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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.

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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 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.

2. Two-phase outflow boundary conditions and algorithm

2.1. Phase field formulation and two-phase outflow boundary conditions

Let Ω denote an open bounded domain in two or three dimensions, and $\partial \Omega$ denote its boundary. Consider a mixture of two immiscible incompressible fluids contained in Ω . Let ρ_1 and ρ_2 respectively denote the densities of the two fluids, and μ_1 and μ_2 denote their dynamic viscosities. This two-phase system can be described by the following coupled system of equations [1]:

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

$$\nabla \cdot \mathbf{u} = \mathbf{0},\tag{1b}$$

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = -\lambda \gamma_1 \nabla^2 \left[\nabla^2 \phi - h(\phi) \right] + g(\mathbf{x}, t).$$
(1c)

In the above equations, $\mathbf{u}(\mathbf{x}, t)$ is velocity, $p(\mathbf{x}, t)$ is pressure, $\mathbf{D}(\mathbf{u}) = \nabla \mathbf{u} + \nabla \mathbf{u}^T$, and $\mathbf{f}(\mathbf{x}, t)$ is a body force, where *t* is time and **x** is the spatial coordinate and $(\cdot)^T$ denotes the transpose of (\cdot) . $\phi(\mathbf{x}, t)$ denotes the phase field function, $-1 \le \phi \le 1$. The flow regions with $\phi = 1$ and $\phi = -1$ respectively represent the first and the second fluids. The iso-surface $\phi(\mathbf{x}, t) = 0$ marks the interface between the two fluids at time *t*. $h(\phi)$ is given by

$$h(\phi) = \frac{1}{\eta^2} \phi \left(\phi^2 - 1 \right) \tag{2}$$

where η is a characteristic length scale of the interface thickness. λ is the mixing energy density coefficient, and is related to the surface tension σ by [30]

$$\lambda = \frac{3}{2\sqrt{2}}\sigma\eta,\tag{3}$$

where σ is assumed to be constant. γ_1 is the mobility of the interface, and is assumed to be constant in this paper. In Eq. (1a) \tilde{J} is given by,

$$\tilde{\mathbf{J}} = \frac{1}{2} (\rho_1 - \rho_2) \lambda \gamma_1 \nabla \left[\nabla^2 \phi - h(\phi) \right], \tag{4}$$

and the term $\tilde{\mathbf{J}} \cdot \nabla \mathbf{u}$ results from the requirement for Galilean invariance of the formulation [1]. The density, ρ , and the dynamic viscosity, μ , are related to the phase field function by,

$$\rho(\phi) = \frac{\rho_1 + \rho_2}{2} + \frac{\rho_1 - \rho_2}{2}\phi, \qquad \mu(\phi) = \frac{\mu_1 + \mu_2}{2} + \frac{\mu_1 - \mu_2}{2}\phi.$$
(5)

Consequently, both the density and the dynamic viscosity in Eq. (1a) are time-dependent field variables. $g(\mathbf{x}, t)$ in Eq. (1c) is a prescribed scalar source term for the purpose of numerical testing only, and it will be set to zero in actual simulations. One can note that Eq. (1c) with g = 0 is the Cahn-Hilliard equation.

We assume that $\partial \Omega = \partial \Omega_d^u \cup \partial \Omega_o = \partial \Omega_d^\phi \cup \partial \Omega_w^\phi \cup \partial \Omega_o$, where $\partial \Omega_d^u = \partial \Omega_d^\phi \cup \partial \Omega_w^\phi$ is the Dirichlet boundary for the velocity and **u** is prescribed on $\partial \Omega_d^u$. $\partial \Omega_d^\phi$ is the Dirichlet boundary for the phase field function and ϕ is prescribed on $\partial \Omega_d^a$. $\partial \Omega_d^\phi$ is the Dirichlet boundary for the phase field function and ϕ is prescribed on $\partial \Omega_d^a$. $\partial \Omega_d^\phi$ is the Dirichlet boundary for the phase field function and ϕ is prescribed on $\partial \Omega_d^\phi$.

- Dirichlet boundaries for the phase field function, such as the inflow boundaries, and
- solid walls, where contact-angle boundary conditions will be imposed for the phase field function.

We refer to $\partial \Omega_o$ as the outflow boundary, where none of the flow variables (**u**, *p*, or ϕ) is known. It should be noted that, because the Cahn-Hilliard equation (1c) has a fourth spatial order, two boundary conditions for the phase field function will be needed on each boundary of the domain.

Specifically, Eqs. (1a)-(1c) are supplemented by the following boundary conditions. For the velocity, we impose

$$\mathbf{u} = \mathbf{w}(\mathbf{x}, t), \text{ on } \partial \Omega_d^u,$$

where **w** is the prescribed boundary velocity on $\partial \Omega_d^u$. For the phase field function, on the wall boundary $\partial \Omega_w^{\phi}$ we impose the dynamic contact-angle boundary conditions from [15,7],

$$\mathbf{n} \cdot \nabla \left[\nabla^2 \phi - h(\phi) \right] = g_w(\mathbf{x}, t), \quad \text{on } \partial \Omega_w^\phi, \tag{7a}$$

$$-D_{w}\left(\frac{\partial\phi}{\partial t}+\mathbf{u}\cdot\nabla\phi\right)=\mathbf{n}\cdot\nabla\phi+\frac{1}{\lambda}f_{w}^{\prime}(\phi)+g_{e}(\mathbf{x},t),\quad\text{on }\partial\Omega_{w}^{\phi},\tag{7b}$$

where **n** is the outward-pointing unit vector normal to $\partial \Omega_w^{\phi}$. g_w and g_e are prescribed scalar functions on $\partial \Omega_w^{\phi}$ for numerical testing purpose, and will be set to $g_w = 0$ and $g_e = 0$ in actual simulations. The constant $D_w \ge 0$ is called the dynamic wall mobility [7]. $f_w(\phi)$ is the fluid-solid interfacial tension function given by [32,7],

$$f_{w}(\phi) = \sigma \cos\theta_{s} \frac{\phi(\phi^{2} - 3)}{4} + \frac{1}{2}(\sigma_{w1} + \sigma_{w2}), \tag{8}$$

where σ is the surface tension between the two fluids, θ_s is the static (equilibrium) contact angle between the fluid interface and the wall measured on the side of the first fluid, the constant σ_{w1} is the interfacial tension between the solid wall and the first fluid, and the constant σ_{w2} is the interfacial tension between the solid wall and the second fluid. $f'_w(\phi)$ denotes the derivative of f_w with respect to ϕ . Note that the unknown constants σ_{w1} and σ_{w2} do not appear in the boundary condition (7b).

We propose the following boundary conditions for the phase-field Dirichlet boundary $\partial \Omega_d^{\phi}$:

$$-\lambda \left[\nabla^2 \phi - h(\phi)\right] + \frac{1}{4}(\rho_1 - \rho_2) |\mathbf{u}|^2 = g_d(\mathbf{x}, t), \quad \text{on } \partial \Omega_d^\phi$$
(9a)

$$\phi = \phi_b(\mathbf{x}, t), \quad \text{on } \partial \Omega_d^{\varphi}, \tag{9b}$$

where ϕ_b is the prescribed phase field function on $\partial \Omega_d^{\phi}$, and $|\mathbf{u}|$ is magnitude of the velocity \mathbf{u} . $g_d(\mathbf{x}, t)$ is a prescribed scalar function on $\partial \Omega_d^{\phi}$ for numerical testing purpose only, and will be set to $g_d = 0$ in actual simulations.

We propose the following boundary conditions for the outflow boundary $\partial \Omega_0$:

for the velocity:

$$-p\mathbf{n} + \mu \mathbf{n} \cdot \mathbf{D}(\mathbf{u}) - \left[\frac{\lambda}{2}\nabla\phi \cdot \nabla\phi + \lambda F(\phi)\right]\mathbf{n} - \left[\frac{1}{2}\rho|\mathbf{u}|^2\Theta_0(\mathbf{n}\cdot\mathbf{u})\right]\mathbf{n} = \mathbf{f}_b(\mathbf{x},t), \quad \text{on } \partial\Omega_o; \tag{10}$$

for the phase field function:

$$\mathbf{n} \cdot \nabla \left[\nabla^2 \phi - h(\phi) \right] = g_0(\mathbf{x}, t), \quad \text{on } \partial \Omega_0, \tag{11a}$$

$$\mathbf{n} \cdot \nabla \phi = -D_0 \frac{\partial \varphi}{\partial t} + g_a(\mathbf{x}, t), \quad \text{on } \partial \Omega_o.$$
(11b)

In the above Eqs. (10)–(11b), **n** is the outward-pointing unit vector normal to $\partial \Omega_0$, μ and ρ are respectively the mixture dynamic viscosity and density given in Eq. (5), and $F(\phi) = \frac{1}{4\eta^2}(\phi^2 - 1)^2$. One can recognize that $(\frac{\lambda}{2}\nabla\phi\cdot\nabla\phi + \lambda F(\phi))$ is the free energy of the two-phase system [18]. One also notes the relation $h(\phi) = F'(\phi)$. $\Theta_0(\mathbf{n} \cdot \mathbf{u})$ represents a smoothed step function about $\mathbf{n} \cdot \mathbf{u}$, and is given by

$$\Theta_0(\mathbf{n} \cdot \mathbf{u}) = \frac{1}{2} \left(1 - \tanh \frac{\mathbf{n} \cdot \mathbf{u}}{U_0 \delta} \right),\tag{12}$$

where U_0 is a characteristic velocity scale, and $\delta > 0$ is a chosen non-dimensional constant that is sufficiently small. As $\delta \to 0$, Θ_0 approaches a step function about $\mathbf{n} \cdot \mathbf{u}$, taking unit value in regions where $\mathbf{n} \cdot \mathbf{u} < 0$ and vanishing elsewhere. $\mathbf{f}_b(\mathbf{x}, t)$ is a prescribed vector function on $\partial \Omega_o$ for the purpose of numerical testing, and will be set to $\mathbf{f}_b = 0$ in actual simulations. $g_o(\mathbf{x}, t)$ and $g_a(\mathbf{x}, t)$ are prescribed scalar functions on $\partial \Omega_o$ for numerical testing, and will be set to $g_o = 0$ and $g_a = 0$ in actual simulations. $D_0 \ge 0$ is a chosen non-negative constant, and will be referred to as the outflow dynamic mobility. $\frac{1}{D_0}$ plays the role of a characteristic convection velocity at $\partial \Omega_o$. When $D_0 = 0$, (11b) becomes the Neumann boundary condition

$$\mathbf{n} \cdot \nabla \phi = g_a(\mathbf{x}, t), \quad \text{on } \partial \Omega_o. \tag{13}$$

The boundary condition (10) has a well-defined physical meaning when $\mathbf{f}_b = 0$. The term $[\frac{\lambda}{2}\nabla\phi \cdot \nabla\phi + \lambda F(\phi)]\mathbf{n}$ represents an effective stress exerting on $\partial \Omega_o$ induced by the flux of free energy of the two-phase system through the outflow boundary. The term $\frac{1}{2}\rho|\mathbf{u}|^2\mathbf{n}$ (when $\mathbf{n} \cdot \mathbf{u} < 0$) represents an effective stress exerting on $\partial \Omega_o$ induced by the *influx* of kinetic energy into the domain through the outflow boundary. The particular form for the kinetic-energy term in (10) is inspired by an outflow boundary condition we have developed recently for *single-phase* incompressible flows [8]. The terms $[-p\mathbf{n} + \mu \mathbf{n} \cdot \mathbf{D}(\mathbf{u})]$ represent the stress on the outflow boundary. Therefore, the boundary condition (10) with $\mathbf{f}_b = 0$ imposes the requirement that, if anywhere on the outflow boundary $\partial \Omega_o$ there is a kinetic energy *influx* into the domain through $\partial \Omega_o$, then the stress on the outflow boundary $\partial \Omega_o$ shall locally balance the total effective stress induced by the total flux of

the free energy and the kinetic energy through $\partial \Omega_o$, otherwise the stress shall locally balance the effective stress induced by the flux of free energy through $\partial \Omega_o$ only.

