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# An Artificial Compressibility Method for 3D Phase-Field Model and its Application to Two-Phase Flows

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In this work, a numerical scheme based on artificial compressibility formulation of a phase-field model is developed for simulating two-phase incompressible flow problems. The coupled nonlinear systems composed of the incompressible Navier–Stokes equations and volume preserving Allen–Cahn-type phase-field equation are recast into conservative form with source terms, which are suited to implement high-resolution schemes originally developed for hyperbolic conservation laws. The Boussinesq approximation is used to account for the buoyancy effect in flow with small density difference. The fifth-order weighted essentially nonoscillatory (WENO) scheme is used for discretizing the convective terms while dual-time stepping (DTS) technique is used for obtaining time accuracy at each physical time step. Beam–Warming approximate factorization scheme is utilized to obtain block tridiagonal system of equations in each spatial direction. The alternating direction implicit (ADI) algorithm is used to solve the resulting system of equations. The performance of the method is demonstrated by its application to some 2D and 3D benchmark viscous two-phase flow problems.

*Keywords*: Two-phase flow; phase-field model; incompressible Navier–Stokes equations; artificial compressibility method; Boussinesq approximation.

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## 1. Introduction

The numerical study of incompressible two-phase interfacial flows is very important in various fields of science and engineering and is applied in many industrial applications. However, several special physical properties like concentrated surface tension, topological change, large density/viscosity difference associated with timeevolving sharp interface make such flows difficult to solve analytically and numerically. From a mathematical point of view, such problems are called moving internal boundary or free surface flows where the interface has varying behaviors due to density and viscosity differences of the two fluids. Several numerical techniques exist to solve such kinds of problems which are usually not easy to implement numerically, especially in three space dimensions.

In incompressible two-phase flows, the physical variables required to describe the motion are velocity, pressure, density, viscosity and surface tension. The density is a very important quantity of fluids since it determines the properties of fluids like acceleration and buoyancy. However, the density variation in the flow-field has complicated effects on the flow and one needs to make some assumptions to reduce the degree of complexity. The Boussinesq approximation [Ferziger and Peric (2002); Liu and Shen (2003)] is one of such assumptions, which is widely used for buoyancy-driven flows. In the Boussinesq approximation, the density variation in space and time is small such that the density occurring in the acceleration terms can be treated as a constant "background density"  $\rho_0$ , and the difference between the actual density and the background density contributes only to the buoyancy force in the momentum equations [Tryggvason (1988); Lee and Kim (2011)].

Phase-field/diffuse-interface models for two-phase flows have gained a lot of attention due to ease in handling the topological changes without explicitly knowing the location of the interface. In our previous work [Shah and Yuan (2011)], we have developed a two-dimensional (2D) artificial compressibility method (ACM) for simulating two-phase flows with constant density and viscosity but different types of fluids embodied by surface tension. The ACM provides a mechanism to march in pseudo-time to get the divergence-free velocity-field such that mass and momentum are conserved in the pseudo-steady state and solves a hyperbolic system to avoid solution of pressure Poisson's equation. Many numerical schemes for hyperbolic conservation laws can easily be transferred to artificial compressibility formulations. The objective of this work is to extend the two-phase numerical method by Shah and Yuan [2011] to three dimension (3D). Due to the inherited simplicity of our formulation, it is not difficult to simulate complicated 3D problems using highperformance computing facilities.

The plan of the paper goes as follows. In Sec. 2, the governing equations for the mixture of two incompressible fluids are provided with relevant details. In Sec. 3, formulations based on the ACM are rewritten in hyperbolic conservative form. Section 4 describes the spatial and temporal discretization and solution algorithm.

Numerical experiments for 2D and 3D problems are given in Sec. 5. Section 6 concludes this work.

# 2. Phase-Field Model for Two Different Fluids

Let  $\Omega$  be a domain filled with two isotropic fluids of different densities and viscosities separated by an interface. The phase-field function  $\phi(\mathbf{x}, t)$  with  $\mathbf{x} \in \Omega$  assumes distinct constant values  $\phi = 1$  in one fluid and  $\phi = -1$  in the other fluid with smooth change in the interfacial region given by a width  $\eta$  as shown in Fig. 1.

