MASTER'S THESIS

Adaptive time-stepping methods for solving the phase field models

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Abstract

In this thesis, we investigate an adaptive time step method for simulating the dynamics of the phase field models. Phase field models are usually constructed in order to reproduce a given interfacial dynamics, which are usually constructed in such a way that in the limit of an infinitesimal interface width (the so-called sharp interface limit) the correct interfacial dynamics are recovered. This approach permits to solve the problem by integrating a set of partial differential equations for the whole system, thus avoiding the explicit treatment of the boundary conditions at the interface. With the increasing power of computers and the theoretical progress in phase field modeling, phase field models have become a useful tool for the numerical simulation of interfacial problems.

In this thesis, we will consider the numerical simulations for a class of the phase field models, namely the phase filed crystal (PFC) model. In the PFC model, a phase-field formulation is introduced that accounts for the periodic structure of a crystal lattice through a free energy functional of Swift-Hohenberg type functions. The model naturally incorporates elastic and plastic deformation of the crystal and the various crystal defects. The idea of the PFC is that a conserved phase variable is introduced to describe a coarse-grained temporal average of the number density of atoms. Consequently, this method represents a significant advantage over other atomistic methods such as molecular dynamics where the time steps are constrained by atomic-vibration time scales.

The PFC equation is a high-order (sixth-order) nonlinear partial differential equation. Except for very special cases, the PFC equation cannot be solved analytically. Therefore, efficient numerical algorithms are essential. Previously, many explicit type time stepping have been proposed for the PFC equation, where a high-order time step restriction is required. In recent years, many stable time-steppings have been also studied. However, all these approaches are based on constant time steps which are generally quite small (say less than $\Delta t < 0.01$ in order to main stable simulations). However, as many practical problems require large time simulations (say $T = 10,000$) in order to obtain dynamical and steady-state behaviors of the physical process. This makes the fixed time-stepping approach questionable due to rounding errors and CPU time restrictions.

It has been realized recently that adaptive time-stepping technique may be useful in long-time simulations of the phase filed problems. The basic idea is to use small time steps in the time regime where the solution energy varies rapidly while larger time steps are employed when the solution energy changes very slowly. In this thesis, we will study the adaptive time-stepping technique for solving the PFC model. Indeed the numerical simulation of the PFC model requires long time simulations. Consequently, adaptive time-stepping method becomes necessary. To this end, we first study unconditionally energy stable schemes for approximating the PFC model. The time steps are adaptively determined based on the variations of the corresponding energy. Our numerical experiments demonstrate that the use of our adaptive time stepping strategy can not only reach the steady state solution but can also resolve

the dynamics of the solutions in an efficiently and accurate manner.

In conclusion, the adaptive time stepping methods should be a useful tool for obtaining efficient and accurate approximations for the phase field models.

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