To elucidate the rationale for these boundary conditions, we briefly look into the energy balance for the two-phase system described by (1a)-(1c). We assume $g(\mathbf{x}, t) = 0$ in (1c) in the following discussion. Let $C(\phi) = -\lambda [\nabla^2 \phi - h(\phi)]$ (i.e. chemical potential). We re-write (1a) into an equivalent but more compact form,

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}\right) + \tilde{\mathbf{J}} \cdot \nabla \mathbf{u} = \nabla \cdot \mathbf{T} + C \nabla \phi + \mathbf{f},\tag{14}$$

where $\mathbf{T} = -[p + \frac{\lambda}{2} \nabla \phi \cdot \nabla \phi + \lambda F(\phi)]\mathbf{I} + \mu \mathbf{D}(\mathbf{u})$ and \mathbf{I} denotes the identity tensor. We have used the relation $h(\phi) = F'(\phi)$ in the above reformulation. We also re-write (1c) into a more compact form

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma_1 \nabla^2 C. \tag{15}$$

By taking the L^2 inner product between Eq. (14) and **u** and the L^2 inner product between Eq. (15) and $C(\phi)$, and summing up the two equations, one can obtain the following energy balance equation for the system,

$$\frac{\partial}{\partial t} \int_{\Omega} \left[\frac{1}{2} \rho |\mathbf{u}|^{2} + \frac{\lambda}{2} \nabla \phi \cdot \nabla \phi + \lambda F(\phi) \right]$$

$$= \int_{\Omega} \mathbf{f} \cdot \mathbf{u} - \int_{\Omega} \frac{\mu}{2} \|\mathbf{D}(\mathbf{u})\|^{2} - \gamma_{1} \int_{\Omega} \|\nabla C\|^{2}$$

$$+ \int_{\partial \Omega_{d}^{u}} \left(\mathbf{n} \cdot \mathbf{T} - \frac{1}{2} \rho |\mathbf{u}|^{2} \mathbf{n} \right) \cdot \mathbf{u} + \int_{\partial \Omega_{0}} \left(\mathbf{n} \cdot \mathbf{T} - \frac{1}{2} \rho |\mathbf{u}|^{2} \mathbf{n} \right) \cdot \mathbf{u}$$

$$+ \gamma_{1} \int_{\partial \Omega_{d}^{\phi}} (\mathbf{n} \cdot \nabla C) \left[C + \frac{1}{4} (\rho_{1} - \rho_{2}) |\mathbf{u}|^{2} \right] + \gamma_{1} \int_{\partial \Omega_{w}^{\phi} \cup \partial \Omega_{0}} (\mathbf{n} \cdot \nabla C) \left[C + \frac{1}{4} (\rho_{1} - \rho_{2}) |\mathbf{u}|^{2} \right]$$

$$+ \lambda \int_{\partial \Omega_{d}^{\phi} \cup \partial \Omega_{w}^{\phi}} (\mathbf{n} \cdot \nabla \phi) \frac{\partial \phi}{\partial t} + \lambda \int_{\partial \Omega_{0}} (\mathbf{n} \cdot \nabla \phi) \frac{\partial \phi}{\partial t}, \qquad (16)$$

where we have used Eqs. (1b) and (5) and the following relations

$$\begin{split} \tilde{\mathbf{J}} &= -\frac{1}{2}(\rho_1 - \rho_2)\gamma_1 \nabla C, \\ \frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho &= -\nabla \cdot \tilde{\mathbf{J}}, \\ \frac{\partial \phi}{\partial t} C &= \frac{\partial}{\partial t} \left[\frac{\lambda}{2} \nabla \phi \cdot \nabla \phi + \lambda F(\phi) \right] - \nabla \cdot \left[\lambda \nabla \phi \frac{\partial \phi}{\partial t} \right] \end{split}$$

In light of this energy balance equation for the two-phase system, we have the following observations:

- By imposing the condition (11a) with g₀ = 0 on ∂Ω₀, the condition (9a) with g_d = 0, and the condition (7a) with g_w = 0 on ∂Ω^φ_w, the surface integrals involving the term **n** · ∇*C* will vanish from the right hand side (RHS) of Eq. (16).
 By imposing the condition (11b) with g_a = 0 on ∂Ω₀, the last surface integral on the RHS of (16) will always be
- non-positive and therefore conducive to stability.
- The surface integral term over the outflow boundary, $\int_{\partial \Omega_0} (\mathbf{n} \cdot \mathbf{T} \frac{1}{2}\rho |\mathbf{u}|^2 \mathbf{n}) \cdot \mathbf{u}$ on the RHS of (16), can potentially cause un-controlled growth in the total energy of the domain, and thus numerical instability, if $\mathbf{n} \cdot \mathbf{u} < 0$ anywhere on the outflow boundary $\partial \Omega_0$, because of the influx of kinetic energy $-\frac{1}{2}\rho |\mathbf{u}|^2 (\mathbf{n} \cdot \mathbf{u})$ into the domain through $\partial \Omega_0$. Requiring that $\mathbf{n} \cdot \mathbf{T} \frac{1}{2}\rho |\mathbf{u}|^2 \mathbf{n} = 0$ in regions of $\partial \Omega_0$ with kinetic energy influx and that $\mathbf{n} \cdot \mathbf{T} = 0$ elsewhere on $\partial \Omega_0$, which give rise to the condition (10), will eliminate this numerical instability. On the other hand, for the Dirichlet boundary $\partial \Omega_d^u$ because the velocity \mathbf{u} is prescribed, the kinetic energy influx through $\partial \Omega_d^u$ (if any) will not cause the numerical instability issue with the surface integral $\int_{\partial \Omega_d^u} (\mathbf{n} \cdot \mathbf{T} \frac{1}{2}\rho |\mathbf{u}|^2 \mathbf{n}) \cdot \mathbf{u}$.

We would like to point out that the outflow boundary conditions, (10)–(11b), and the Dirichlet boundary condition for the phase field function (9a), proposed here can also be applied to other phase-field models in which the term $\tilde{J} \cdot \nabla u$ is absent from the Navier–Stokes equation (1a), see e.g. [14,4,18,30,10]. The only slight change that is necessary will be for the

phase-field Dirichlet condition (9a). For those phase field models in which $\tilde{\mathbf{J}} \cdot \nabla \mathbf{u}$ term is absent, we employ the following modified boundary condition on $\partial \Omega_d^{\phi}$ to replace (9a),

$$-\lambda \left[\nabla^2 \phi - h(\phi)\right] = g_d(\mathbf{x}, t), \quad \text{on } \partial \Omega_d^{\phi}, \tag{17}$$

where g_d is a prescribed function and will be set to $g_d = 0$ in actual simulations. We will show simulation results of the proposed boundary conditions for both types of phase field models in Section 3.

For the phase-field Dirichlet boundary $\partial \Omega_d^{\phi}$, it is tempting to employ the zero-flux condition for the chemical potential, $\mathbf{n} \cdot \nabla C = 0$, to replace the current condition (9a). However, we observe that the zero-flux condition for the chemical potential, together with the usual Dirichlet condition (9b), fails to work for the phase-field Dirichlet boundary in actual simulations when the density ratio becomes large. This combination induces a numerical instability at the inflow boundary in such situations.

We would also like to mention a variant form for the outflow boundary condition. An alternative form to the boundary condition (10) is the following

$$-p\mathbf{n} + \mu \mathbf{n} \cdot \mathbf{D}(\mathbf{u}) - \left[\frac{\lambda}{2}\nabla\phi \cdot \nabla\phi + \lambda F(\phi)\right]\mathbf{n} - \left[\frac{1}{2}\rho(\mathbf{n}\cdot\mathbf{u})\mathbf{u}\right]\Theta_0(\mathbf{n}\cdot\mathbf{u}) = \mathbf{f}_b(\mathbf{x},t), \quad \text{on } \partial\Omega_o.$$
(18)

The alternative form, $\frac{1}{2}\rho(\mathbf{n} \cdot \mathbf{u})\mathbf{u}$, results from a reformulation of the kinetic-energy flux term in (16) as follows, $(\mathbf{n} \cdot \mathbf{T} - \frac{1}{2}\rho|\mathbf{u}|^2\mathbf{n}) \cdot \mathbf{u} = [\mathbf{n} \cdot \mathbf{T} - \frac{1}{2}\rho(\mathbf{n} \cdot \mathbf{u})\mathbf{u}] \cdot \mathbf{u}$. This form has a connection with the boundary condition developed in [5] for single-phase incompressible Navier–Stokes equations.

In addition to the boundary conditions discussed above, the coupled system of equations, (1a)-(1c), should also be supplemented by appropriate initial conditions for the velocity **u** and the phase field function ϕ .

2.2. Algorithm formulation

Eqs. (1a)–(1c), the boundary conditions (6)–(7b) and (9a)–(11b), and the appropriate initial conditions for the velocity **u** and phase field function ϕ , together constitute the system that need to be solved in two-phase flow simulations. We next present an algorithm for solving this system. The main idea for discretizing Eqs. (1a)–(1c) is based on the splitting scheme we developed in [10]. Our emphasis in the following discussions is on how to numerically treat the outflow boundary conditions (10) and (11a)–(11b), as well as the Dirichlet boundary conditions for the phase field function (9a)–(9b).

We reformulate Eq. (1a) into an equivalent form,

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \Lambda \frac{1}{\rho} \tilde{\mathbf{J}} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla P + \frac{\mu}{\rho} \nabla^2 \mathbf{u} + \frac{1}{\rho} \nabla \mu \cdot \mathbf{D}(\mathbf{u}) - \frac{\lambda}{\rho} \nabla^2 \phi \nabla \phi + \frac{1}{\rho} \mathbf{f}(\mathbf{x}, t),$$
(19)

where

$$P = p + \frac{\lambda}{2} \nabla \phi \cdot \nabla \phi$$

is an auxiliary pressure, and will also be loosely referred to as the pressure where no confusion arises. We have included a constant Λ in the $\tilde{\mathbf{J}} \cdot \nabla \mathbf{u}$ term so that Eq. (19) can apply to both types of phase field models where the $\tilde{\mathbf{J}} \cdot \nabla \mathbf{u}$ term is present, such as in the system (1a)–(1c), or is absent, such as in those of [14,4,18,30,10]. Specifically,

$$\Lambda = \begin{cases} 1, & \text{for phase-field models in which } \tilde{\mathbf{J}} \cdot \nabla \mathbf{u} \text{ term is present,} \\ 0, & \text{for phase-field models in which } \tilde{\mathbf{J}} \cdot \nabla \mathbf{u} \text{ term is absent.} \end{cases}$$
(20)

Accordingly, the boundary condition (10) is reformulated into

$$-P\mathbf{n} + \mu \mathbf{n} \cdot \mathbf{D}(\mathbf{u}) - \lambda F(\phi)\mathbf{n} - \left[\frac{1}{2}\rho|\mathbf{u}|^2\Theta_0(\mathbf{n}\cdot\mathbf{u})\right]\mathbf{n} = \mathbf{f}_b(\mathbf{x},t), \quad \text{on } \partial\Omega_o.$$
(21)

We use the constant Λ introduced above to consolidate the boundary conditions (9a) and (17) into a single form applicable to both types of phase field models,

$$-\lambda \left[\nabla^2 \phi - h(\phi)\right] + \Lambda \frac{1}{4} (\rho_1 - \rho_2) |\mathbf{u}|^2 = g_d(\mathbf{x}, t), \quad \text{on } \partial \Omega_d^\phi.$$
⁽²²⁾

We also combine the boundary conditions (7a) and (11a) into a compact single equation

$$\mathbf{n} \cdot \nabla \left[\nabla^2 \phi - h(\phi) \right] = g_c(\mathbf{x}, t), \quad \text{on } \partial \Omega_w^\phi \cup \partial \Omega_o,$$
(23)

where

$$g_{c}(\mathbf{x},t) = \begin{cases} g_{w}(\mathbf{x},t), & \text{on } \partial \Omega_{w}^{\phi}, \\ g_{o}(\mathbf{x},t), & \text{on } \partial \Omega_{o}, \end{cases}$$
(24)

and in actual simulations g_c will be set to zero.

We next present an algorithm for solving the system consisting of Eqs. (19), (1b)–(1c), and boundary conditions (6), (21), (22), (9b), (23), (7b), and (11b). Let $(\mathbf{u}^n, P^n, \phi^n)$ denote the velocity, pressure, and phase field function at time step n, respectively. To compute these variables at time step (n + 1), we successively solve for the phase field function, pressure and velocity in a *de-coupled* fashion as follows:

For phase field function ϕ^{n+1}

$$\frac{\gamma_0 \phi^{n+1} - \hat{\phi}}{\Delta t} + \mathbf{u}^{*,n+1} \cdot \nabla \phi^{*,n+1} = -\lambda \gamma_1 \nabla^2 \bigg[\nabla^2 \phi^{n+1} - \frac{S}{\eta^2} (\phi^{n+1} - \phi^{*,n+1}) - h(\phi^{*,n+1}) \bigg] + g^{n+1},$$
(25a)

$$-\lambda \left[\nabla^2 \phi^{n+1} - h(\phi^{n+1})\right] + \Lambda \frac{1}{2}(\rho_1 - \rho_2) \left| \mathbf{u}^{n+1} \right|^2 = g_d^{n+1}, \quad \text{on } \partial \Omega_d^{\phi},$$
(25b)

$$\phi^{n+1} = \phi_b^{n+1}, \quad \text{on } \partial \Omega_d^{\phi}, \tag{25c}$$

$$\mathbf{n} \cdot \nabla \left[\nabla^2 \phi^{n+1} - \frac{S}{\eta^2} (\phi^{n+1} - \phi^{*,n+1}) - h(\phi^{*,n+1}) \right] = g_c^{n+1}, \quad \text{on } \partial \Omega_w^\phi \cup \partial \Omega_o,$$
(25d)

$$-D_{w}\left(\frac{\partial\phi}{\partial t}\Big|^{*,n+1} + \mathbf{u}^{*,n+1} \cdot \nabla\phi^{*,n+1}\right) = \mathbf{n} \cdot \nabla\phi^{n+1} + \frac{1}{\lambda}f'_{w}(\phi^{*,n+1}) + g_{e}^{n+1}, \quad \text{on } \partial\Omega_{w}^{\phi}, \tag{25e}$$

$$-D_{w}\left(\frac{\gamma_{0}\phi^{n+1}-\hat{\phi}}{\Delta t}+\mathbf{u}^{*,n+1}\cdot\nabla\phi^{*,n+1}\right)=\mathbf{n}\cdot\nabla\phi^{n+1}+\frac{1}{\lambda}f_{w}'(\phi^{*,n+1})+g_{e}^{n+1},\quad\text{on }\partial\Omega_{w}^{\phi},\tag{25f}$$

$$\mathbf{n} \cdot \nabla \phi^{n+1} = -D_0 \frac{\partial \phi}{\partial t} \Big|_{a}^{*,n+1} + g_a^{n+1}, \quad \text{on } \partial \Omega_0,$$
(25g)

$$\mathbf{n} \cdot \nabla \phi^{n+1} = -D_0 \frac{\gamma_0 \phi^{n+1} - \hat{\phi}}{\Delta t} + g_a^{n+1}, \quad \text{on } \partial \Omega_o.$$
(25h)