The elastic mixing free-energy of two-component fluids can be expressed by the Ginzburg–Landau free-energy functional of the form:

$$F(\phi, \nabla \phi) = \int_{\Omega} \left( \frac{1}{2} |\nabla \phi|^2 + \frac{1}{4\eta^2} (\phi^2 - 1)^2 \right) d\mathbf{x},$$
 (1)

where the constant  $\eta$  is an artificial thickness for the diffusive interface. Actually, the gradient term for  $\phi$  in the integrand leads to a diffuse liquid-liquid interface, a feature observed both experimentally and numerically [Tegze *et al.* (2005); Tan *et al.* (2007)], while the latter term in the integrand leads to a sharp interface. The energy minimization in one-dimensional (1D) case yields the equilibrium with  $\phi = \pm 1$  in the two bulk phases and  $\phi(x) = \tanh(\frac{x}{\sqrt{2\eta}})$  across the interface at x = 0. The avaluation of  $\phi$  is groupped by the Allen Cohen ture equation:

The evolution of  $\phi$  is governed by the Allen–Čahn-type equation:

$$\phi_t + (\mathbf{u} \cdot \nabla)\phi = -\gamma \frac{\delta F}{\delta \phi} = \gamma (\Delta \phi - f(\phi)).$$
<sup>(2)</sup>

Here,  $\delta F/\delta \phi$  represents the variation of the energy F with respect to  $\phi$ ,  $f(\phi)$  is the double well potential  $(f(\phi) = \frac{\phi(\phi^2 - 1)}{\eta^2})$ , and  $\gamma$  is the elastic relaxation time-scale of the two fluids. We used a modified Allen–Cahn formulation [Yang *et al.* (2006); Di *et al.* (2008)] by introducing  $\xi(t)$  that allows to enforce the condition  $|\phi| = 1$  as a remedy to conserve the mass. We can see that Eq. (2) tends to the classical volume of fluid (VOF) equation  $\phi_t + (\mathbf{u} \cdot \nabla)\phi = 0$ , provided that both  $\eta$  and  $\gamma$  tend to 0.



Fig. 1. A schematic diagram showing the distribution of phase variable across an interface ( $\phi = 0$ ) while ( $\phi = 1$ ) and ( $\phi = -1$ ) represent two phases separated by a diffusive region with a thickness  $\eta$ .

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The momentum equation for the fluid mixture with small density difference can be described by the Boussinesq approximation:

$$\rho_0[\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u}] = -\nabla \tilde{p} + \nabla \cdot \boldsymbol{\sigma} + \mathbf{b}(\boldsymbol{\phi}), \tag{3}$$

where  $\rho_0$  is the "background" density treated as constant in the whole flow-field and the difference between the actual density and  $\rho_0$  contributes only to the buoyancy force  $\mathbf{b}(\phi)$ .  $\tilde{p}$  is the pressure that has absorbed  $\rho_0 gz$  from original gravity term.  $\boldsymbol{\sigma}$ is the lumped stress tensor that includes the viscous stress tensor and the induced elastic stress tensor, and is given by

$$\sigma = \mu(\phi) [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] - \lambda \nabla \phi \otimes \nabla \phi, \qquad (4)$$

where  $\mu(\phi) = \frac{1+\phi}{2}\mu_1 + \frac{1-\phi}{2}\mu_2$  is the dynamic viscosity of the mixture,  $\lambda$  is the surface tension coefficient and  $(\nabla\phi\otimes\nabla\phi)_{ij} = \nabla_i\phi\nabla_j\phi$  is the usual tensor product. By using the identity,

$$\nabla \cdot (\nabla \phi \otimes \nabla \phi) = \Delta \phi \nabla \phi + \nabla \left(\frac{1}{2} |\nabla \phi|^2\right),\tag{5}$$

the momentum equation is further simplified by redefining the pressure term:  $p = \tilde{p} + \frac{1}{2}\lambda |\nabla \phi|^2$ . The buoyancy force with gravitational acceleration g in the negative z-direction is given as

$$\mathbf{b}(\phi) = (0, 0, -g(\rho - \rho_0))^{\mathrm{T}},\tag{6}$$

where  $\rho = \frac{1+\phi}{2}\rho_1 + \frac{1-\phi}{2}\rho_2$  is used. In this work, we restrict ourself to a simpler type of incompressible two-fluid mixture [Liu and Shen (2003); Di *et al.* (2008)] with a viscosity constant  $\mu_1 = \mu_2 = \mu$ . We used the incompressibility condition to convert the convective term in Eq. (3) to a conservative form, divide it by  $\rho_0$  but still denote  $(p, \mu, \mathbf{b}, \lambda) = (p, \mu, \mathbf{b}, \lambda)/\rho_0$ , the system of governing equations consisting of the continuity equation, the momentum equation, and the phase-field equation are as follows:

$$\nabla \cdot \mathbf{u} = 0, \tag{7a}$$

$$\mathbf{u}_t + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) + \nabla p - \mu \Delta \mathbf{u} = \mathbf{b}(\phi) - \lambda \Delta \phi \nabla \phi, \tag{7b}$$

$$\phi_t + \mathbf{u} \cdot \nabla \phi - \gamma \Delta \phi = \gamma (-f(\phi) + \xi(t))$$
(7c)

with initial conditions

 $\mathbf{u}|_{t=0} = \mathbf{u}_0, \quad \phi|_{t=0} = \phi_0$ 

and appropriate boundary conditions. The phase-field model Eq. (7) for two-phase incompressible viscous flows has received a lot of attention recently and some authors [Liu and Shen (2003); Chiu and Lin (2011); Yue *et al.* (2005); Liu *et al.* (2005); Tan *et al.* (2006); Zhang and Tang (2007); Sun and Beckermann (2007); Ding *et al.* (2007); Sun *et al.* (2009); Feng *et al.* (2005); Zhao *et al.* (2016)] among others have developed different numerical methods to solve this type of coupled system of equations.

# 3. Artificial Compressibility Formulation

The mass conservation is the main difficulty in solving the incompressible Navier– Stokes equations in primitive variables. To relax this constraint, the ACM [Chorin (1967)] provides a mechanism to march in pseudo-time towards the divergence-free velocity-field such that the mass and momentum are conserved in the pseudo-steady state. The method gives an artificial relation between pressure and density in order to bring a pseudo-time derivative to the mass conservation equation, i.e.,  $p \sim \beta \rho^*$  implies that  $\beta \frac{\partial \rho^*}{\partial \tau} = \frac{\partial p}{\partial \tau}$ , where  $\beta$  is the artificial compressibility parameter. Now that the system of equations become hyperbolic in pseudo-time, numerical methods for hyperbolic conservation laws can be used. Adding the artificial compressibility terms with dual-time stepping (DTS) technique [Shah and Yuan (2011)] to the governing equations (7), we obtain

$$\frac{\partial p}{\partial \tau} + \beta (\nabla \cdot \mathbf{u}) = 0, \tag{8a}$$

$$\frac{\partial \mathbf{u}}{\partial \tau} + \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) + \nabla p - \mu \Delta \mathbf{u} = \mathbf{b}(\phi) - \lambda \Delta \phi \nabla \phi, \tag{8b}$$

$$\frac{\partial \phi}{\partial \tau} + \frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u}) - \gamma \Delta \phi = \gamma (-f(\phi) + \xi(t)).$$
(8c)

After  $\xi(t)$  in Eq. (8c) is modified as  $\xi(t)(1 - \phi^2)$  as per Di *et al.* [2008] to keep  $\phi \in [-1, 1]$ , the above equations can be written in the following conservative form:

$$\frac{\partial \mathbf{D}}{\partial \tau} + \mathbf{I}_m \frac{\partial \mathbf{D}}{\partial t} + \frac{\partial (\mathbf{E} - \mathbf{E}_v)}{\partial x} + \frac{\partial (\mathbf{F} - \mathbf{F}_v)}{\partial y} + \frac{\partial (\mathbf{G} - \mathbf{G}_v)}{\partial z} = \mathbf{S}_b \tag{9}$$

with

$$\mathbf{D} = \begin{bmatrix} p \\ u \\ v \\ w \\ \phi \end{bmatrix}, \quad \mathbf{E} = \begin{bmatrix} \beta u \\ u^2 + p \\ uv \\ uw \\ u\phi \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} \beta v \\ uv \\ v^2 + p \\ vw \\ v\phi \end{bmatrix}, \quad \mathbf{G} = \begin{bmatrix} \beta w \\ uw \\ vw \\ w^2 + p \\ w\phi \end{bmatrix}$$

and

$$\mathbf{I}_{m} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{E}_{v} = \begin{bmatrix} 0 \\ \mu u_{x} \\ \mu v_{x} \\ \mu w_{x} \\ \gamma \phi_{x} \end{bmatrix}, \quad \mathbf{F}_{v} = \begin{bmatrix} 0 \\ \mu u_{y} \\ \mu v_{y} \\ \mu w_{y} \\ \gamma \phi_{y} \end{bmatrix}, \quad \mathbf{G}_{v} = \begin{bmatrix} 0 \\ \mu u_{z} \\ \mu v_{z} \\ \mu w_{z} \\ \gamma \phi_{z} \end{bmatrix},$$

