Numerical Analysis of a Continuous Interior Penalty Method for the Phase Field Crystal Equation

Abstract

In this talk, we consider the phase field crystal (PFC) equation which is a phase field model describing the dynamical formation of crystalline structures. This PFC equation is derived from an energy functional that is minimized by periodic density fields, naturally incorporating the periodicity of a crystal lattice. The model is then expressed as a sixth-order nonlinear parabolic equation that locally minimizes this energy functional under the constraint of mass conservation. The numerical simulation of this equation presents challenges such as the spatial discretization of the nonlinear higher-order differential operators that appear in the equation and the approximation of dynamic interfaces that travel over the entire material. To cope with these challenges, we propose an unconditionally stable and uniquely solvable numerical scheme and prove these theoretical properties. We close the talk by presenting the numerical results of some benchmark problems to verify the practical performance of the proposed approach and discuss some exciting current and future applications.

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