For pressure P^{n+1}

$$\frac{\gamma_{0}\tilde{\mathbf{u}}^{n+1}-\hat{\mathbf{u}}}{\Delta t} + \frac{1}{\rho_{0}}\nabla P^{n+1} = -\mathbf{N}(\mathbf{u}^{n}) - \Lambda \frac{1}{\rho^{n+1}}\tilde{\mathbf{J}}^{n+1} \cdot \nabla \mathbf{u}^{n} + \left(\frac{1}{\rho_{0}} - \frac{1}{\rho^{n+1}}\right)\nabla P^{n} - \frac{\mu^{n+1}}{\rho^{n+1}}\nabla \times \nabla \times \mathbf{u}^{n} + \frac{1}{\rho^{n+1}}\nabla \mu^{n+1} \cdot \mathbf{D}(\mathbf{u}^{n}) - \frac{\lambda}{\rho^{n+1}}\nabla^{2}\phi^{n+1}\nabla \phi^{n+1} + \frac{1}{\rho^{n+1}}\mathbf{f}^{n+1},$$
(26a)

$$\nabla \cdot \tilde{\mathbf{u}}^{n+1} = \mathbf{0},\tag{26b}$$

$$\mathbf{n} \cdot \tilde{\mathbf{u}}^{n+1} = \mathbf{n} \cdot \mathbf{w}^{n+1}, \quad \text{on } \partial \Omega_d^u, \tag{26c}$$

$$P^{n+1} = \mu^{n+1} \mathbf{n} \cdot \mathbf{D}(\mathbf{u}^{*,n+1}) \cdot \mathbf{n} - \lambda F(\phi^{n+1}) - \frac{1}{2} \rho^{n+1} |\mathbf{u}^{*,n+1}|^2 \Theta_0^{*,n+1} - \mathbf{f}_b^{n+1} \cdot \mathbf{n}, \quad \text{on } \partial \Omega_o.$$
(26d)

For velocity \mathbf{u}^{n+1}

 $\mathbf{u}^{n+1} = \mathbf{w}^{n+1}, \quad \text{on } \partial \Omega_d^u,$

$$\frac{\gamma_{0}\mathbf{u}^{n+1} - \gamma_{0}\tilde{\mathbf{u}}^{n+1}}{\Delta t} - \nu_{m}\nabla^{2}\mathbf{u}^{n+1} = -\mathbf{N}(\mathbf{u}^{*,n+1}) + \mathbf{N}(\mathbf{u}^{n}) + \nu_{m}\nabla\times\nabla\times\mathbf{u}^{*,n+1}$$
$$-\Lambda\frac{1}{\rho^{n+1}}\tilde{\mathbf{J}}^{n+1} \cdot (\nabla\mathbf{u}^{*,n+1} - \nabla\mathbf{u}^{n})$$
$$+ \left(\frac{1}{\rho_{0}} - \frac{1}{\rho^{n+1}}\right)\nabla(P^{n+1} - P^{n}) - \frac{\mu^{n+1}}{\rho^{n+1}}\nabla\times\nabla\times(\mathbf{u}^{*,n+1} - \mathbf{u}^{n})$$
$$+ \frac{1}{\rho^{n+1}}\nabla\mu^{n+1} \cdot [\mathbf{D}(\mathbf{u}^{*,n+1}) - \mathbf{D}(\mathbf{u}^{n})], \qquad (27a)$$

(27b)

$$\mathbf{n} \cdot \mathbf{D}(\mathbf{u}^{n+1}) = \left(1 - \frac{\mu^{n+1}}{\mu_0}\right) \mathbf{n} \cdot \mathbf{D}(\mathbf{u}^{*,n+1}) + \frac{1}{\mu_0} \left[P^{n+1}\mathbf{n} + \lambda F(\phi^{n+1})\mathbf{n} + \mathbf{f}_b^{n+1} + \left(\frac{1}{2}\rho^{n+1}|\mathbf{u}^{*,n+1}|^2\Theta_0^{*,n+1}\right)\mathbf{n} - \mu_0(\nabla \cdot \mathbf{u}^{*,n+1})\mathbf{n}\right], \quad \text{on } \partial\Omega_o,$$
(27c)

$$\mathbf{n} \cdot \nabla \mathbf{u}^{n+1} = \mathbf{n} \cdot \mathbf{D} (\mathbf{u}^{n+1}) - \mathbf{n} \cdot (\nabla \mathbf{u}^{*,n+1})^T, \quad \text{on } \partial \Omega_o.$$
(27d)

The meanings of the symbols involved in the above equations are as follows. Let χ denote a generic variable. Then χ^n denotes χ at time step n. $\chi^{*,n+1}$ denotes a *J*-th order explicit approximation, where J = 1 or 2 denotes the order of temporal accuracy of scheme, of χ at time step (n + 1) as follows,

$$\chi^{*,n+1} = \begin{cases} \chi^n, & \text{if } J = 1\\ 2\chi^n - \chi^{n-1}, & \text{if } J = 2. \end{cases}$$
(28)

In (25a), (25f), (25h), and (26a) the expression $\frac{1}{\Delta t}(\gamma_0\chi^{n+1} - \hat{\chi})$ represents an approximation of the time derivative $\frac{\partial \chi}{\partial t}$ at time step (n + 1) using the *J*-th order backward differentiation formula, where Δt is the time step size and γ_0 and $\hat{\chi}$ are given by

$$\hat{\chi} = \begin{cases} \chi^n, & \text{if } J = 1\\ 2\chi^n - \frac{1}{2}\chi^{n-1}, & \text{if } J = 2, \end{cases} \qquad \gamma_0 = \begin{cases} 1, & \text{if } J = 1\\ \frac{3}{2}, & \text{if } J = 2. \end{cases}$$
(29)

In (25e) and (25g) the expression $\frac{\partial \chi}{\partial t}|^{*,n+1}$ denotes a *J*-th order explicit approximation of $\frac{\partial \chi}{\partial t}$ at time step (n+1) as follows,

$$\frac{\partial \chi}{\partial t}\Big|^{*,n+1} = \begin{cases} \frac{1}{\Delta t} (\chi^n - \chi^{n-1}), & \text{if } J = 1\\ \frac{1}{\Delta t} (\frac{5}{2} \chi^n - 4 \chi^{n-1} + \frac{3}{2} \chi^{n-2}), & \text{if } J = 2. \end{cases}$$
(30)

n is the outward-pointing unit vector normal to the domain boundary $\partial \Omega$. **N**(**u**) = **u** · ∇ **u** denotes the nonlinear convection term. $\Theta_0^{*,n+1} = \Theta_0(\mathbf{n} \cdot \mathbf{u}^{*,n+1})$, where the function Θ_0 is defined in (12). The auxiliary velocity, $\tilde{\mathbf{u}}^{n+1}$, is an approximation of \mathbf{u}^{n+1} .

In (25a) S is a chosen constant that satisfies the condition

$$S \ge \eta^2 \sqrt{\frac{4\gamma_0}{\lambda\gamma_1 \Delta t}}.$$
(31)

 ρ_0 is a chosen constant that satisfies the condition

$$0 < \rho_0 \leqslant \min(\rho_1, \rho_2). \tag{32}$$

 v_m is a chosen constant that satisfies the condition

$$\nu_m \ge \frac{1}{2} \left(\frac{\mu_1}{\rho_1} + \frac{\mu_2}{\rho_2} \right). \tag{33}$$

The derivation of the condition (31) and the importance of the conditions (32) and (33) have been discussed in detail in [10] and [7]. In (26a) and (27a),

$$\tilde{\mathbf{J}}^{n+1} = \frac{1}{2} (\rho_1 - \rho_2) \lambda \gamma_1 \nabla \left[\nabla^2 \phi^{n+1} - \frac{S}{\eta^2} (\phi^{n+1} - \phi^{*,n+1}) - h(\phi^{*,n+1}) \right]$$
(34)

is an approximation of $\tilde{\mathbf{J}}$ at time step (n + 1).

 μ_0 in Eq. (27c) is a chosen constant that satisfies

$$\mu_0 > \min(\mu_1, \mu_2) \quad \text{if } \mu_1 \neq \mu_2, \quad \text{and} \quad \mu_0 = \mu_1 = \mu_2 \quad \text{if } \mu_1 = \mu_2.$$
 (35)

From numerical simulations it is observed that the scheme is unstable if $\mu_0 \leq \min(\mu_1, \mu_2)$ when $\mu_1 \neq \mu_2$.

The density ρ^{n+1} and viscosity μ^{n+1} involved in Eqs. (26a), (26d), (27a) and (27c) are computed from Eq. (5), once ϕ^{n+1} is known, with an exception for very large (or conversely very small) density ratios (ρ_2/ρ_1 or ρ_1/ρ_2). For very large (or conversely very small) density ratios (μ^{n+1} and μ^{n+1} as follows,

$$\rho = \frac{1}{2}(\rho_1 + \rho_2) + \frac{1}{2}(\rho_1 - \rho_2)\tilde{\phi}, \qquad \mu = \frac{1}{2}(\mu_1 + \mu_2) + \frac{1}{2}(\mu_1 - \mu_2)\tilde{\phi}, \qquad \tilde{\phi} = \begin{cases} \phi, & \text{if } |\phi| \le 1\\ \text{sign}(\phi), & \text{if } |\phi| > 1. \end{cases}$$
(36)

The need for using (36) to compute ρ^{n+1} and μ^{n+1} at large density ratios has been discussed in [10]. Basically, the interplay between the mass conservation and the energy minimization inherent in the dynamics of the Cahn-Hilliard equation (1c)

tends to induce a slight shift of the phase field function in the bulk phases [31], which may cause the numerically-computed phase field function to go slightly out of range (i.e. [-1, 1]) at certain points in the domain. This at very large (or conversely very small) density ratios can produce un-physical negative density/viscosity values at those points and cause numerical difficulties.

Let us first comment on the numerical treatment of the outflow boundary condition (21) in the above algorithm. In the pressure step, we impose a Dirichlet condition (26d) for the pressure P^{n+1} on the outflow boundary $\partial \Omega_o$. This pressure Dirichlet condition is obtained by taking the inner product between **n** and the outflow boundary condition (21) and by treating the velocity **u** explicitly. In the velocity step, we impose a discrete Neumann-type condition (27d) for **u**ⁿ⁺¹ on the outflow boundary $\partial \Omega_o$. In this velocity Neumann condition, the term **n** · **D**(**u**ⁿ⁺¹) is approximated using Eq. (27c), which largely stems from the outflow boundary condition (21) but contains two key constructions:

• The particular forms of (27c) for those terms involving the constant μ_0 . The introduction of the constant μ_0 for treating the variable dynamic viscosity μ^{n+1} in the outflow boundary condition, and these particular algorithmic forms, are critical to the stability of the scheme. We observe that, owing to the variable viscosity μ^{n+1} , the following alternative and straightforward treatment of the boundary condition (21)

$$\mathbf{n} \cdot \mathbf{D}(\mathbf{u}^{n+1}) = \frac{1}{\mu^{n+1}} \left[P^{n+1} \mathbf{n} + \lambda F(\phi^{n+1}) \mathbf{n} + \mathbf{f}_b^{n+1} + \left(\frac{1}{2} \rho^{n+1} |\mathbf{u}^{*,n+1}|^2 \Theta_0^{*,n+1} \right) \mathbf{n} - \mu^{n+1} (\nabla \cdot \mathbf{u}^{*,n+1}) \mathbf{n} \right]$$
(37)

is unstable when the viscosity ratio of the two fluids $(\mu_2/\mu_1 \text{ or } \mu_1/\mu_2)$ is large or conversely small (beyond ~20 or below $\sim \frac{1}{20}$).

• The extra term $(\nabla \cdot \mathbf{u})\mathbf{n}$ in (27c), which prevents a numerical locking on the outflow boundary $\partial \Omega_o$ for time-dependent problems. If this term is absent and $\mathbf{f}_b = 0$, and further if the two fluids have matched dynamic viscosities, then by combining Eqs. (26d) and (27c) one can show that $\mathbf{n} \cdot \mathbf{D}(\mathbf{u}^{n+1}) = \mathbf{n} \cdot \mathbf{D}(\mathbf{u}^n) = \cdots = \mathbf{n} \cdot \mathbf{D}(\mathbf{u}^1) = [\mathbf{n} \cdot \mathbf{D}(\mathbf{u}^0) \cdot \mathbf{n}]\mathbf{n}$, leading to a numerical locking on the outflow boundary $\partial \Omega_o$ for time-dependent problems.

We would also like to point out that the approximation form (27d) for $\mathbf{n} \cdot \nabla \mathbf{u}^{n+1}$ on $\partial \Omega_0$ is important. An alternative approximation, $\mathbf{n} \cdot \nabla \mathbf{u}^{n+1} = \frac{1}{2} \mathbf{n} \cdot \mathbf{D}(\mathbf{u}^{n+1}) + \frac{1}{2} \boldsymbol{\omega}^{*,n+1} \times \mathbf{n}$, where $\boldsymbol{\omega} = \nabla \times \mathbf{u}$ is the vorticity, is observed to lead to an instability in flow simulations.