$$\mathbf{S}_{b} = \begin{bmatrix} 0 \\ -\lambda\phi_{x}(\phi_{xx} + \phi_{yy} + \phi_{zz}) \\ -\lambda\phi_{y}(\phi_{xx} + \phi_{yy} + \phi_{zz}) \\ -\lambda\phi_{z}(\phi_{xx} + \phi_{yy} + \phi_{zz}) - \frac{1}{2}g\left[(1+\phi)\frac{\rho_{1}-\rho_{0}}{\rho_{0}} - (1-\phi)\frac{\rho_{2}-\rho_{0}}{\rho_{0}}\right] \\ \gamma(1-\phi^{2})(\phi/\eta^{2} + \xi(t)) \end{bmatrix}, \quad (10)$$

where **D** is the solution vector (u, v, w) are velocity components in each spatial directions, respectively,  $\tau$  is the pseudo-time, t is the physical time,  $\mathbf{I}_m$  is a modified identity matrix and  $\mathbf{S}_b$  represents the effects of nonlinear surface tension terms and buoyancy terms. The Jacobian matrices **A**, **B** and **C** of the inviscid flux vectors **E**, **F** and **G**, respectively, are given by

$$\mathbf{A} = \frac{\partial \mathbf{E}}{\partial \mathbf{D}} = \begin{bmatrix} 0 & \beta & 0 & 0 & 0 \\ 1 & 2u & 0 & 0 & 0 \\ 0 & v & u & 0 & 0 \\ 0 & w & 0 & u & 0 \\ 0 & \phi & 0 & 0 & u \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 0 & 0 & \beta & 0 & 0 \\ 0 & v & u & 0 & 0 \\ 1 & 0 & 2v & 0 & 0 \\ 0 & 0 & w & v & 0 \\ 0 & 0 & \phi & 0 & v \end{bmatrix},$$
$$\mathbf{C} = \begin{bmatrix} 0 & 0 & 0 & \beta & 0 \\ 0 & w & 0 & u & 0 \\ 0 & 0 & w & v & 0 \\ 1 & 0 & 0 & 2w & 0 \\ 0 & 0 & 0 & \phi & w \end{bmatrix}.$$

The viscous Jacobian matrices  $\mathbf{A}_v$ ,  $\mathbf{B}_v$  and  $\mathbf{C}_v$  of the viscous flux vectors  $\mathbf{E}_v$ ,  $\mathbf{F}_v$ and  $\mathbf{G}_v$ , respectively, which will be utilized in the approximate factorization (AF) scheme are

$$\mathbf{A}_{v} = \frac{\partial \mathbf{E}_{v}}{\partial \mathbf{D}} = \operatorname{diag}(0, \mu, \mu, \mu, \gamma) \partial_{x}, \quad \mathbf{B}_{v} = \frac{\partial \mathbf{F}_{v}}{\partial \mathbf{D}} = \operatorname{diag}(0, \mu, \mu, \mu, \gamma) \partial_{y}$$
  
d 
$$\mathbf{C}_{v} = \frac{\partial \mathbf{G}_{v}}{\partial \mathbf{D}} = \operatorname{diag}(0, \mu, \mu, \mu, \gamma) \partial_{z}.$$

It is possible to diagonalize **A**, **B** and **C** as

an

$$\mathbf{A} = \mathbf{X} \mathbf{\Lambda}_A \mathbf{X}^{-1}, \quad \mathbf{B} = \mathbf{Y} \mathbf{\Lambda}_B \mathbf{Y}^{-1}, \quad \mathbf{C} = \mathbf{Z} \mathbf{\Lambda}_C \mathbf{Z}^{-1},$$

where diagonal matrices  $\Lambda_A$ ,  $\Lambda_B$  and  $\Lambda_C$  contain the eigenvalues of matrices **A**, **B** and **C**, respectively, e.g.,  $\Lambda_A = \text{diag} = \{u - c_1, u, u, u, u + c_1\}$  with  $c_1 = \sqrt{u^2 + \beta}$  being the pseudo-speed of sound. The matrices **X** and **Y** and **Z** are the right eigenvectors matrices, while  $\mathbf{X}^{-1}$  and  $\mathbf{Y}^{-1}$  and  $\mathbf{Z}^{-1}$  are their inverses, respectively.

