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An outflow boundary condition and algorithm for incompressible two-phase flows with phase field approach

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ABSTRACT

We present an effective outflow boundary condition, and an associated numerical algorithm, within the phase-field framework for dealing with two-phase outflows or open boundaries. The set of two-phase outflow boundary conditions for the phase-field and flow variables are designed to prevent the un-controlled growth in the total energy of the two-phase system, even in situations where strong backflows or vortices may be present at the outflow boundaries. We also present an additional boundary condition for the phase field function, which together with the usual Dirichlet condition can work effectively as the phase-field inflow conditions. The numerical algorithm for dealing with these boundary conditions is developed on top of a strategy for de-coupling the computations of all flow variables and for overcoming the performance bottleneck caused by variable coefficient matrices associated with variable density/viscosity. The algorithm contains special constructions, for treating the variable dynamic viscosity in the outflow boundary condition, and for preventing a numerical locking at the outflow boundaries for time-dependent problems. Extensive numerical tests with incompressible two-phase flows involving inflow and outflow boundaries demonstrate that, the two-phase outflow boundary conditions and the numerical algorithm developed herein allow for the fluid interface and the two-phase flow to pass through the outflow or open boundaries in a smooth and seamless fashion, and that our method produces stable simulations when large density ratios and large viscosity ratios are involved and when strong backflows are present at the outflow boundaries.

1. Introduction

The present work concerns *two-phase outflows*, where the interface between two immiscible incompressible fluids passes through open portions of the domain boundary and where the field variables are unknown and need to be computed. Two-phase outflows are widely encountered in two-phase jets, wakes, shear layers, and other spatially-developing flows involving un-bounded physical domains. To numerically simulate such flows, it is necessary to artificially truncate the domain to a finite size. Therefore, an outflow or open boundary condition will be required for the two-phase artificial boundary. Many desirable properties for single-phase outflow boundary conditions [23] can carry over to two-phase outflows. It is desired that an ideal two-phase outflow boundary condition would allow the information carried with the two-phase flow to exit

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the domain smoothly without adverse upstream effects, and that it should allow for stable computations of the two-phase flow.

The design of effective techniques for treating two-phase outflows presents new challenges beyond those encountered for single-phase outflows. Two-phase outflows involve density contrast, viscosity contrast, fluid interface, and surface tension on the open boundaries, and the density ratio and viscosity ratio of the two fluids may be large. While a large volume of work on outflow conditions for single-phase flows exist in the literature (see e.g. [12,23,29,6,11] for related reviews and the references therein), a survey of literature indicates that the work on two-phase outflows is very scarce. Some recent efforts employ a convective boundary condition for the lattice-Boltzmann equations [19] or level set method [2]. Other previous work involves only a single type of fluid on the outflow boundary, even though the flow inside the domain involves two fluid phases, and therefore a usual single-phase outflow condition would suffice; see e.g. [28].

The two-phase outflow boundary conditions and numerical algorithm in the current work are developed within the phase field framework. In the phase field approach the sharp interface between two immiscible incompressible fluids is replaced by a thin smooth transition layer (i.e. diffuse interface), and the two-phase system is characterized by a phase field function, which varies continuously over the transition layer and is mostly uniform in the bulk phases; see e.g. [3,20,14,18] for reviews and more detailed discussions of related concepts. The governing equations consist of the variable-density Navier–Stokes equations and the Cahn–Hilliard equation (or Allen–Cahn equation) which describes the evolution of the phase field function [20,15,18,26,25]. The surface tension effect is naturally and implicitly accounted for in the phase field formulation.

One faces several challenges when designing boundary conditions and numerical algorithms for dealing with two-phase outflows, and also inflows, with the phase field approach. First, because the phase field formulation implicitly incorporates the surface tension effect, at the outflow boundary one must also take into account the surface tension in the boundary conditions. How to achieve this is not immediately clear. Second, strong vortices or backflows may occur on portions of the two-phase outflow boundaries, especially with large density ratios or at high Reynolds numbers. The outflow boundary conditions should facilitate stable computations in such situations. Third, the variable mixture properties, and in particular the variable viscosity, pose a significant issue to the algorithmic treatment of the outflow boundary conditions. Large viscosity ratios have been observed to lead to a numerical instability at the two-phase outflow boundaries. Fourth, it is desired that the outflow conditions should not induce significant artificial distortions of the fluid interface when it passes through the outflow boundaries. Finally, the fourth spatial order of the Cahn–Hilliard equation requires two independent boundary conditions for the phase field function on each boundary, which creates additional difficulties on the inflow boundaries where Dirichlet type conditions are desired.

In the current work, we present a set of effective two-phase outflow boundary conditions for the phase-field and flow variables, a boundary condition for the phase field function (in addition to the usual Dirichlet condition) for the inflow boundaries, and an efficient numerical algorithm for treating these outflow and inflow boundary conditions. These boundary conditions are developed based on considerations of the energy relation of the two-phase system. They are designed to prevent the un-controlled growth in the total energy of the domain, even when energy influx or backflows into the domain may exist at the outflow boundaries. The numerical algorithm for dealing with these boundary conditions are developed on top of a scheme for the coupled Navier–Stokes and Cahn–Hilliard equations we developed previously in [10]. The algorithm contains special treatments for the variable dynamic viscosity at the outflow boundaries, and a special construction for preventing the numerical locking on the two-phase outflow boundaries.

The method developed herein is effective for dealing with two-phase outflows where the fluid interface may pass through the outflow boundaries and when large density ratios and large viscosity ratios may be involved. It is also effective when there are strong backflows or vortices at the two-phase outflow boundaries. The method retains several crucial features inherited from [10], which makes the current method computationally very efficient. For example, the method de-couples the computations for all flow variables, and involves only constant and time-independent coefficient matrices for the linear algebraic systems for each flow variable after discretization. Therefore, these coefficient matrices can be pre-computed, which effectively overcomes the performance bottleneck caused by variable coefficient matrices associated with variable mixture properties.

The novelties of the presented method lie in three aspects: the outflow boundary condition for the velocity, the additional phase-field boundary condition for inflows (beyond the usual phase-field Dirichlet condition), and the numerical algorithm for treating the outflow and inflow boundary conditions. The outflow boundary condition for the phase field function presented here is also new in the context of phase field approach. On the other hand, the contact-angle boundary conditions for solid walls discussed here are largely based on techniques we developed previously in [7].

The algorithm developed herein has been implemented using the spectral elements [27,16,17,33] for spatial discretizations, because of the high-order numerical accuracy and geometric flexibility. While the algorithm is formulated for C^0 spectral elements, it can also apply to low-order C^0 finite elements without any change. We would like to point out that the outflow and inflow boundary conditions and the numerical algorithm presented herein are general. They are independent of the particular spatial discretization schemes. The implementation with finite difference type methods is also briefly discussed in the paper.