We next comment on the numerical treatments of the outflow boundary conditions for the phase field function, (11a) (or equivalently (23)) and (11b). The main issue lies in the treatment of the term $\frac{\partial \phi}{\partial t}$ in (11b). Our goal is two-fold: (1) the treatment should allow for the re-formulation of the 4th-order Cahn-Hilliard equation into two *de-coupled* Helmholtz type equations after discretization (see Section 2.3), and (2) it should be stable when D_0 becomes large. A straightforward treatment of this term (implicit or explicit) leads to two difficulties. It will either result in, when solving the 4th-order Cahn-Hilliard equation, two Helmholtz type equations that are coupled with each other through the outflow boundary, or it will be unstable unless D_0 is extremely small. The dilemma here is similar in nature to that encountered in [7] for discretization of the dynamic contact-angle boundary conditions. The numerical treatments here for the phase-field outflow boundary conditions. The explicit treatment of $\frac{\partial \phi}{\partial t}$ in (25g), and the implicit treatment of this term in (25h), will be employed at different stages of the implementation (see Section 2.3). This allows for the re-formulation of the semi-discretized 4th-order Cahn-Hilliard equation into two Helmholtz-type equations that are completely de-coupled from each other, and simultaneously it can deal with large D_0 values.

Another issue related to the phase-field outflow boundary condition is the numerical treatment of the condition (23) on the outflow boundary (or on solid walls). A key point lies in the incorporation of the extra term, $\frac{S}{\eta^2}(\phi^{n+1} - \phi^{*,n+1})$, in the discrete form (25d). Absence of this extra term in the discrete form results in a catastrophic loss of mass for one of the fluid phases in simulations.

The numerical treatment of the additional boundary condition, (9a), for the phase-field Dirichlet boundary $\partial \Omega_d^{\phi}$ is quite straightforward. In the current discretization of this condition, (25b), note that both \mathbf{u}^{n+1} and ϕ^{n+1} are known on $\partial \Omega_d^{\phi}$, due to Eqs. (25c) and (27b). The discrete form (25b) will give rise to a Dirichlet type condition for an auxiliary phase field variable; see Section 2.3.

We would like to mention that the numerical treatments of the dynamic contact-angle boundary conditions on $\partial \Omega_{w}^{\phi}$, (25e) and (25f), have followed the ideas developed in [7]; see [7] for details.

Let us next briefly comment on the discretization of the system of governing equations consisting of (19), (1b) and (1c). The discrete formulations for these equations ((25a), (26a) and (27a)) employ a strategy that we developed in [10]. Overall, the computation for the phase field function ϕ^{n+1} is de-coupled from those for the pressure and the velocity due to the explicit treatment of the convection terms in the phase field equation (1c) and in the dynamic contact-angle boundary condition (7b). The computations for the pressure P^{n+1} and the velocity \mathbf{u}^{n+1} are further de-coupled by a rotational velocity-correction type strategy [13,9]. There are three key constructions in these discrete formulations:

• The reformulation of the pressure term

$$\frac{1}{\rho}\nabla P \approx \frac{1}{\rho_0}\nabla P + \left(\frac{1}{\rho} - \frac{1}{\rho_0}\right)\nabla P^*,\tag{38}$$

where ρ_0 is a constant satisfying condition (32) and P^* is an explicit approximation of P. By treating the term $\frac{1}{\rho_0} \nabla P$ implicitly and the ∇P^* term explicitly, this reformulation leads to a *constant* and *time-independent* coefficient matrix for the linear algebraic system for the pressure P^{n+1} . The condition (32) on ρ_0 is critical for the stability of the scheme [7]. • The reformulation of the viscous term

$$\frac{\mu}{\rho} \nabla^2 \mathbf{u} \approx \nu_m \nabla^2 \mathbf{u} - \left(\frac{\mu}{\rho} - \nu_m\right) \nabla \times \nabla \times \mathbf{u}^*,\tag{39}$$

where v_m is a constant satisfying condition (33) and \mathbf{u}^* is an explicit approximation of \mathbf{u} . This reformulation leads to a *constant* and *time-independent* coefficient matrix for the linear algebraic system for the velocity \mathbf{u}^{n+1} . See [4,24] for the use of similar strategies by other researchers. • The additional term $\frac{S}{\eta^2}(\phi^{n+1} - \phi^{*,n+1})$ in (25a), where *S* is a constant satisfying the condition (31). This term enables

a reformulation of the 4th-order phase field equation (1c) into two nominally-decoupled Helmholtz-type equations. Furthermore, if the boundary conditions are numerically treated appropriately, the two nominally-decoupled Helmholtz-type equations can be completely decoupled [7]. This strategy allows for a successful treatment of the large spatial order of the phase field equation using C^0 spectral elements or finite elements. See [30,26] for the use of this strategy by other researchers.

2.3. Implementation

We employ C^0 spectral elements [16,33] for spatial discretizations in the current paper. In this subsection we concentrate on the implementation of the algorithm, (25a)-(27d), using C^0 spectral elements or finite elements. We will also briefly discuss the implementation using finite difference-type methods.

We will reformulate the algorithm in order to facilitate the implementation using C^0 spectral elements or finite elements. The reformulation will eliminate the auxiliary velocity $\tilde{\mathbf{u}}^{n+1}$, and appropriately treat the terms involving derivatives of order two or higher (e.g. $\nabla \times \nabla \times \mathbf{u}$, $\nabla^2 \phi \nabla \phi$, $\nabla^2 (\nabla^2 \phi)$), which cannot be computed directly using C^0 elements.

Let us first consider the solution for the phase field function ϕ^{n+1} . We re-write (25a) into

$$\nabla^2 \left[\nabla^2 \phi^{n+1} - \frac{S}{\eta^2} \phi^{n+1} \right] + \frac{\gamma_0}{\lambda \gamma_1 \Delta t} \phi^{n+1} = Q = Q_1 + \nabla^2 Q_2, \tag{40}$$

where

$$Q_{1} = \frac{1}{\lambda \gamma_{1}} \left[g^{n+1} - \mathbf{u}^{*,n+1} \cdot \nabla \phi^{*,n+1} + \frac{\hat{\phi}}{\Delta t} \right]$$

$$Q_{2} = h(\phi^{*,n+1}) - \frac{S}{n^{2}} \phi^{*,n+1}.$$
(41)

Eq. (40) can be reformulated into (see [30,10]):

$$\nabla^2 \psi^{n+1} - \left(\alpha + \frac{S}{\eta^2}\right) \psi^{n+1} = Q,$$
(42a)

$$\nabla^2 \phi^{n+1} + \alpha \phi^{n+1} = \psi^{n+1}.$$
(42b)

 $=\psi$

where ψ^{n+1} is an auxiliary variable and α is a constant given by

$$\alpha = -\frac{S}{2\eta^2} \left[1 - \sqrt{1 - \frac{4\gamma_0}{\lambda\gamma_1 \Delta t} \left(\frac{\eta^2}{S}\right)^2} \right].$$
(43)

Note that $\alpha < 0$ and $\alpha + \frac{S}{\eta^2} > 0$ under the condition (31). One can also note that (42a) and (42b) are *nominally decoupled*. If appropriate boundary conditions for ψ^{n+1} and ϕ^{n+1} are available, to compute ϕ^{n+1} from (25a) one can successively solve (42a) for ψ^{n+1} , and then solve (42b) for ϕ^{n+1} . Let $H^1_{\phi 0}(\Omega) = \{ v \in H^1(\Omega) : v |_{\partial \Omega^{\phi}_d} = 0 \}$, and $\varpi \in H^1_{\phi 0}(\Omega)$ denote the test function. Taking the L^2 inner product between

(42a) and ϖ , we have the weak form about ψ^{n+1} ,

$$\int_{\Omega} \nabla \psi^{n+1} \cdot \nabla \varpi + \left(\alpha + \frac{S}{\eta^2}\right) \int_{\Omega} \psi^{n+1} \varpi$$

$$= -\int_{\Omega} Q_1 \varpi + \int_{\Omega} \nabla Q_2 \cdot \nabla \varpi + \int_{\partial \Omega_w^{\phi} \cup \partial \Omega_0} \left(-\mathbf{n} \cdot \nabla Q_2 + \mathbf{n} \cdot \nabla \psi^{n+1}\right) \varpi \quad \forall \varpi \in H^1_{\phi 0}(\Omega), \tag{44}$$

where we have used integration by part, and the fact that $\int_{\partial \Omega_{d}^{\phi}} (-\mathbf{n} \cdot \nabla Q_{2} + \mathbf{n} \cdot \nabla \psi^{n+1}) \boldsymbol{\varpi} = 0$, because $\boldsymbol{\varpi} \in H^{1}_{\phi 0}(\Omega)$.

Let $\vartheta \in H^1_{\phi 0}(\Omega)$ denote the test function. Taking the L^2 inner product between (42b) and ϑ , we have the weak form about ϕ^{n+1} ,

$$\int_{\Omega} \nabla \phi^{n+1} \cdot \nabla \vartheta - \alpha \int_{\Omega} \phi^{n+1} \vartheta = -\int_{\Omega} \psi^{n+1} \vartheta + \int_{\partial \Omega_{w}^{\phi}} \mathbf{n} \cdot \nabla \phi^{n+1} \vartheta + \int_{\partial \Omega_{o}} \mathbf{n} \cdot \nabla \phi^{n+1} \vartheta, \quad \forall \vartheta \in H^{1}_{\phi 0}(\Omega),$$
(45)

where we have used integration by part and the fact that $\int_{\partial \Omega_{\tau}^{\phi}} \mathbf{n} \cdot \nabla \phi^{n+1} \vartheta = 0$ because $\vartheta \in H^{1}_{\phi 0}(\Omega)$.

The discrete boundary condition (25d) can be written as

$$\mathbf{n} \cdot \nabla \psi^{n+1} - \mathbf{n} \cdot \nabla Q_2 = \left(\alpha + \frac{S}{\eta^2}\right) \mathbf{n} \cdot \nabla \phi^{n+1} + g_c^{n+1}, \quad \text{on } \partial \Omega_w^\phi \cup \partial \Omega_o, \tag{46}$$

where we have used Eq. (41), and the relation $\nabla^2 \phi^{n+1} = \psi^{n+1} - \alpha \phi^{n+1}$ due to (42b). In light of (46), we can transform (44) into

$$\int_{\Omega} \nabla \psi^{n+1} \cdot \nabla \overline{\omega} + \left(\alpha + \frac{S}{\eta^2}\right) \int_{\Omega} \psi^{n+1} \overline{\omega}$$

$$= -\int_{\Omega} Q_1 \overline{\omega} + \int_{\Omega} \nabla Q_2 \cdot \nabla \overline{\omega} + \int_{\partial \Omega_w^{\phi} \cup \partial \Omega_0} g_c^{n+1} \overline{\omega} + \left(\alpha + \frac{S}{\eta^2}\right) \left[\int_{\partial \Omega_w^{\phi}} \mathbf{n} \cdot \nabla \phi^{n+1} \overline{\omega} + \int_{\partial \Omega_0} \mathbf{n} \cdot \nabla \phi^{n+1} \overline{\omega}\right],$$

$$\forall \overline{\omega} \in H^1_{\phi 0}(\Omega). \tag{47}$$

One can note that the weak form for ψ^{n+1} , (47), and the weak form for ϕ^{n+1} , (45), are now coupled with each other due to the surface integral terms on $\partial \Omega_w^{\phi}$ and $\partial \Omega_o$ involving $\mathbf{n} \cdot \nabla \phi^{n+1}$.

We now employ an idea developed in [7]. On wall boundary $\partial \Omega_w^{\phi}$, we approximate the $\mathbf{n} \cdot \nabla \phi^{n+1}$ term in Eq. (47) using the discrete dynamic contact-angle condition (25e), and approximate the $\mathbf{n} \cdot \nabla \phi^{n+1}$ term in Eq. (45) using a different discrete dynamic contact-angle condition (25f). Similarly, on the outflow boundary $\partial \Omega_o$, we approximate the $\mathbf{n} \cdot \nabla \phi^{n+1}$ term in Eq. (45) using a different discrete outflow condition (25g), and approximate the $\mathbf{n} \cdot \nabla \phi^{n+1}$ term in Eq. (45) using a different discrete outflow condition (25g), and approximate the $\mathbf{n} \cdot \nabla \phi^{n+1}$ term in Eq. (45) using a different discrete outflow condition (25h). This will de-couple the computations for ψ^{n+1} and ϕ^{n+1} , and simultaneously can deal with large values for D_w and D_o . Therefore we obtain the final weak form for the ψ^{n+1} equation,

$$\int_{\Omega} \nabla \psi^{n+1} \cdot \nabla \varpi + \left(\alpha + \frac{S}{\eta^2}\right) \int_{\Omega} \psi^{n+1} \varpi$$

$$= -\int_{\Omega} Q_1 \varpi + \int_{\Omega} \nabla Q_2 \cdot \nabla \varpi + \left(\alpha + \frac{S}{\eta^2}\right) \int_{\partial \Omega_w^{\phi}} \left[-D_w \left(\frac{\partial \phi}{\partial t}\right)^{*,n+1} + \mathbf{u}^{*,n+1} \cdot \nabla \phi^{*,n+1} \right) - \frac{1}{\lambda} f'_w (\phi^{*,n+1}) - g_e^{n+1} \right] \varpi$$

$$+ \left(\alpha + \frac{S}{\eta^2}\right) \int_{\partial \Omega_o} \left(-D_0 \frac{\partial \phi}{\partial t} \right|^{*,n+1} + g_a^{n+1} \right) \varpi + \int_{\partial \Omega_w^{\phi}} g_w^{n+1} \varpi + \int_{\partial \Omega_o} g_o^{n+1} \varpi, \quad \forall \varpi \in H^1_{\phi 0}(\Omega), \quad (48)$$

where $\frac{\partial \phi}{\partial t}|^{*,n+1}$ is given by (30), and we have used expression (24). We also obtain the final weak form for the ϕ^{n+1} equation,

$$\int_{\Omega} \nabla \phi^{n+1} \cdot \nabla \vartheta - \alpha \int_{\Omega} \phi^{n+1} \vartheta + \frac{\gamma_0 D_w}{\Delta t} \int_{\partial \Omega_w^{\phi}} \phi^{n+1} \vartheta + \frac{\gamma_0 D_0}{\Delta t} \int_{\partial \Omega_0} \phi^{n+1} \vartheta$$

$$= -\int_{\Omega} \psi^{n+1} \vartheta + \int_{\partial \Omega_w^{\phi}} \left[-D_w \left(-\frac{\hat{\phi}}{\Delta t} + \mathbf{u}^{*,n+1} \cdot \nabla \phi^{*,n+1} \right) - \frac{1}{\lambda} f'_w (\phi^{*,n+1}) - \mathbf{g}_e^{n+1} \right] \vartheta$$

$$+ \int_{\partial \Omega_0} \left(\frac{D_0}{\Delta t} \hat{\phi} + \mathbf{g}_a^{n+1} \right) \vartheta, \quad \forall \vartheta \in H^1_{\phi 0}(\Omega).$$
(49)

One can observe that the two equations, (48) and (49), are both Helmholtz-type equations in weak forms, and that they are completely decoupled from each other.

