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Energy Law Preserving Finite Element Scheme for the Cahn-Hilliard Equation with Dynamic Boundary Conditions†

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Abstract. In this paper, we develop the energy law preserving method for a phase-field model of Cahn-Hilliard type describing binary mixtures. A new class of dynamic boundary conditions in a rather general setting proposed in [1] is adopted here. The model equations are discretized by a continuous finite element method in space and a midpoint scheme in time. The discrete energy law of the numerical method for the model with the dynamic boundary conditions is derived. By a few two-phase examples, we demonstrate the performance of the energy law preserving method for the computation of the phase-field model with the new class of dynamic boundary conditions, even in the case of relatively coarse mesh.

AMS subject classifications: 65M06, 76T10

Key words: Cahn-Hilliard equation, dynamic boundary condition, energy law preservation, finite element method.

1 Introduction

Multiphase flow is common and important in our daily life, for example, bubbles in water, droplets falling from air, mixtures of oil and water, mixtures of polymers, biological liquids and cells. Multiphase fluid motion is involved in many important biological and

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industrial processes and has become an active interdisciplinary research field. Many different methods can be found in the literature to model and simulate multiphase problems(e.g. [2–15]). We can roughly divided them into two categories: sharp interface and diffuse interface (or phase-field) models. The traditional sharp interface model consists of an independent hydrodynamic system for each component and a free interface for separating them. In the diffusion interface model, the interface is considered to have thickness and the flow parameters vary continuously from one stage to another. Different from the sharp interface model, the two kinds of fluid in the phase-field model are considered to be one kind of fluid, they are mixed smoothly near the interface, and the phase parameter changes rapidly. These two fluid mixtures can also be considered a special non-Newtonian fluid. This not only leads to a more easily analyzed differential equation system, but also can naturally handle possible interface topology changes (e.g. [14, 16]). With the development of advanced algorithms and computing technologies, the application of phase-field models has gradually expanded and has become an effective modeling and calculation tool for dealing with complex topologies of interfaces between different material components.

The Cahn-Hilliard equation is the basic diffusion interface model for multiphase systems. Since the system is usually evolved within the boundary region, appropriate boundary conditions need to be considered. In recent years, various dynamic boundary conditions have been proposed to account for possible short-range interactions of materials with solid walls. The dynamic boundary conditions studied in this paper are recently proposed in [1]. It is closely related to moving contact line conditions (e.g. [17–19]). Comparing with the existing dynamic boundary conditions in the literature (e.g. [20–23]), an interesting feature of the boundary condition is that it is not chosen as a sufficient condition for the energy dissipation, but uniquely determined by the kinematic and energetic relations together with the force balance law. As a consequence, for more general boundary force relations, this type of boundary conditions naturally fulfills important physical constraints such as conservation of mass, dissipation of energy and force balance relations. They can be naturally applied to the moving contact line problem.

As we all know, the phase-field model equations are generally nonlinear equations with high-order spatial derivatives, so it is difficult to find the exact analytical solution. The numerical simulation of the phase-field model becomes an important means to visually describe the multiphase flow and its dynamics intuitively. Over the years, many numerical methods have been developed to solve the phase-field model. For examples, Fourier-spectral method (e.g. [11, 24, 25]), spectral method (e.g. [26–28]), adaptive moving mesh method (e.g. [29–31]), finite difference method ((e.g. [32–35])), finite element method (e.g. [36–40]), and discontinuous finite element method ([41, 42]). There are also error analysis of finite element approximation for phase-field models without coupling the flow field or coupled with the Stokes flow (e.g. [43–48]). However, these efforts did not pay close attention to the preservation of the energy law inherited in the fully discrete system. The maintenance of energy law is very important in numerical calculation. This is because preserving the law of energy allows the numerical scheme to capture the