## 4. Numerical Method

The fifth-order weighted essentially nonoscillatory (WENO) scheme [Jiang and Shu (1996); Yang *et al.* (1998)] for the discretization of the convective terms while second-order central scheme for the viscous and surface tension terms are used. Forward difference scheme for pseudo time derivative and two-point backward difference scheme for the physical time derivative are used, i.e.,

$$\frac{\mathbf{D}^{n+1,m+1} - \mathbf{D}^{n+1,m}}{\Delta \tau} + \mathbf{I}_m \frac{3\mathbf{D}^{n+1,m+1} - 4\mathbf{D}^n + \mathbf{D}^{n-1}}{2\Delta t} + \left[\frac{\partial(\mathbf{E} - \mathbf{E}_v)}{\partial x} + \frac{\partial(\mathbf{F} - \mathbf{F}_v)}{\partial y} + \frac{\partial(\mathbf{G} - \mathbf{G}_v)}{\partial z}\right]^{n+1,m+1} = \mathbf{S}_b^{n+1,m+1}, \quad (11)$$

where n is the physical time level and m is the pseudo-time level. The objective is to solve for  $\mathbf{D}^{m+1}$  at level n + 1 (knowing the solution at level n and n - 1) which is nonlinear in nature, so first we linearize it using the first-order Taylor's series expansion

$$\mathbf{E}^{m+1} \approx \mathbf{E}^m + \left(\frac{\partial \mathbf{E}}{\partial \mathbf{D}}\right)^m (\mathbf{D}^{m+1} - \mathbf{D}^m), \tag{12}$$

where second and higher-order terms are neglected. Since  $\left(\frac{\partial \mathbf{J}}{\partial \mathbf{D}}\right)^m = \mathbf{A}^m$ , Eq. (12) becomes

$$\mathbf{E}^{m+1} \approx \mathbf{E}^m + \mathbf{A}^m \Delta \mathbf{D}^m. \tag{13}$$

Similarly, we expand  $\mathbf{F}^{m+1}$ ,  $\mathbf{G}^{m+1}$ ,  $\mathbf{E}^{m+1}_{\nu}$ ,  $\mathbf{F}^{m+1}_{\nu}$ ,  $\mathbf{G}^{m+1}_{\nu}$  with respect to pseudo-time level *m* like Eq. (13). From now on, superscript n + 1 is omitted for brevity. After substituting Eq. (13) and similar expansions in Eq. (11), the following rearranged form is obtained:

$$\begin{bmatrix} \mathbf{I} + 1.5\frac{\Delta\tau}{\Delta t}\mathbf{I}_m + \Delta\tau \left(\frac{\partial(\mathbf{A} - \mathbf{A}_v)}{\partial x} + \frac{\partial(\mathbf{B} - \mathbf{B}_v)}{\partial y} + \frac{\partial(\mathbf{C} - \mathbf{C}_v)}{\partial z} - \mathbf{\Phi} - \widetilde{\mathbf{P}} \right) \end{bmatrix} \Delta \mathbf{D}^m$$
$$= -\Delta\tau \left(\frac{\partial(\mathbf{E} - \mathbf{E}_v)}{\partial x} + \frac{\partial(\mathbf{F} - \mathbf{F}_v)}{\partial y} + \frac{\partial(\mathbf{G} - \mathbf{G}_v)}{\partial z} - \mathbf{S}_b \right)^m$$
$$-\frac{\Delta\tau}{2\Delta t} \mathbf{I}_m (3\mathbf{D}^m - 4\mathbf{D}^n + \mathbf{D}^{n-1}). \tag{14}$$

In Eq. (14),  $\Phi$  is a Jacobian matrix resulting from the nonlinear function in the  $\phi$  equation and the buoyancy term in the momentum equations, and  $\tilde{\mathbf{P}} = (\mathbf{P}_x + \mathbf{P}_y + \mathbf{P}_z)$ , where  $\mathbf{P}_x$ ,  $\mathbf{P}_y$  and  $\mathbf{P}_z$  are the Jacobian matrix *operators* resulting from the *x*-, *y*- and *z*-derivative operators of the surface tension terms in the momentum equations, respectively.