Finally, the boundary condition (25b) can be transformed into, in light of Eq. (42b),

$$\psi^{n+1} = \alpha \phi_b^{n+1} + h(\phi_b^{n+1}) + \Lambda \frac{1}{4\lambda} (\rho_1 - \rho_2) |\mathbf{w}^{n+1}|^2 - \frac{1}{\lambda} g_d^{n+1}, \quad \text{on } \partial \Omega_d^{\phi},$$
(50)

where we have used (25c) and (27b), and the assumption $\partial \Omega_d^u = \partial \Omega_d^\phi \cup \partial \Omega_w^\phi$. This is a Dirichlet type condition for ψ^{n+1} .

Therefore, in order to compute ϕ^{n+1} , we first solve Eq. (48) for ψ^{n+1} , together with the Dirichlet condition (50) on $\partial \Omega_d^{\phi}$. Then we solve Eq. (49) for ϕ^{n+1} , together with the Dirichlet condition (25c) on $\partial \Omega_d^{\phi}$. Let us now consider how to compute P^{n+1} and \mathbf{u}^{n+1} , assuming that ϕ^{n+1} and ψ^{n+1} are known. Re-write (26a) as

$$\frac{\gamma_0}{\Delta t}\tilde{\mathbf{u}}^{n+1} + \frac{1}{\rho_0}\nabla P^{n+1} = \mathbf{G}^{n+1} - \frac{\mu^{n+1}}{\rho^{n+1}}\nabla \times \boldsymbol{\omega}^n$$
(51)

where $\boldsymbol{\omega} = \nabla \times \mathbf{u}$ is the vorticity, and

$$\mathbf{G}^{n+1} = \frac{1}{\rho^{n+1}} \mathbf{f}^{n+1} + \frac{\hat{\mathbf{u}}}{\Delta t} - \mathbf{N}(\mathbf{u}^n) - \Lambda \frac{1}{\rho^{n+1}} \tilde{\mathbf{J}}^{n+1} \cdot \nabla \mathbf{u}^n + \left(\frac{1}{\rho_0} - \frac{1}{\rho^{n+1}}\right) \nabla P^n + \frac{1}{\rho^{n+1}} \nabla \mu^{n+1} \cdot \mathbf{D}(\mathbf{u}^n) - \frac{\lambda}{\rho^{n+1}} (\psi^{n+1} - \alpha \phi^{n+1}) \nabla \phi^{n+1},$$
(52)

$$\tilde{\mathbf{J}}^{n+1} = \frac{1}{2} (\rho_1 - \rho_2) \lambda \gamma_1 \nabla \left[\psi^{n+1} - \left(\alpha + \frac{S}{\eta^2} \right) \phi^{n+1} - Q_2 \right].$$
(53)

Note that in deriving the expressions (52) and (53) we have used Eq. (42b), and that Q_2 is given by (41).

Let $H_{p0}^1(\Omega) = \{v \in H^1(\Omega): v|_{\partial \Omega_0} = 0\}$, and $q \in H_{p0}^1(\Omega)$ denote the test function. Taking the L^2 inner product between (51) and ∇q , we have the weak form about the pressure P^{n+1}

$$\int_{\Omega} \nabla P^{n+1} \cdot \nabla q = \rho_0 \int_{\Omega} \left[\mathbf{G}^{n+1} + \nabla \left(\frac{\mu^{n+1}}{\rho^{n+1}} \right) \times \boldsymbol{\omega}^n \right] \cdot \nabla q - \rho_0 \int_{\partial \Omega_o} \frac{\mu^{n+1}}{\rho^{n+1}} \mathbf{n} \times \boldsymbol{\omega}^n \cdot \nabla q - \rho_0 \int_{\partial \Omega_d^u} \frac{\mu^{n+1}}{\rho^{n+1}} \mathbf{n} \times \boldsymbol{\omega}^n \cdot \nabla q - \frac{\gamma_0 \rho_0}{\Delta t} \int_{\partial \Omega_d^u} \mathbf{n} \cdot \mathbf{w}^{n+1} q, \quad \forall q \in H^1_{p0}(\Omega),$$
(54)

where we have used integration by part, Eqs. (26b) and (26c), the identity

$$\frac{\mu}{\rho} \nabla \times \boldsymbol{\omega} \cdot \nabla q = \nabla \cdot \left(\frac{\mu}{\rho} \boldsymbol{\omega} \times \nabla q\right) - \nabla \left(\frac{\mu}{\rho}\right) \times \boldsymbol{\omega} \cdot \nabla q,$$
(55)

and the fact that $\int_{\partial \Omega_0} \mathbf{n} \cdot \tilde{\mathbf{u}}^{n+1} q = 0$ because $q \in H^1_{p0}(\Omega)$. Eq. (54) is a Poisson type equation in weak form, whose RHS can be explicitly computed. This equation can be used for computing P^{n+1} .

Summing up Eqs. (27a) and (26a) and collecting the explicit terms to the RHS, one can get the following equation for n^{n+1}

$$\frac{\gamma_0}{\nu_m \Delta t} \mathbf{u}^{n+1} - \nabla^2 \mathbf{u}^{n+1} = \frac{1}{\nu_m} \mathbf{R}^{n+1} - \frac{1}{\nu_m} \left(\frac{\mu^{n+1}}{\rho^{n+1}} - \nu_m \right) \nabla \times \boldsymbol{\omega}^{*,n+1},\tag{56}$$

where

$$\mathbf{R}^{n+1} = \frac{1}{\rho^{n+1}} \mathbf{f}^{n+1} + \frac{\hat{u}}{\Delta t} - \mathbf{u}^{*,n+1} \cdot \nabla \mathbf{u}^{*,n+1} - \Lambda \frac{1}{\rho^{n+1}} \tilde{\mathbf{J}}^{n+1} \cdot \nabla \mathbf{u}^{*,n+1} - \frac{1}{\rho^{n+1}} \nabla P^{n+1} + \frac{1}{\rho^{n+1}} \nabla \mu^{n+1} \cdot \mathbf{D}(\mathbf{u}^{*,n+1}) - \frac{\lambda}{\rho^{n+1}} (\psi^{n+1} - \alpha \phi^{n+1}) \nabla \phi^{n+1}.$$
(57)

Let $H^1_{u0}(\Omega) = \{ v \in H^1(\Omega) : v |_{\partial \Omega^u_d} = 0 \}$ and $\varphi \in H^1_{u0}(\Omega)$ denote the test function. Taking the L^2 inner product between (56) and φ , we obtain the weak form about \mathbf{u}^{n+1}

$$\int_{\Omega} \nabla \varphi \cdot \nabla \mathbf{u}^{n+1} + \frac{\gamma_0}{\nu_m \Delta t} \int_{\Omega} \varphi \mathbf{u}^{n+1}$$
$$= \frac{1}{\nu_m} \int_{\Omega} \left[\mathbf{R}^{n+1} + \nabla \left(\frac{\mu^{n+1}}{\rho^{n+1}} \right) \times \boldsymbol{\omega}^{*,n+1} \right] \varphi$$
$$- \frac{1}{\nu_m} \int_{\Omega} \left(\frac{\mu^{n+1}}{\rho^{n+1}} - \nu_m \right) \boldsymbol{\omega}^{*,n+1} \times \nabla \varphi - \frac{1}{\nu_m} \int_{\partial \Omega_0} \left(\frac{\mu^{n+1}}{\rho^{n+1}} - \nu_m \right) \mathbf{n} \times \boldsymbol{\omega}^{*,n+1} \varphi$$

$$+ \int_{\partial \Omega_{0}} \left\{ \left(1 - \frac{\mu^{n+1}}{\mu_{0}} \right) \mathbf{n} \cdot \mathbf{D}(\mathbf{u}^{*,n+1}) + \frac{1}{\mu_{0}} \left[\left(P^{n+1} + \lambda F(\phi^{n+1}) \right) \mathbf{n} + \frac{1}{2} \rho^{n+1} |\mathbf{u}^{*,n+1}|^{2} \Theta_{0}^{*,n+1} \mathbf{n} + \mathbf{f}_{b}^{n+1} - \mu_{0} (\nabla \cdot \mathbf{u}^{*,n+1}) \mathbf{n} \right] - \mathbf{n} \cdot (\nabla \mathbf{u}^{*,n+1})^{T} \right\} \varphi, \quad \forall \varphi \in H_{u0}^{1}(\Omega),$$
(58)

where we have used integration by part, Eqs. (27d) and (27c), the identities (B denoting a scalar field function)

$$\begin{cases} \int_{\Omega} B\nabla \times \boldsymbol{\omega}\varphi = \int_{\partial\Omega} B\mathbf{n} \times \boldsymbol{\omega}\varphi - \int_{\Omega} \nabla B \times \boldsymbol{\omega}\varphi + \int_{\Omega} B\boldsymbol{\omega} \times \nabla\varphi; \\ \int_{\partial\Omega} B\mathbf{n} \times \boldsymbol{\omega}\varphi = \int_{\partial\Omega_{q}} B\mathbf{n} \times \boldsymbol{\omega}\varphi, \quad \forall \varphi \in H^{1}_{u0}(\Omega) \end{cases}$$
(59)

and the fact that $\int_{\partial \Omega_d^u} \mathbf{n} \cdot \nabla \mathbf{u}^{n+1} \varphi = 0$ because $\varphi \in H^1_{u0}(\Omega)$. Eq. (58) is a Helmholtz-type equation in weak form, and can be solved for \mathbf{u}^{n+1} .

One can note that Eqs. (48), (49), (54) and (58) involve no derivatives of order two or higher, and that they are already in weak forms. These equations can be directly discretized in space using C^0 spectral elements or finite elements.

The re-formulated algorithm therefore consists of the following procedure. Given $(\mathbf{u}^n, P^n, \phi^n)$, we successively compute ϕ^{n+1} , P^{n+1} , \mathbf{u}^{n+1} as follows:

- 1. Solve Eq. (48), together with the Dirichlet condition (50) on $\partial \Omega_d^{\phi}$, for ψ^{n+1} ;
- 2. Solve Eq. (49), together with the phase-field Dirichlet condition (25c) on $\partial \Omega_d^{\phi}$, for ϕ^{n+1} ;
- 3. Compute ρ^{n+1} and μ^{n+1} based on (5), or based on (36) in the case of large density ratios;
- 4. Compute $\tilde{\mathbf{I}}^{n+1}$ based on Eq. (53);
- 5. Solve Eq. (54), together with the pressure Dirichlet condition (26d) on $\partial \Omega_0$, for P^{n+1} ;
- 6. Solve Eq. (58), together with the velocity Dirichlet condition (27b) on $\partial \Omega_d^u$, for \mathbf{u}^{n+1} .

This algorithm has the following characteristics:

- The auxiliary velocity $\tilde{\mathbf{u}}^{n+1}$ is eliminated.
- The computations for different flow variables (ψ^{n+1} , ϕ^{n+1} , P^{n+1} , \mathbf{u}^{n+1}) are completely decoupled.
- The computations for different components of the velocity **u**ⁿ⁺¹ from Eq. (58) are completely decoupled.
 The linear algebraic systems for all flow variables (ψⁿ⁺¹, φⁿ⁺¹, Pⁿ⁺¹, **u**ⁿ⁺¹) involve only constant and time-independent coefficient matrices after spatial discretization. These coefficient matrices can be pre-computed during pre-processing.
- Only Helmholtz (including Poisson) type equations need to be solved within each time step.

We now briefly comment on imposing the pressure Dirichlet condition (26d) on the outflow boundary $\partial \Omega_0$ in step (5) of the reformulated algorithm. The pressure expression (26d) involves velocity derivatives due to the term containing D(u). Consequently, with C^0 spectral elements or finite elements, the pressure data computed directly from (26d) may not be continuous across the element boundaries on $\partial \Omega_{0}$. Therefore, we need to project the pressure data computed based on (26d) to the $H^1(\partial \Omega_0)$ space, and use the projected pressure data as the pressure Dirichlet condition. This projection amounts to the solution of a small linear algebraic system on the outflow boundary $\partial \Omega_0$, with the coefficient matrix being the mass matrix on $\partial \Omega_0$.

