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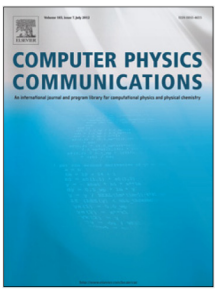

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Parallel energy-stable phase field crystal simulations based on domain decomposition methods

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Abstract

In this paper, we present a parallel numerical algorithm for solving the phase field crystal equation. In the algorithm, a semi-implicit finite difference scheme is derived based on the discrete variational derivative method. Theoretical analysis is provided to show that the scheme is unconditionally energy stable and can achieve second-order accuracy in both space and time. An adaptive time step strategy is adopted such that the time step size can be flexibly controlled based on the dynamical evolution of the problem. At each time step, a nonlinear algebraic system is constructed from the discretization of the phase field crystal equation and solved by a domain decomposition based, parallel Newton–Krylov–Schwarz method with improved boundary conditions for subdomain problems. Numerical experiments with several two and three dimensional test cases show that the proposed algorithm is second-order accurate in both space and time, energy stable with large time steps, and highly scalable to over ten thousands processor cores on the Sunway TaihuLight supercomputer.

Keywords: phase field crystal equation, discrete variational derivative method, unconditionally energy stable scheme, domain decomposition method

1. Introduction

The phase field crystal (PFC) equation is a popular model for simulating microstructural evolution in material sciences. As an atomic description of crystalline materials on the diffusive time scale, the PFC equation was originally proposed to model the dynamics of crystal growth by Elder et. al. [1, 2]. Since then, during the past decade, it has been applied with significant successes for the simulation of phenomena found in various solid-liquid

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