Denoting the RHS of Eq. (14) as  $\mathbf{R}^m$  and  $\mathbf{H} = \mathbf{I} + 1.5 \frac{\Delta \tau}{\Delta t} \mathbf{I}_m - \Delta \tau \boldsymbol{\Phi}$  in the LHS, we get

$$\left[\mathbf{H} + \Delta \tau \left(\frac{\partial (\mathbf{A} - \mathbf{A}_v)}{\partial x} + \frac{\partial (\mathbf{B} - \mathbf{B}_v)}{\partial y} + \frac{\partial (\mathbf{C} - \mathbf{C}_v)}{\partial z} - \widetilde{\mathbf{P}}\right)\right]^m \Delta \mathbf{D}^m = \mathbf{R}^m.$$
 (15)

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Therefore, we have linearized the nonlinear system of Eqs. (11) by using Taylor's series expansion to obtain the linearized system of equations given by Eq. (15). Next, we split the matrices **A**, **B** and **C** into positive and negative parts and discretize the split parts with the first-order upwind scheme, and discretize the viscous terms and surface tension matrix operator terms in the LHS with the second-order central difference as follows:

$$[\mathbf{H} + \Delta \tau (\delta_x^- \mathbf{A}^+ + \delta_x^+ \mathbf{A}^- - \delta_x^2 \mathbf{A}_v - \mathbf{P}_x) + \Delta \tau (\delta_y^- \mathbf{B}^+ + \delta_y^+ \mathbf{B}^- - \delta_y^2 \mathbf{B}_v - \mathbf{P}_y)$$
  
+  $\Delta \tau (\delta_z^- \mathbf{C}^+ + \delta_z^+ \mathbf{C}^- - \delta_z^2 \mathbf{C}_v - \mathbf{P}_z)]^m \Delta \mathbf{D}^m = \mathbf{R}^m.$  (16)

In the LHS of Eq. (16), the first-order upwind difference and the second-order central difference schemes used are

$$\delta_x^+ f_i = \frac{f_{i+1} - f_i}{\Delta x}, \quad \delta_x^- f_i = \frac{f_i - f_{i-1}}{\Delta x} \quad \text{and} \quad \delta_x^2 f_i = \frac{(f_{i+1} - f_i) - (f_i - f_{i-1})}{\Delta x^2}.$$

The Beam–Warming AF scheme [Beam and Warming (1978)] which converts a 3D problem into three 1D problems, symbolically written as

$$\pounds \cdot \Delta \mathbf{D}^m \approx \pounds_x \pounds_y \pounds_z \cdot \Delta \mathbf{D}^m = \mathbf{R}^m.$$
<sup>(17)</sup>

In a standard fashion to add cross-derivative terms to the LHS of Eq. (16), which are the same order of  $\Delta \tau^3$  as the truncated terms of the original equations, one can obtain the AF scheme in the form which can be easily solved by alternating direction implicit (ADI) method, i.e.,

$$[\mathbf{H} + \Delta \tau (\delta_x^- \mathbf{A}^+ + \delta_x^+ \mathbf{A}^- - \delta_x \mathbf{A}_v - \mathbf{P}_x)] \Delta \mathbf{D}^{**} = \mathbf{R}^m,$$
(18)

$$[\mathbf{H} + \Delta \tau (\delta_y^- \mathbf{B}^+ + \delta_y^+ \mathbf{B}^- - \delta_y \mathbf{B}_v - \mathbf{P}_y)] \Delta \mathbf{D}^* = \Delta \mathbf{D}^{**}, \tag{19}$$

$$[\mathbf{H} + \Delta \tau (\delta_z^- \mathbf{C}^+ + \delta_z^+ \mathbf{C}^- - \delta_z \mathbf{C}_v - \mathbf{P}_z)] \Delta \mathbf{D}^m = \Delta \mathbf{D}^*.$$
(20)

That is, first solve Eq. (18) for  $\Delta \mathbf{D}^{**}$  then solve Eq. (19) for  $\Delta \mathbf{D}^{*}$  and finally solve Eq. (20) for  $\Delta \mathbf{D}^{m}$  to update the solution at m + 1 pseudo-time level ( $\mathbf{D}^{m+1} = \mathbf{D}^{m} + \Delta \mathbf{D}^{m}$ ). The resulting block tri-diagonal linear system in each direction is

$$\alpha_i \Delta U_{i-1} + \beta_i \Delta U_i + \gamma_i \Delta U_{i+1} = R_i, \quad i = 2, \dots, i \max - 1$$

with appropriate boundary conditions at i = 1 and i = imax.