So far we have concentrated on the implementation of the algorithm using C^0 spectral elements (or finite elements), which have been used for spatial discretizations in the current paper. We next briefly discuss the implementation of the algorithm using finite difference-type methods.

Using finite-difference schemes, one can successively solve the Helmholtz equations (42a) and (42b) for ψ^{n+1} and ϕ^{n+1} , with the following boundary conditions. For the field function ψ^{n+1} , we impose the Dirichlet condition (50) on $\partial \Omega_{4}^{\phi}$, and the following conditions according to Eq. (46),

$$\mathbf{n} \cdot \nabla \psi^{n+1} = \left(\alpha + \frac{S}{\eta^2}\right) \left[-D_w \left(\frac{\partial \phi}{\partial t}\Big|^{*,n+1} + \mathbf{u}^{*,n+1} \cdot \nabla \phi^{*,n+1}\right) - \frac{1}{\lambda} f'_w (\phi^{*,n+1}) - g_e^{n+1} \right] \\ + \mathbf{n} \cdot \nabla Q_2 + g_w^{n+1}, \quad \text{on } \partial \Omega_w^{\phi}, \tag{60a}$$

$$\mathbf{n} \cdot \nabla \psi^{n+1} = \left(\alpha + \frac{S}{\eta^2}\right) \left(-D_0 \frac{\partial \phi}{\partial t}\Big|^{*,n+1} + g_a^{n+1}\right) + \mathbf{n} \cdot \nabla Q_2 + g_o^{n+1}, \quad \text{on } \partial \Omega_o, \tag{60b}$$

where we have used Eqs. (25e) and (25g). For the field function ϕ^{n+1} , we impose the conditions (25c), (25f) and (25h) to supplement Eq. (42b).

For pressure P^{n+1} , we take the divergence of Eq. (51) and obtain the Poisson equation

$$\nabla^2 P^{n+1} = \rho_0 \nabla \cdot \mathbf{G}^{n+1} - \rho_0 \nabla \left(\frac{\mu^{n+1}}{\rho^{n+1}}\right) \cdot \nabla \times \boldsymbol{\omega}^n,\tag{61}$$

Table 1

Non-dimensional physical parameters resulting from normalization of governing equations and boundary conditions.

$\rho^* = \frac{\rho_2}{\rho_1}$ (density ratio)	$Pe = \frac{U_0 \eta L}{\sigma \gamma_1}$ (Peclet number)
$\mu^* = \frac{\mu_2}{\mu_1}$ (viscosity ratio)	$We = \frac{\rho_1 U_0^2 L}{\sigma}$ (Weber number)
$C_n = \frac{\eta}{L}$ (Cahn number)	$D_w^* = D_w U_0$ (dynamic wall mobility)
$Re = \frac{\rho_1 U_0 L}{\mu_1}$ (Reynolds number)	$D_0^* = D_0 U_0$ (dynamic outflow mobility)
θ_s (static contact angle)	

where we have used Eq. (26b). Take the inner product between Eq. (51) and the directional vector **n** of $\partial \Omega_d^u$, and we get the following condition

$$\frac{\partial P^{n+1}}{\partial n} = \rho_0 \mathbf{n} \cdot \mathbf{G}^{n+1} - \rho_0 \frac{\mu^{n+1}}{\rho^{n+1}} \mathbf{n} \cdot \nabla \times \boldsymbol{\omega}^n - \frac{\gamma_0 \rho_0}{\Delta t} \mathbf{n} \cdot \mathbf{w}^{n+1}, \quad \text{on } \partial \Omega_d^u, \tag{62}$$

where we have used condition (26c). Therefore, the pressure P^{n+1} can be computed using finite-difference type methods by solving the Poisson equation (61), together with the pressure Neumann condition (62) on $\partial \Omega_d^u$ and the pressure Dirichlet condition (26d) on $\partial \Omega_o$.

Finally, for velocity \mathbf{u}^{n+1} one can solve the Helmholtz equation (56) using finite-difference type methods, together with the velocity Dirichlet condition (27b) on $\partial \Omega_d^u$ and the velocity Neumann condition (27d) on $\partial \Omega_0$, in which $\mathbf{n} \cdot \mathbf{D}(\mathbf{u}^{n+1})$ is given by (27c).

3. Representative numerical tests

In this section we consider several two-phase flow problems in two dimensions to demonstrate the capabilities of the boundary conditions and the numerical algorithm developed in Section 2. These problems involve two-phase outflow boundaries, inflow boundaries, as well as large viscosity ratios and large density ratios. We first demonstrate the spatial and temporal convergence rates of our algorithm using an analytic solution to the system. Then we consider the instability of an oil jet in water, which involves a large viscosity ratio. We will also consider an air jet in water, and the bubble motion across the open domain boundaries, which involves a large density ratio. Our phase field model and methods have previously been verified and validated by comparing with theory, physically exact solutions, as well as experimental data; see [10] and [7] for details.

3.1. Convergence rates

The goal of the first test is to demonstrate the temporal and spatial convergence rates of our algorithm from Section 2 for problems involving two-phase outflow boundaries.

Let us first briefly discuss the non-dimensionalization of the flow variables, the governing equations, and the boundary conditions. For a more detailed dimensional analysis, we refer to [7] (Section 3.1). We choose a characteristic length scale *L* and a characteristic velocity scale U_0 . Then we normalize all velocity variables by U_0 , all length variables by *L*, the time by L/U_0 , pressure by $\rho_1 U_0^2$, ψ introduced in (42a) and (42b) by $1/L^2$, the density variables by ρ_1 , and the dynamic viscosity variables by μ_1 . The normalization procedure leads to the set of non-dimensional physical parameters listed in Table 1. In addition, we normalize the numerical parameters v_m as $v_m^* = \frac{v_m}{\mu_1/\rho_1} \frac{1}{Re}$, ρ_0 as $\rho_0^* = \frac{\rho_0}{\rho_1}$, and μ_0 introduced in (27c) as $\mu_0^* = \frac{\mu_0}{\mu_1}$. Note that δ in (12) and *S* in (25a) are non-dimensional. Note also that the mixing energy density coefficient λ is normalized by $\lambda^* = \frac{\lambda}{\rho_1 U_0^2 L} = \frac{3}{2\sqrt{2}} \frac{C_n}{We}$ in light of Eq. (3). When gravity is considered in subsequent test problems, the non-dimensional Froude number will also be involved, $Fr = \frac{U_0}{\sqrt{g_r L}}$, where g_r is the gravitational acceleration. By default, the variables are all given in non-dimensional forms subsequently.

We consider the flow domain \overline{ABCD} shown in Fig. 1(a), which is defined by $\Omega = \{(x, y): 0 \le x \le 2, -1 \le y \le 1\}$, and the following analytic solution to the two-phase governing equations on Ω ,

$$u = A\cos \pi y \sin ax \sin \beta t$$

$$v = -\frac{Aa}{\pi} \sin \pi y \cos ax \sin \beta t$$

$$P = A\sin \pi y \sin ax \cos \beta t$$

$$\phi = A_1 \cos a_1 x \cos b_1 y \cos \beta_1 t.$$
(63)

In the above expressions, (u, v) are the velocity components, and A, A₁, a, a₁, b₁, β and β_1 are all prescribed constants.

The problem configuration is shown in Fig. 1(a). The flow domain is discretized using two quadrilateral spectral elements of equal size (\overline{AEFD} and \overline{EBCF}). On the sides \overline{AD} , \overline{AB} and \overline{BC} we impose a Dirichlet boundary condition for the velocity, chosen according to the analytic expressions in (63). For the phase field function, we impose the wall contact-angle boundary conditions (7a) and (7b) on \overline{AD} and \overline{BC} , and impose the Dirichlet conditions (9a) and (9b) on \overline{AB} . On the side \overline{DC} we



Fig. 1. Convergence rates (analytic solution): (a) Mesh and boundary conditions; (b) numerical errors (fixed $\Delta t = 0.001$) versus element order showing spatial exponential convergence rate and error saturation at large element orders due to temporal truncation error; (c) numerical errors (fixed element order 18) versus time step size showing temporal second-order convergence rate.

impose the outflow boundary conditions, (10)-(11b), for the velocity and the phase field function. The initial conditions for the velocity **u** and the phase field function ϕ are chosen by setting t = 0 to the analytic solutions (63).

The external body force and source terms in the governing equations and boundary conditions, including **f** in (19), *g* in (1c), **w** in (6), **f**_b in (21), g_c (g_w and g_o) in (23), g_d in (22), ϕ_b in (9b), g_e in (7b), g_a in (11b), are chosen such that the analytic expressions in (63) satisfy the governing equations (19), (1b) and (1c), as well as the boundary conditions (6), (21), (23), (22), (9b), (7b), and (11b).

We employ the following parameter values for this problem:

$$A = 2.0, \quad A_{1} = 1.0, \quad a = a_{1} = b_{1} = \pi, \quad \beta = \beta_{1} = 1.0,$$

$$\frac{\rho_{2}}{\rho_{1}} = 3.0, \quad \frac{\mu_{2}}{\mu_{1}} = 5.0, \quad Re = 100, \quad C_{n} = 0.1, \quad We = 10.607, \quad Pe = 106.07$$

(contact angle) $\theta_{s} = 90^{\circ}$, (wall mobility) $D_{w}^{*} = 0$, (outflow mobility) $D_{0}^{*} = 0.2,$
 $\rho_{0}^{*} = \frac{\rho_{0}}{\rho_{1}} = \frac{1}{\rho_{1}} \min(\rho_{1}, \rho_{2}) = 1, \quad \mu_{0}^{*} = \frac{\mu_{0}}{\mu_{1}} = \frac{\max(\mu_{1}, \mu_{2})}{\mu_{1}} = 5.0,$
 $\nu_{m}^{*} = \frac{\nu_{m}}{\mu_{1}/\rho_{1}} \frac{1}{Re} = \frac{1}{2} \left(\frac{\mu_{1}}{\rho_{1}} + \frac{\mu_{2}}{\rho_{2}} \right) \frac{1}{\mu_{1}/\rho_{1}} \frac{1}{Re} = 1.333 \times 10^{-2},$
 $\delta = \frac{1}{20}, \quad S = 77.46,$
 $A = 1$ (phase field model with $\tilde{\mathbf{J}} \cdot \nabla \mathbf{u}$ term)
(integration order) $J = 2.$



Fig. 2. Oil jet in water: (a) Problem configuration; (b) time histories of maximum and average velocity magnitudes showing that the flow has reached a statistically stationary state. Results obtained using the phase field model with $\Lambda = 1$ (i.e. with the $\tilde{J} \cdot \nabla u$ term).

We integrate the system of governing equations from t = 0 to $t = t_f$ using the algorithm developed in Section 2, and compute the errors of the numerical solutions at $t = t_f$ against the analytic solutions (63). In the first set of tests, we use a fixed $t_f = 0.1$, and fix the time step size at $\Delta t = 0.001$ (i.e. 100 time steps). Then we vary the element order systematically between 2 and 20. Fig. 1(b) shows the L^{∞} and L^2 errors of all the flow variables at $t = t_f$ as a function of the element order. It is evident that the numerical errors decrease exponentially with increasing element order when it is below order 10. As the element order increases beyond 10 or 12, the numerical errors saturate due to the temporal truncation error. These results demonstrate the spatial exponential convergence rate of our scheme for two-phase problems involving outflow boundaries.

In the second set of tests, we use a fixed $t_f = 0.2$ and a fixed large element order 18. Then we vary the time step size systematically between $\Delta t = 0.0015625$ and $\Delta t = 0.1$. In Fig. 1(c) we show the L^{∞} and L^2 errors of the flow variables at $t = t_f$ as a function of Δt , both in logarithmic scales. The results show a temporal second-order convergence rate of our scheme for two-phase flows with outflow boundaries. We also observe that the L^{∞} errors for the velocity and the pressure show a non-monotonic behavior around the intermediate time step size $\Delta t = 0.0125-0.025$, producing a "bump" in their respective error curves.

3.2. Instability of an oil jet in water

For the second test problem we simulate the instability of an oil jet in water. The goal is to demonstrate the effectiveness of our method for two-phase outflows involving large viscosity ratios.

We consider the flow domain shown in Fig. 2(a), $-\frac{l}{2} \le x \le \frac{l}{2}$ and $0 \le y \le 2L$, where L = 6 cm. The bottom side of the domain (y = 0) is a solid wall, while the other three sides (left $x = -\frac{L}{2}$, right $x = \frac{l}{2}$, and top y = 2L) are all open where the flow can enter or leave the domain freely. The domain initially contains water inside. The bottom wall has an orifice of diameter $\frac{l}{5}$ in its center, and a jet of oil enters the domain through the orifice. The setup of this problem therefore models an oil jet in an infinite expanse of water. At the orifice, the oil jet has a parabolic profile for its *y* velocity component with a centerline velocity $U_0 = 24.495$ cm/s, and it has no *x* velocity component. The gravity is along the vertical (y) direction, pointing downward. The contact angle between the oil–water interface and the bottom wall, if they intersect, is assumed to be 90°. The oil jet develops an instability in the water, and oil drops break up from the jet. The purpose is to the simulate the long-time behavior of the oil jet in water.

The values for the physical parameters involved in this problem, including the oil/water densities and dynamic viscosities, and their surface tension, are obtained from the literature, and they are provided in Table 2.

In the simulations, we consider the oil as the first fluid and water as the second fluid. The boundary conditions are set up as follows:

• At the bottom wall (excluding the orifice), we impose the Dirichlet condition (6) for the velocity with $\mathbf{w} = 0$, and the contact-angle boundary conditions (7a) and (7b) for the phase field function, with $g_w = g_e = 0$, $D_w = 0$ and $\theta_s = \frac{\pi}{2}$.

