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A phase-field method for 3D simulation of two-phase heat transfer

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ABSTRACT

We formulate new multi-phase convective heat transfer equations by combining the three-dimensional (3D) Navier–Stokes equations, the energy equation and the Cahn–Hilliard equation for the phase field variable $\phi(\mathbf{x}, t)$. The density, viscosity, heat capacity and conductivity are functions of $\phi(\mathbf{x}, t)$. The equations are solved in time with a splitting scheme that decouples the flow and temperature variables, yielding time-independent coefficient matrices after discretization, which can be computed during preprocessing. Here, a spectral element method is employed for spatial discretization but any other Eulerian grid discretization scheme is also suitable. We test the new method in several 3D benchmark problems for convergence in time/space including a conjugate heat transfer problem and also for a realistic transient cooling of a 3D hot object in a cavity with a moving air–water interface. These applications demonstrate the efficiency of the new method in simulating 3D multi-phase convective heat transfer on stationary grids, different modes of heat transfer (e.g. convection/conduction), as well as its robustness in handling different fluids with large contrasts in physical properties.

1. Introduction

Heat transfer in conjunction with multi-phase flow is ubiquitous in many engineering and scientific applications involving phase change, distillation, extraction, absorption and drying. The modeling and numerical simulation of multi-phase flow systems have therefore been the subject of numerous theoretical and computational studies [1–5].

The common modeling approaches can be broadly divided into two basic types of *sharp-* and *diffuse-interface* models. The sharp-interface models assume a zero-thickness layer that separates the two fluids. This layer is endowed with properties such as surface tension, and matching boundary conditions are imposed on either side of this surface. For numerical simulation of two-phase flow systems with sharp-interface models, moving-grid methods are commonly used with conformal elements on either side of the interface [6,7]. However, the possibility of mesh entanglement restricts the moving-grid approaches to cases with mild deformation of the interface. Such a limitation forbids any morphological changes, unless a new grid is generated "on-the-fly", which significantly hampers the efficiency of the method.

More recently, Smoothed Particle Hydrodynamics (SPH) has also been successfully used in modeling two-phase flow system. The SPH model employs a purely Lagrangian viewpoint in which the particles are moving as interpolation points, and the inner-particle forces (viscous, pressure, etc.) are calculated by smoothing the properties of its neighboring particles while satisfying the Navier–Stokes equations. This approach provides a suitable framework for tracking different phases, in multi-phase flow systems. For the application of SPH method in multi-phase flow systems see for instance [8–10].

The diffuse-interface models, however, assume a finite-thickness layer between the two phases. The interfacial tension between the two fluids spreads over this narrow layer. This approach yields a unified set of governing equations for two phases, instead of formulating the flow in two separate domains. Numerical methods such as *Volume-of-Fluid (VOF)* [11–14] and *level-set* [14–16] have been successfully employed by utilizing diffuse-interface models to simulate two-phase systems.

From the modeling perspective, the energy-based variational framework of phase-field formulation makes it a thermodynamically-consistent and physically attractive approach to modeled multi-phase flow systems (see for instance [17]). Unlike the level-set model, where an artificial smoothing function is prescribed for the interface, the Cahn–Hilliard model describes the interface by a mixing energy, and in that sense, the phase-field

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model can be viewed as a physically motivated level-set method. The energy-based description of phase-field model can also allow complex rheology of non-Newtonian fluids to be easily incorporated into the formulation [18]. On the other hand, from the numerical viewpoint, the phase-field method provides a single set of partial differential equations for two phases that can be discretized on a *fixed grid* in an Eulerian framework. It can also handle morphological changes such as breakup, coalescence and reconnection, which extends the application of the method to complex two-phase flow systems. An example of a 2D simulation of a cold water jet impinging on a hot air–water interface is shown in Fig. 1. Initially we have cold water (10 °C) issuing from the middle of the upper wall. Hot water (50 °C) fills up the bottom half of the domain. There are two outlets at the two corners of the upper wall. Upper and lower walls assume adiabatic temperature boundary conditions and periodic in horizontal direction. As shown in Fig. 1(b), blue color represents water, which corresponds to $\phi(\mathbf{x},t) = -1$, while white color represents air, which corresponds to $\phi(\mathbf{x},t) = 1$. The interface between water and air is provided by the solution of $\phi(\mathbf{x},t)$ from the Cahn–Hilliard equation but not tracked, which is different from the interface tracking/capturing techniques.