# 5. Numerical Results

In this section, a number of flow problems in 2D and 3D are simulated to validate the numerical method and test the application of phase-field model for two-phase flows. Relevant details for convergence and volume conservation properties of the method are presented in our previous work [Shah and Yuan (2011)].

#### 5.1. 2D rising bubbles

In our first numerical experiment, we investigate the bubble deformation due to the buoyancy effect and elastic relaxation. The parameters for this problem are:  $\eta = 0.01, \Delta t = 0.01, \beta = 200, \rho_1 - \rho_2 = -1.0$  and g = 9.8. Here,  $\rho_1$  refers to the fluid density inside the bubble,  $\rho_2$  refers to the density of the surrounding fluid that can be taken as the "background" density,  $\rho_0 = \rho_2$ , and this will simplify the buoyancy term to  $-\frac{1+\phi}{2}g(\rho_1 - \rho_2)$  in Eq. (10). We consider a circular bubble of radius  $R_0 = 0.25$  with center at  $\mathbf{x}_c = (0.5, 0.35)$  in the rectangle domain of size  $[0, 1] \times [0, 2.5]$ . Grid resolutions of  $201 \times 551$  can give reasonable results for smaller width  $\eta = 0.01$ . Initially, zero velocity is assumed and the phase function is given by

$$\phi(\mathbf{x}, 0) = \tanh\left(\frac{\|\mathbf{x} - \mathbf{x}_c\| - R_0}{\sqrt{2\eta}}\right)$$

so that  $\phi \approx 1$  inside the bubble and  $\phi \approx -1$  in the surrounding fluid. We performed 60 sub-iterations to get converged solution in pseudo-time at each physical time-step.

From Figs. 2(a)-2(d), we display the time evolution and shape deformation of a rising bubble by plotting  $\phi = 0$ . It can be seen that for surface tension  $\lambda = 0.0$ , viscosity  $\mu = 0.05$  and elastic relaxation  $\gamma = 0.05$ , the bubble rise in the upward y-direction because of the buoyancy force. It attains a steady state with somewhat kidney-shaped bubble as shown in Figs. 2(d)-2(f). In Fig. 3, however, with zero surface tension and  $\mu = \gamma = 0.005$ , a bubble starts rising in the upward direction with a breakup of primary and secondary liquid drops as shown in Figs. 3(f)and 3(h), respectively. Soon, the primary and secondary drops start shrinking as shown in Figs. 3(i)-3(j) and eventually disappear given in Fig. 3(k). The shrinking phenomena which is similar to the Ostwald ripening phenomenon in liquid solutions [https://en.wikipedia.org/wiki/Ostwald\_ripening] is actually due to Allen-Cahn-type (diffusive) approximation of the sharp interface. It causes the smaller bubble to dissolve into the fluid while the bigger bubble to absorb mass from the fluid. It is to be noted that the overall mass of the bubble is still conserved due to the mass transfer from smaller to the lager bubble. It is noted that for large value of surface tension coefficient, the bubble remains nearly circular and rise in a steady state fashion with constant velocity and shape [Rizwan et al. (2016)] while larger values



Fig. 2. Time evolution of the rising 2D bubble interface for  $\lambda = 0.0$  and  $\mu = \gamma = 0.05$ .



Fig. 3. Time evolution of the rising 2D bubble interface for  $\lambda = 0$  and  $\gamma = 0.005$ .

of elastic relaxation parameter can control the breakup of smaller drops. Although, our results agree well with the results in Sussman and Smereka (1997) and Unverdi and Tryggvason (1992) qualitatively, however for accurate representations of the interface location and flow-field require more studies and high resolution (adaptive) grids to better resolve the thin interface profile ( $\eta \rightarrow 0$ ). High grid resolution and smaller width  $\eta$  both may help minimize the coarsening effect of the Allen–Cahntype approximation due to potential difference at the interface Jamet (2001).

## 5.2. 3D rising bubble

As a second numerical experiment, we show the deformation of a fully 3D rising bubble to validate our 3D code. We choose  $\eta = 0.04$ ,  $\lambda = 0.005$ ,  $\mu = \gamma = 0.05$ while  $\Delta t$  and  $\beta$  remain the same as in Sec. 5.1 with a 3D domain of size  $[0, 1] \times [0, 1] \times [0, 2.5]$ . The mesh size is  $101 \times 101 \times 251$ . Similar to previous 2D case, as the simulation starts, the 3D spherical bubble deforms and starts to rise and reach to steady state with a constant shape as shown in Fig. 4.