Table 2

Physical parameter values concerning air, water and oil employed in the current paper.

Air density 1.204 kg/m ³	Air dynamic viscosity $1.78 \times 10^{-5} \text{ kg/(m s)}$
Water density 998.207 kg/m ³	Water dynamic viscosity $1.002 \times 10^{-3} \text{ kg/(m s)}$
Oil density 870 kg/m ³	Oil dynamic viscosity $9.15 \times 10^{-2} \text{ kg/(m s)}$
Air–water surface tension $7.28 \times 10^{-2} \text{ kg/s}^2$	Oil–water surface tension $2.356 \times 10^{-2} \text{ kg/s}^2$
Gravitational acceleration $g_r = 9.8 \text{ m/s}^2$	

• At the orifice, we impose the Dirichlet condition (6) for the velocity, where **w** has a parabolic profile for the *y* component and is zero for the *x* component; On the other hand, we impose the Dirichlet conditions (9a) and (9b) for the phase field function, with $g_d = 0$ and

$$\phi_b = -\tanh\frac{x - R_0}{\sqrt{2\eta}} \Big[H(x) - H(x - R_0) \Big] + \tanh\frac{x + R_0}{\sqrt{2\eta}} \Big[H(x + R_0) - H(x) \Big], \quad \text{(at orifice)}$$
(65)

where $R_0 = \frac{L}{10}$ is the radius of the orifice, and H(x) is the heaviside step function (taking unit value for $x \ge 0$ and zero otherwise).

• On the left, right and top sides of the domain, we impose the outflow boundary condition (10) for the velocity with $\mathbf{f}_b = 0$, and for the phase field function we impose the outflow conditions (11a) and (11b) with $g_o = 0$, $g_a = 0$, and $D_0 = 0$.

In the simulations, we apply an external pressure gradient $\left(-\frac{\Delta P}{L}\right)$ in the y direction to the entire domain,

$$-\frac{\Delta P}{L} = \rho_w g_r,\tag{66}$$

where ρ_w is the water density, in order to balance the gravity of the water. Therefore, the region occupied by water experiences no net external body force.

We employ L as the characteristic length scale, U_0 as the characteristic velocity scale, and normalize the problem based on the procedure outlined in Section 3.1. This results in the following non-dimensional physical parameter values

$$\frac{\rho_2}{\rho_1} = 1.147, \qquad \frac{\mu_2}{\mu_1} = 1.095 \times 10^{-2},
Re = 1.397 \times 10^2,
We = 1.329 \times 10^2, \qquad Pe = 2.652 \times 10^2, \qquad C_n = 5 \times 10^{-3},
(Froude number) Fr = 0.319,
D_w^* = 0, \qquad \theta_s = \frac{\pi}{2}, \qquad D_0^* = 0.$$
(67)

To simulate the problem, we discretize the flow domain using 800 quadrilateral spectral elements, with 20 elements along the *x* direction and 40 elements along the *y* direction. The element order is 14 for all elements in the simulations. The algorithm developed in Section 2 is employed for marching in time. We use $\rho_0 = \min(\rho_1, \rho_2)$, $\nu_m = \frac{1}{2}(\frac{\mu_1}{\rho_1} + \frac{\mu_2}{\rho_2})$, $\mu_0 = \max(\mu_1, \mu_2)$, and $S = \eta^2 \sqrt{\frac{4\gamma_0}{\lambda\gamma_1 \Delta t}}$ in the algorithm. In addition, the non-dimensional constant δ in the smoothed step function (12) is $\delta = \frac{1}{20}$ in the simulations. As shown in [8], the simulation result is not sensitive to δ when it is sufficiently small. The non-dimensional time step size is $\Delta t = 2 \times 10^{-5}$ in the simulations.

We have performed a long-time simulation of the problem, and the oil-water two-phase flow has reached a statistically stationary state. We compute the following maximum magnitudes (U_{max} , V_{max}) and average magnitudes (U_{ave} , V_{ave}) of the x and y velocity components at each time step,

$$\begin{aligned} U_{\max}(t) &= \max_{\mathbf{x} \in \Omega} |u(\mathbf{x}, t)|, \\ V_{\max}(t) &= \max_{\mathbf{x} \in \Omega} |v(\mathbf{x}, t)|, \\ U_{\text{ave}}(t) &= \left(\frac{1}{V_{\Omega}} \int_{\Omega} |u|^2 \, d\Omega\right)^{\frac{1}{2}}, \\ V_{\text{ave}}(t) &= \left(\frac{1}{V_{\Omega}} \int_{\Omega} |v|^2 \, d\Omega\right)^{\frac{1}{2}}, \end{aligned}$$
(68)

where (u, v) are the *x* and *y* velocity components, and $V_{\Omega} = \int_{\Omega} d\Omega$ is the volume of the flow domain. We have monitored these quantities over time. Fig. 2(b) shows a window of the time histories of these velocity magnitudes. The result is



Fig. 3. Oil jet in water: temporal sequence of snapshots of oil-water interface (contour level $\phi = 0$) at (a) t = 69.212, (b) t = 69.312, (c) t = 69.412, (d) t = 69.512, (e) t = 69.612, (f) t = 69.732, (g) t = 69.812, (h) t = 69.912, (i) t = 70.012. Results obtained using the phase field model with $\Lambda = 1$.

obtained using the phase field model in which the $\tilde{\mathbf{J}} \cdot \nabla \mathbf{u}$ term is present (i.e. $\Lambda = 1$ in (19)). One can observe that these velocities fluctuate over time, but always about some constant mean values. The fluctuations in the maximum velocities are more significant. These velocity histories indicate that the oil–water two-phase flow has reached a statistically stationary state.

Let us next consider the dynamical characteristics of the two-phase oil jet in water. In Fig. 3 we show a temporal sequence of snapshots of the oil-jet configurations, where the oil-water interface is represented by the contour level $\phi = 0$.

These results are obtained using the phase field model with $\Lambda = 1$. The oil jet exhibits distinct characteristics in different regions, depending on the distance from the oil inlet. In the region near the orifice $(y/L \leq 1 \text{ in this case})$ the oil jet maintains a stable configuration. The jet tapers off in this stable region along the vertical direction, due to the velocity increase caused by buoyancy. Beyond this stable region, a Plateau–Rayleigh [21,22] type instability develops. The jet exhibits a wavy pattern in its profile, and the jet diameter modulates along the vertical direction (Figs. 3(a)–(e)), forming bulges as a result. As the oil moves downstream, the bulges deform significantly, and the thin oil bridge connecting subsequent bulges can sometimes be observed to pinch off (Fig. 3(f)). Further downstream, the dramatic deformation of the oil bulge leads to configurations with branches forming from the oil jet (Figs. 3(g)–(i)). The branches may break off from the main jet to form oil drops; see e.g. Figs. 3(a)–(b). The process of forming oil bulges, branches and drops repeats itself.

Fig. 4 shows a temporal sequence of snapshots of the velocity fields of the oil-water flow, at the same time instants as those of the phase field plots in Fig. 3. These results are obtained using the phase field model with $\Lambda = 1$. One can observe several characteristics. First, the region occupied by the jet, as shown by the velocity patterns, is wider than the actual region the material oil occupies (see Fig. 3), especially in the upper half of domain where the material oil jet becomes unstable. This indicates that the water in the immediate regions surrounding the material oil jet has been accelerated to form a wider high-speed region. The jet region shows a lateral spread along the streamwise direction, as can be observed from the velocity patterns. Pairs of vortices can be observed to form along the jet, in regions where the oil jet becomes unstable. These vortices reside behind the oil bulges, at the same vertical locations as the thin oil bridges that connect consecutive bulges (see Fig. 3). These vortices form periodically as new oil bulges form, and travel downstream along with the bulges. Finally, one can note that on the side boundaries the velocity generally points into the domain, indicating that the water has in general been sucked into the domain from both sides. Note that in the simulations we have used the outflow boundary conditions on both the upper and the side boundaries.

We have also performed simulations using the phase field model in which the $\tilde{\mathbf{J}} \cdot \nabla \mathbf{u}$ term is absent, that is, $\Lambda = 0$ in (19). Our results indicate that for the oil-water problem the phase field models with or without the $\tilde{\mathbf{J}} \cdot \nabla \mathbf{u}$ term in the variable-density Navier–Stokes equation produce quite similar results in terms of the dynamic characteristics of the oil jet and the velocity distributions. Indeed, one can observe that when the mobility γ_1 is sufficiently small (or Peclet number is large), the contribution from the term $\tilde{\mathbf{J}} \cdot \nabla \mathbf{u}$ will tend to be insignificant.

3.3. Air jet in water and bubble motion through open boundaries

In the next test we consider a continuous stream of air injected into the water, the formation of a train of air bubbles, and the bubble motion across open domain boundaries. The goal of this test is to demonstrate the performance of our method for two-phase outflows when large density ratios are involved. This problem is significantly more challenging than the problem of the previous section, because of the large density contrast between the air and water.

The configuration of this problem has some similarity to the oil-jet problem of Section 3.2. We consider the flow domain shown in Fig. 5, $-\frac{L}{2} \le x \le \frac{L}{2}$ and $0 \le y \le \frac{3}{2}L$, where *L* is to be specified later. The bottom of the domain is a solid wall, while the other three sides (left, right, top) of the domain are open boundaries. The domain is filled with water. The bottom wall has an orifice of diameter $\frac{L}{5}$ in its center. A stream of air is continuously injected into the domain through the orifice. At the orifice, the incoming air velocity has a parabolic profile, with a centerline velocity U_0 . We assume that, if the air-water interface intersects the bottom wall the static contact angle would be 90°, and that $D_w = 0$. The gravity is assumed to be along the vertical direction (downward). The air stream feeds a train of bubbles, which rise through the water and move out of the domain due to buoyancy. The objective of this test is to simulate the long-time behavior of this air-water flow.

The physical parameters involved in this problem, such as the air/water densities, dynamic viscosities and surface tension, are provided in Table 2. Similar to that for the oil-water problem of Section 3.2, in simulations we impose a pressure gradient in the vertical direction to balance the water gravity, such that no net external body force is experienced in the region occupied by water.

We treat air as the first fluid and water as the second fluid in the simulations. The boundary conditions are set up in a way similar to that for the oil-jet-water problem of Section 3.2. Specifically,

- On the bottom wall we impose a zero-velocity condition, and a contact-angle boundary condition for the phase field function with $\theta_s = \frac{\pi}{2}$ and $D_w = 0$. g_w and g_e in (7a), (7b) have been set to zero.
- At the inlet orifice, a parabolic profile has been set for the *y* velocity, and the *x* velocity is set to zero. The Dirichlet conditions, (9a) and (9b), have been imposed on the phase field function, where ϕ_b is given by (65) and g_d is set to zero.
- On the left, right and top sides of the domain, the outflow boundary conditions, (10)–(11b), have been imposed for the velocity and the phase field function. We set \mathbf{f}_b , g_o and g_a to zeros in these boundary conditions. The outflow dynamic mobility D_0 in (11b) is determined from preliminary simulations. Preliminary simulations (using $D_0 = 0$) indicate that the non-dimensional convection velocity of the air bubble at the upper domain boundary is about 2.0–3.0. So we have used an outflow dynamic mobility $D_0^* = D_0 U_0 = \frac{1}{2.5} = 0.4$ in the simulations.

The problem normalization follows the discussions in Section 3.1, using L as the characteristic length scale and U_0 as the velocity scale.



Fig. 4. Oil jet in water: temporal sequence of snapshots of velocity fields at (a) t = 69.212, (b) t = 69.312, (c) t = 69.412, (d) t = 69.512, (e) t = 69.612, (f) t = 69.732, (g) t = 69.812, (h) t = 69.912, (i) t = 70.012. Results obtained using the phase field model with A = 1. Velocity vectors are plotted on every ninth quadrature point in each direction within each element.



Fig. 5. Air jet in water: problem configurations.

To simulate this problem we discretize the domain with 600 quadrilateral spectral elements, with 20 elements in the x direction and 30 elements in the y direction. The element order is 14 for all elements in the simulations. We employ the algorithm from Section 2 for time integration, with the parameters

$$\begin{cases} \rho_{0} = \min(\rho_{1}, \rho_{2}) \\ \nu_{m} = 2 \max\left(\frac{\mu_{1}}{\rho_{1}}, \frac{\mu_{2}}{\rho_{2}}\right) \\ \mu_{0} = \frac{1}{4} \max(\mu_{1}, \mu_{2}) + \frac{3}{4} \min(\mu_{1}, \mu_{2}) \\ S = \eta^{2} \sqrt{\frac{4\gamma_{0}}{\lambda \gamma_{1} \Delta t}} \end{cases}$$
(69)

in the algorithm. We use $\delta = \frac{1}{20}$ in the smoothed step function (12) for the outflow boundary condition (10). The nondimensional time step size is $\Delta t = 2 \times 10^{-6}$ in the simulations. We employ the phase field model without the $\tilde{\mathbf{J}} \cdot \nabla \mathbf{u}$ term for the simulations of this section, i.e. $\Lambda = 0$.