However, there are several challenges in the numerical simulation of the Cahn-Hilliard equation coupled with convective heat transfer equations that must be remedied for the model to be used in realistic applications. In cases with large thermal conductivity and density ratios, the discretization of the phase-field formulation combined with heat transfer equations leads to highly stiff discrete systems, causing numerical stability issues. The cases with large ratios of physical properties are plentiful in realistic applications such as water–air systems or most systems where phase change is involved. On the other hand, the phase-field formulation renders physical properties (such as density, thermal conductivity, viscosity, ...) as time-dependent variables through their dependence on the phase field $\phi(\mathbf{x},t)$. The time-dependence of these properties makes the coefficient matrices time-dependent accordingly, requiring an expensive computing/assembling of these matrices at each time step, and thus significantly hampering the numerical efficiency of the algorithm. Moreover, the convective heat transfer equations combined with Cahn-Hilliard equation form a fully coupled system of partial differential equations. Hence, a *de-coupling* strategy is very desirable in order to avoid the high computational cost incurred by solving such a coupled system of equations.

Among the existing methods of discretizing the phase-field formulation for convective heat transfer problems, the spectral/hp element method, in particular, is very promising [19]. The smooth transition of phase field and physical properties between the two phases makes this method compliant with sufficient regularity required in spectral-type element discretizations. The low dispersion error of spectral/hp discretization compared to low-order methods is also attractive in convection-dominated problems. For more details on spectral/hp element method see reference [20]. However, any other finite difference, finite volume or finite element method can be combined with the approach proposed here.

In this paper we present an efficient numerical algorithm for discretizing multi-phase convective heat transfer equations. We employ a splitting scheme as a decoupling strategy to efficiently solve the system of PDEs obtained from phase-field formulation. Our method results in time-independent coefficient matrices that can be pre-computed during the pre-processing. We verify our method by comparing the numerical results with analytical solutions. We also demonstrate the capability of our method by simulating the flow of a water–air system with density ratio of 1000 around a hot object.

This paper is organized as follows. In the next section we develop the numerical algorithm for discretizing multi-phase convective heat transfer equation using the phase-field methodology. In the third section, we demonstrate the spatial and time convergence of the proposed method. In the fourth section, we verify the accuracy of the numerical temperature field with an exact solution for a two-phase flow convection problem in a pipe and a conjugate heat transfer problem in a channel. In the last section we show the results of simulation of a transient cooling of a hot object immersed in water–air flow with a moving interface.

2. Numerical method

2.1. Governing equations and boundary conditions

Let Ω denote an open bounded domain in two or three dimensions (2-D or 3-D), and let $\partial\Omega$ denote its boundary. We consider a mixture of two immiscible incompressible fluids, with different viscous and thermal properties, contained in Ω. Let ρ_1 and ρ_2, respectively, denote the densities of the two fluids, μ_1 and μ_2 denote their dynamic viscosities, c_1 and c_2 denote their specific heat coefficients, and k_1 and k_2 denote their thermal conductivities. We assume that there is no phase change in the system. This two-phase system can be described by the following system of equations:

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla p + \nabla\cdot\left[\mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T)\right] - \lambda\nabla \cdot(\nabla\phi\nabla\phi) + \mathbf{f}(\mathbf{x},t), \quad (1a)$$

$$\nabla\cdot\mathbf{u} = 0, \quad (1b)$$

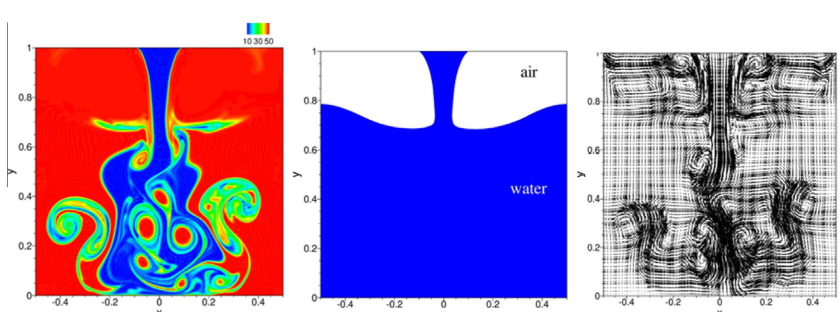

Fig. 1. Cold water jet 10 °C issuing from the middle of the upper wall into a hot air–water pool 50 °C: (a) temperature snapshot; (b) air–water interface snapshot in terms of the phase field. Initially $\phi(\mathbf{x},t) = 1$ for air and $\phi(\mathbf{x},t) = -1$ for water; (c) velocity snapshot. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)