# 5.3. Coalesces of two bubbles

In this example, coalesces and changes in topology of two 3D interacting bubbles due to the surface tension are considered. Coalescence is the process by which two



Fig. 4. Iso-surface of a 3D rising bubble at time t = 0, 0.5, 1.0, 1.5 and 1.75.



Fig. 5. Coalesces of two bubbles at time t = 0, 0.1, 0.2, 0.5 and 2.0.

or more droplets, bubbles or particles merge during contact to form a larger single droplet, bubble or particle. It can take place in many processes, e.g., the formation of rain drop is due to the coalesces of small droplets in clouds. When the droplets become heavy not to be sustained in the air, it begin to fall as rain. Let the 3D domain is of size  $[0, 2] \times [0, 2] \times [0, 2]$  with a computational grids  $101 \times 101 \times 101$ , respectively, in which two 3D spherical bubbles of equal radius are taken as shown in Fig. 5. As the computation starts, the two bubbles coalesce and first they transform into one elliptic shape bubble, which then transfigures and deforms into a steady state single larger circular bubble.

In Figs. 6(a)-6(c), results from literature for the interaction of two spherical rising bubbles are shown. For comparison purpose, we take two spherical bubbles of radii 0.5 which are centered at (0.7, 0.7, 0.5) and (1.2, 1.4, 1.65), respectively, as shown in Fig. 7 with the density ratio  $\rho_1/\rho_2 = 1/20$ . Now the background density  $\rho_0$  is taken to be  $0.5(\rho_1 + \rho_2)$  such that the buoyancy force  $b = -g\phi(\rho_1 - \rho_2)/(\rho_1 + \rho_2)$  in Eq. (10). Other parameters are  $\eta = 0.04, \lambda = \gamma = 0.01, g = 9.8$  and the solution domain is of size  $[0, 2] \times [0, 2] \times [0, 4]$  with computational grids of  $101 \times 101 \times 201$ , respectively, so that the interfacial zone is fairly resolved by two grid points. This setting is roughly similar to the one used by Di *et al.* [2008], Sussman and Puckett [2000] and Unverdi and Tryggvason [1992]. The topological deformation "mushroom"-like shape can be seen when the bubbles start rising. The top bubble continues deform and draws the lower bubble, a similar behavior given



Fig. 6. Reference results at different time-level for coalescence of two rising bubbles (a) Di *et al.* [2008], (b) Sussman and Puckett [2000] and (c) Unverdi and Tryggvason (1992).



Fig. 7. Coalescence of two rising viscous bubbles in a continuous phase at time t = 0, 0.4, 0.8, 1.0 and 1.2, when the bubbles are not aligned.

in Di *et al.* [2008], Sussman and Puckett [2000] and Unverdi and Tryggvason [1992]. We see a very close resemblance of our results with that of Sussman and Puckett [2000]. Nevertheless, the method, time-scale and parameter settings used and 3D image view may slightly different from the reference solution resulting the difference qualitatively in Figs. 6 and 7. Further studies of parameter estimations and method may help us to establish relation between numerical simulation and experimental results.

# 6. Conclusions

Based on a phase-field model, an implicit 3D method is developed for simulating two-phase flow problems which is capable of capturing essential features of interfacial dynamics and topological changes. The model consists of the incompressible Navier–Stokes equations coupled with mass preserving Allen–Cahn phase-field equation through surface tension term and buoyancy force (Boussinesq approximation). The numerical algorithm is based on ACM which recast the governing equations into conservative form for using numerical methods developed for hyperbolic conservation laws. The high-order high-resolution WENO scheme can capture the sharp interface correctly and avoid spurious oscillation. A number of numerical simulations were performed to validate the method. The major limitation of the method is, of course, insufficient resolution of small interfacial width  $\eta$  if using fixed coarse grid. Also, in spite of being implicit mostly, the numerical scheme still has restricted physical time step because the source terms are hard to be fully implicit. More studies are needed to establish accurately the correspondence between the parameters in the model and those in experiments and sharp interface modeling. In future work, we intend to use adaptive meshes to increase the grid scale locally for phase-field simulation and to go beyond the Boussinesq approximation to solve more challenging multi-phase flow problems with large density and viscosity differences.

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