We have considered two values for the characteristic length: L = 3 cm and L = 4 cm. These lead to two different sizes for the flow domain and the inlet orifice. The first domain has a dimension 3 cm × 4.5 cm, with an orifice of diameter 6 mm at the bottom wall. The second domain has a dimension 4 cm × 6 cm, with an orifice of diameter 8 mm at the bottom wall. The air velocities at the centerline of the orifice are respectively $U_0 = 17.32$ cm/s and $U_0 = 20$ cm/s for these two cases. After normalization, for the smaller domain we have the following non-dimensional parameter values:

$$\begin{cases} \frac{\rho_2}{\rho_1} = 829, & \frac{\mu_2}{\mu_1} = 56.29, \\ Re = 3.515 \times 10^2, \\ We = 1.489 \times 10^{-2}, & Pe = 1.061 \times 10^3, \\ (Froude number) Fr = 0.319, \\ D_w^* = 0, & \theta_s = \frac{\pi}{2}. \end{cases}$$
(70)

For the larger domain, we have the parameter values

$$Re = 5.412 \times 10^{2},$$

$$We = 2.646 \times 10^{-2},$$
(71)

while the rest of the non-dimensional parameters have the same values as those for the smaller domain. We will look into the characteristics of the air-water flow for these two cases individually in the following.

Smaller domain Let us first consider the smaller domain of 3 cm \times 4.5 cm with an orifice of diameter 6 mm. We have performed a long-time simulation of the problem, and have monitored the evolution of the maximum and average magnitudes of the *x* and *y* velocities of the domain as defined by (68). Fig. 6 shows a window of the maximum and average velocity histories of the two velocity components. One can observe that both the maximum and the average velocity magnitudes fluctuate quasi-periodically over time, but approximately around some constant mean levels. They indicate that the air-water flow has reached a statistically stationary state.



Fig. 6. Air jet in water (smaller domain): Time histories of the maximum and averaged magnitudes of x and y velocities.

The time histories of the maximum velocities seem to suggest the presence of two distinct states in the flow, which alternate in time with each other. At one flow state, the maximum velocities exhibit relatively low values, e.g. at the instant marked by the arrow "B" in Fig. 6. At the other state, the maximum velocities exhibit generally higher values, and in particular the maximum velocity peaks at certain time instants; see e.g. the time interval marked by "snapshot sequence" in Fig. 6.

We first look into the characteristics of the flow at a state with relatively higher maximum velocities. Fig. 7 provides a temporal sequence of snapshots of the air-water interface, in the time interval marked by "snapshot sequence" in Fig. 6. Fig. 7(a) shows a free air bubble rising through water, and that a second bubble is forming at the orifice but still attached to the bottom wall. Figs. 7(b)–(c) show the process when the second bubble breaks away from the wall to form a distinct free bubble. As the second bubble grows owing to the incoming air stream through the orifice, its lower portion shrinks to form a thin channel (throat), which connects the bulk of the air bubble and the orifice. The connecting thin channel then pinches off, and a distinct free bubble forms and breaks away from the bottom wall (Fig. 7(c)). Subsequently, the feeding air stream gradually inflates another bubble at the orifice attached to the wall, and the process of bubble formation repeats itself. Once breaking free from the wall, the second air bubble rises through water in the wake of the first bubble. It can be observed that the second bubble is dramatically distorted, see Figs. 7(e)–(j), by the presence of a pair of vortices in the wake of the first bubble, which will become clear from Fig. 8 subsequently. Figs. 7(g)–(j) show the passing of the first air bubble through the upper open boundary of the domain. Fig. 7(l) shows that the dramatically deformed second bubble is crossing the upper boundary, and that it is about to pinch off in the middle and break into two.

Fig. 8 shows the corresponding temporal sequence of snapshots of the velocity fields at the same time instants as those of Fig. 7. Comparison between Fig. 8(b) and Fig. 7(b) indicates that, as the channel between the bulk of air bubble and the orifice shrinks, a strong jet of air with large velocity magnitudes forms in the thin channel. This strong jet of air correspond to some of the peaks observed in the maximum-velocity histories in Fig. 6. This air jet also produces violent velocity fields and strong vortices inside the air bubble shortly before and after the bubble breaks away from the wall; see Figs. 8(a)–(d). Figs. 8(a)–(f) clearly show the pair of vortices in the wake of the first air bubble. The interaction between the second bubble and the wake of the first bubble is responsible for the significant deformations of the second bubble; see Figs. 8(e)–(j) and also Fig. 7. Figs. 8(g)–(j) show the velocity distributions as the first air bubble passes through the upper open boundary. It is also observed that on the side boundaries the flow is generally into the domain (backflow).

Subsequently, as the second bubble moves out of the domain, while another bubble is still forming at the orifice, the flow domain is essentially depleted of free air bubbles. This is shown by Fig. 9(a) with a snapshot of the air-water interface at a time instant marked by the arrow "A" in Fig. 6.

Figs. 9(b) and (c) show the air bubble configurations at two time instants that are marked by the arrows "B" and "C" respectively in Fig. 6. They correspond to the flow state with relatively low values of maximum velocities in the history plot. The free air bubble in these two plots corresponds to the bubble in Fig. 9(a) that is about to break away from the wall. The rising speed of this free bubble is relatively low, because the flow field in the upper part of the domain has gradually died down due to the depletion of free bubbles in the domain. The low rising speed of this free bubble in turn allows enough time for a second bubble to form and subsequently break away from the wall. After that, the scenario shown by Figs. 7(a)–(b) and subsequent scenarios will repeat.

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Fig. 7. Air jet in water: temporal sequence of snapshots of air-water interface: (a) t = 5.054, (b) t = 5.093, (c) t = 5.150, (d) t = 5.183, (e) t = 5.243, (f) t = 5.303, (g) t = 5.351, (h) t = 5.372, (i) t = 5.402, (j) t = 5.432, (k) t = 5.456, (l) t = 5.483.

The results suggest that the alternation of the two flow states, with relatively lower and higher maximum velocities, observed from the velocity time histories is owing to the different rising speeds of the free air bubbles. When two or more free bubbles are present in the domain, the interaction between these bubbles and their synergistic effect will markedly accelerate the flow and the bubble motion, causing the free bubbles to move out of the domain in a relatively short period of time. Because the interval at which a new free bubble breaks away from the wall is relatively regular, the rapid bubble motion out of the domain may periodically deplete the domain (or at least the near-wall region of domain) of free bubbles. As the flow field caused by the bubble passage dies down upon depletion of free bubbles, the free bubble generated at the wall at that point will rise at a relatively low speed. This in turn allows enough time for the formation and accumulation of new free bubbles in the domain, thus accelerating the flow and bubble rising. The above cycle repeats itself, resulting in the alternation of the two states observed from the velocity histories.

Larger domain We next consider the larger flow domain of dimension $4 \text{ cm} \times 6 \text{ cm}$ with an 8 mm-diameter orifice on the bottom wall. A long-time simulation has been performed for this case to ensure that the air–water flow has reached a statistically stationary state. This is demonstrated by the time histories of the maximum and average magnitudes of the *x* and *y* velocities in Fig. 10. The basic characteristics in the time histories are similar to those on the smaller domain. For example, the large fluctuations in time of the maximum velocities, and the alternation in time between two flow states



Fig. 8. Air jet in water: temporal sequence of snapshots of velocity fields: (a) t = 5.054, (b) t = 5.093, (c) t = 5.150, (d) t = 5.183, (e) t = 5.243, (f) t = 5.303, (g) t = 5.351, (h) t = 5.372, (i) t = 5.402, (j) t = 5.432, (k) t = 5.456, (l) t = 5.483. Velocity vectors are plotted on every ninth quadrature point in each direction on each element.

with generally lower or higher maximum velocities, can also be observed with the larger domain here. A difference is that the alternation period between the two states appears noticeably shorter for this case in non-dimensional time.

Fig. 11 shows a temporal sequence of snapshots of configurations of the air–water interface over the time interval marked by "snapshot sequence" in Fig. 10. The figure shows the formation of free air bubbles near the orifice, and the motion of a cluster of air bubbles across and out of the flow domain. Figs. 11(a)-(c) show a free bubble rising in the domain and the formation of a second free bubble near the bottom wall. Once formed, the second bubble rises rapidly in the domain, and catches up with the first bubble (Figs. 11(d)-(e)). The two free bubbles then appear to rise through the water together as a cluster (Figs. 11(e)-(f)). The second bubble experiences severe deformations in the process. Subsequently, the second bubble breaks up into two daughter bubbles (Fig. 11(g)). The cluster of these bubbles rises along the vertical direction and eventually moves out of the domain (Figs. 11(g)-(1)). In the process it can be observed that one of the daughter bubbles merges with the first bubble (Figs. 11(i)). One can also observe that a third bubble forms at the orifice and breaks free from the bottom wall (Figs. 11(j)-(1)).

The above results indicate that the overall scenario about the bubble motions observed on the smaller domain manifests in a similar way for the larger domain. The presence of a free bubble inside the domain (not far from the bottom wall)



Fig. 9. Snapshots of air-water interface at time instants marked in Fig. 6 by (a) arrow A, (b) arrow B, (c) arrow C.



Fig. 10. Air jet in water (larger domain): Time histories of the maximum and average magnitudes of x and y velocities.

will accelerate the rising of the free bubble subsequently generated at the wall. Their rapid movement across the domain ultimately depletes the near-wall region or even the entire flow domain of free bubbles. This in turn slows down the motion of the free bubble that is subsequently generated at the wall. The main difference with the larger domain appears to lie in that the free bubbles in the domain have formed a cluster in this case and rise together through the water. The cluster of bubbles also exhibits more complicated dynamics, such as bubble breakup and coalescence.

The results of this section demonstrate that the outflow boundary conditions we developed in Section 2 can effectively deal with two-phase outflows where large density ratios and viscosity ratios are involved. They also show that the Dirichlet conditions we developed in Section 2 for the phase field function can effectively deal with two-phase inflows. Our method allows the bubbles and the air-water interface to move freely and seamlessly through the outflow and open boundaries.

Because of the large density ratio between the air and water, the simulation of the air-water flow involving outflow boundaries is very challenging. Besides the usual factors that affect the stability (such as spatial resolution and time step size), we observe that the constant v_m in the algorithm also has an effect on the stability of computation. A larger v_m makes the computation more stable, while with a small v_m one may encounter numerical instability. For example, we observe that the constant μ_0 on the stability of computation, and a smaller μ_0 tends to improve the stability. In addition, we observe that, if the $[\frac{1}{2}\rho|\mathbf{u}|^2\Theta_0]\mathbf{n}$ term is absent from the outflow boundary condition (10), the simulation for this air-water flow is unstable.

4. Concluding remarks

In this paper we have presented a set of outflow boundary conditions, and an associated numerical algorithm, within the phase field framework for simulating incompressible two-phase flows involving outflow or open boundaries. The two-phase outflow boundary conditions for the velocity and for the phase field function are designed in a fashion such that they will



Fig. 11. Air jet in water (larger domain): temporal sequence of snapshots of the air-water interface at (a) t = 6.927, (b) t = 7.007, (c) t = 7.047, (d) t = 7.087, (e) t = 7.167, (f) t = 7.223, (g) t = 7.303, (h) t = 7.383, (i) t = 7.423, (j) t = 7.463, (k) t = 7.515, (l) t = 7.575.

not cause un-controlled growth in the total energy of the two-phase system, even in situations where energy influx or backflows into the domain through the outflow boundaries may be present.

In addition, we have also presented an extra boundary condition, together with the usual Dirichlet condition, for the phase field function on inflow boundaries. We observe that the often-used zero-flux condition on the chemical potential fails to work for phase-field Dirichlet boundaries. A combination of the zero-flux condition on the chemical potential, together with the usual Dirichlet condition for the phase field function, has been observed to cause a numerical instability at the inflow boundaries, when the density ratio of the two fluids becomes large (e.g. the air–water problem).

Our numerical algorithm for dealing with these boundary conditions is developed on top of a strategy we developed previously in [10] for de-coupling the computations of all flow variables and for overcoming the performance bottleneck caused by variable coefficient matrices associated with variable mixture properties. The algorithm contains special constructions for treating the variable viscosity at the outflow boundaries and for preventing a numerical locking on the outflow boundaries for time-dependent problems. We observe that the current algorithmic treatment of the variable dynamic viscosity in the outflow boundary condition is extremely important. Without this treatment, the computation is unstable when the fluid interface touches the outflow boundaries for high and moderate viscosity ratios. The numerical treatment of the outflow boundary condition for the phase field function also warrants special care, due to the inertial term $\frac{\partial \phi}{\partial t}$. A straightforward treatment of this term on the outflow boundaries will cause a numerical instability unless D_0 is extremely small, or will couple up the computations for the auxiliary phase-field variable ψ and the phase field function ϕ , which are naturally de-coupled if no outflow boundary is present. In our algorithm, we have treated this term on the outflow boundaries by borrowing an idea from [7] for dealing with the dynamic contact-angle boundary conditions on solid walls. This allows for stable computations in the case of large D_0 values, and simultaneously de-couples the computations for ψ and ϕ .

Extensive numerical experiments have been presented for incompressible two-phase flows involving inflow and outflow boundaries. These results demonstrate that the two-phase outflow boundary conditions and the numerical algorithm developed herein allow the fluid interface and the two-phase flow to pass through the outflow or open boundaries in a smooth and seamless fashion. Our method achieves stable computations when large density ratios and large viscosity ratios are involved and when strong backflows are present at the outflow boundaries.

The method developed herein provides an effective and efficient technique for simulating a large class of crucial twophase flows, for example, two-phase jets, wakes, shear layers, and other spatially-developing two-phase flows involving inflow/outflow boundaries. It can facilitate and potentially enable new investigations into the statistical features of twophase flows, since the technique allows for long-time simulations such that statistically stationary flow states can be examined. It is observed that numerical studies of the statistical aspect of two-phase flows (involving inflows/outflows) seem still severely lacking, at least for the phase field community. The presented method can facilitate new applications in this direction.

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