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Diffuse Interface Methods for Multiple Phase Materials: An Energetic Variational Approach

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Abstract. In this paper, we introduce a diffuse interface model for describing the dynamics of mixtures involving multiple (two or more) phases. The coupled hydrodynamical system is derived through an energetic variational approach. The total energy of the system includes the kinetic energy and the mixing (interfacial) energies. The least action principle (or the principle of virtual work) is applied to derive the conservative part of the dynamics, with a focus on the reversible part of the stress tensor arising from the mixing energies. The dissipative part of the dynamics is then introduced through a dissipation function in the energy law, in line with Onsager's principle of maximum dissipation. The final system, formed by a set of coupled time-dependent partial differential equations, reflects a balance among various conservative and dissipative forces and governs the evolution of velocity and phase fields. To demonstrate the applicability of the proposed model, a few two-dimensional simulations have been carried out, including (1) the force balance at the three-phase contact line in equilibrium, (2) a rising bubble penetrating a fluid-fluid interface, and (3) a solid particle falling in a binary fluid. The effects of slip at solid surface have been examined in connection with contact line motion and a pinch-off phenomenon.

AMS subject classifications: 65F10, 65N22, 65N55

Key words: multiphase flow, energetic variational approach

1. Introduction

Phase field methods (PFM), also known as diffuse interface methods, have been widely used in modeling two-phase problems and free interface motion of mixtures. The methods are based on a labeling function $\phi(x)$, which usually takes values as ± 1, to distinguish between the two different materials (phases). Du et. al. applied phase

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field methods in their studies of the configurations and the deformations of elastic bio-membranes [7]. Liu and Shen investigated the use of two-phase models for studying bubble relaxation, rise, and coalescence [18]. Qian et al. studied the moving contact line problem using phase field methods in [19]. Yue et. al. [25] studied a general approach for modeling two-phase complex fluids, with numerical examples simulating emulsion of nematic drops in a Newtonian matrix. Recently Shen and Yang applied the phase field method to two-phase incompressible flows with different densities and viscosities [22].

The basic idea of the two-phase PFM is to use a coarse graining (mean field) model to describe the microscopic dynamics of the mixtures. In the hydrodynamical (macroscopic) time scale, such dynamics involve the deformations of each phase, the interaction between the two, and their interactions with the surrounding environment. The underlying dynamical system is derived from applying variational principles to a certain free energy, e.g. the classical Ginzburg-Landau type energy [4]

$$\mathcal{F}_{CH} = \int \gamma \Big\{ \frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{4\varepsilon} \left(\phi^2 - 1\right)^2 \Big\} dx,$$

where $\phi(x)$ is the phase field function and ε is the width of the diffuse interface. The two parts in the above integrand represent the "philic" and "phobic" interactions between the two materials. The parameter γ can be associated to the surface tension in the conventional sharp interface formulations. The applicability of this model has been demonstrated for many different applications (see [8] [9] [20] and references theirin). Although analytically it is still an open question whether the the sharp interface model can be recovered by the phase field model via a rigorous proof, the latter has been applied theoretically and numerically for a long time. Moreover, from a practical and more physical point of view, the sharp interface models can be viewed as the simplification or idealization of phase field models.

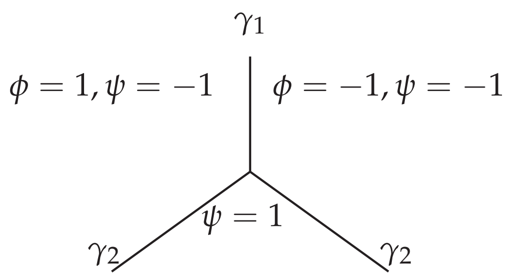

Figure 1: A Schematic illustration for three phases distinguished/labelled by two phase fields ϕ and ψ.

In this paper, we show that for problems in which more than two phases are involved, we can introduce additional labeling functions to distinguish among them, as illustrated in Fig. 1. The derivation follows from applying the energetic variational framework as in [25]. Here, in the region at the bottom of the figure, a single phase is characterized by $\{\psi = 1\}$ and ϕ is not defined. In the top region of the figure, there are two phases distinguished by different values of ϕ, while sharing the same ψ value. In