Simulation of gas bubble dynamics using a phase-field model

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Abstract. The modeling and simulation of gas bubble dynamics is still an active research area, mainly when surface tension is present. One way to model the gas and fluid phases is with interface capturing methods. Three well-established interface capturing models are the Volume-of-Fluid (VOF), level-set, and phase-field models. The main advantage of the VOF method is mass conservation, while the implementation of the surface tension may be challenging. The level-set is known for its ability to compute the surface tension accurately, and phase-field models are known for satisfying the second law of thermodynamics. This work uses a conservative Allen-Cahn equation to model and simulates the effects of the surface tension in gas bubble dynamics. We include concepts of the level-set and VOF methods and verify the energetic stability of the methodology. We also compare the results with the convected level-set method. Results are analyzed and discussed.

Keywords: Phase-Field, Bubble dynamics, Surface tension

1 Introduction

The modeling and simulation of two-phase flows is still an area of active research. Among the several engineering problems involving two-phase flows, the study of bubbles' motion is of fundamental importance in many physical, chemical, and biological processes. Several experimental studies on the bubbles' motion in liquids have been conducted. Although experiments provide reliable results, they are difficult to reproduce, and measuring all quantities of interest can be challenging. Thus, numerical simulation has become an alternative approach for such complicated studies.

In numerical simulations, one of the main issues is to model the motion and deformation of the interface between the two phases. Several methods are used for this purpose, and different approaches have been used to model bubble problems. Three important methods used in this kind of study are the Volume of Fluid (VOF) method [1], the Phase-Field method [2] and the Level-Set method [3].

In this work, we use a conservative Allen-Cahn equation based on [4] to model and simulate the effects of the surface tension in gas bubble dynamics. This method is coupled with the Navier-Stokes equations, which are discretized by the residual-based variational multiscale finite element formulation. Moreover, we consider adaptive mesh refinement based on the flux jump of the phase-field variable errors in our simulations. All implementations in this work uses the `libMesh` library. `libMesh` is an open-source library that provides a platform for parallel, adaptive, multiphysics finite element simulations [5]. The main advantage of `libMesh` is the possibility to focus on the implementation of the modeling-specific features without worrying about issues such as adaptivity and code parallelization. Consequently, it tends to minimize the effort to build a high-performance computing code.

This study aims to predict the behavior of two-phase flows correctly and thus, represent bubbles rising in viscous liquids. The remainder of this paper is organized as follows. Section 2 presents the conservative Allen-Cahn model. Section 3 discusses the governing equations for two-phase incompressible fluid flow. Numerical results for the two-dimensional rising bubble problem are shown in Section 4. The paper ends with a summary of our main findings.

2 Phase-Field model

The phase-field method is used to model the interface between two phases, which considers a diffuse representation of the interface geometry and describes the minimization of the free energy functional [6]. The diffuse interface between the two phases is described as a region where the phases are mixed and store the free energy. Concerning the computational efficiency and stability, we employ the Allen-Cahn phase-field equation with a Lagrange multiplier for solving two-phase flow problems in the current study. Therefore, the motion of the phase-field is described by:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi - \gamma(t)\left(\epsilon^2 \nabla^2 \phi - F'(\phi) + \beta(t)\sqrt{F(\phi)}\right) = 0 \tag{1}$$

where ϕ represents the mixture of the phases (pure phases are ϕ = 1 and ϕ = -1), $\mathbf{u}$ is the velocity field, $\gamma(t)$ is a time-dependent mobility coefficient, given by,

$$\gamma(t) = \frac{1}{\eta}\mathcal{F}\left(\left|\frac{\nabla \phi \cdot \mathbf{u} \cdot \nabla \phi}{|\nabla \phi|^2}\right|\right) \tag{2}$$

where $\mathcal{F}(\psi(\mathbf{x}, t)) = \sqrt{\frac{\int_\Omega (\psi(\mathbf{x},t))^2 d\Omega}{\int_\Omega 1 d\Omega}}$ and η is the RMS convective distortion parameter. ϵ is the thickness of the diffuse interface layer (we define $\epsilon = h_e$). The term $F'(\phi)$ denotes the derivative of $F(\phi)$ with respect to ϕ, being $F(\phi)$ the double-well energy potential $F(\phi) = \frac{1}{4}(\phi^2 - 1)^2$. The parameter $\beta(t)$ is the time dependent part of the Lagrange multiplier, given by,

$$\beta(t) = \frac{\int_\Omega F'(\phi) d\Omega}{\int_\Omega \sqrt{F(\phi)} d\Omega} \tag{3}$$

$$\phi(R) = \tanh\left(\frac{R}{\sqrt{2}\epsilon}\right) \tag{4}$$

3 Navier-Stokes equations

The Navier-Stokes equations govern the fluid flow, which lead to the following nonlinear mathematical problem to be solved: let us consider a space-time domain in which the flow takes place along the interval $[0, t_f]$ given by $\Omega \subset R^{nsd}$, where nsd is the number of space dimensions. Let Γ denote the boundary of Ω. Find the pressure p and the velocity $\mathbf{u}$ satisfying the following equations [4]:

$$\rho(\phi)\frac{\partial \mathbf{u}}{\partial t} + \rho(\phi)\mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - \nabla \cdot (\mu(\phi)\nabla \mathbf{u}) - \rho(\phi)\mathbf{g} + \mathbf{sf}(\phi) = 0 \text{ in } \Omega \times [0, t_f] \tag{5}$$

$$\nabla \cdot \mathbf{u} = 0 \text{ in } \Omega \times [0, t_f]. \tag{6}$$

where ρ is the density, μ is the dynamic viscosity and $\mathbf{sf}(\phi)$ is the surface tension force, given by:

$$\rho(\phi) = \frac{1+\phi}{2}\rho_1 + \frac{1-\phi}{2}\rho_2 \tag{7}$$

$$\mu(\phi) = \frac{1+\phi}{2}\mu_1 + \frac{1-\phi}{2}\mu_2 \tag{8}$$

$$\mathbf{sf}(\phi) = \sigma \kappa \mathbf{n}_\phi \delta_S \tag{9}$$

The implementation is done considering $\kappa = \nabla \cdot \left(\frac{\nabla \phi}{|\nabla \phi|}\right)$, $\mathbf{n}_\phi = \frac{\nabla \phi}{|\nabla \phi|}$, $\delta_S = \alpha \epsilon |\nabla \phi|^2$ and $\alpha = \frac{3\sqrt{2}}{4}$, that leads to [7, 8]:

$$\mathbf{sf}(\phi) = \sigma \nabla \cdot (\mathbf{n}\phi) \nabla \phi \frac{3\sqrt{2}}{4}\epsilon |\nabla \phi| \tag{10}$$

where σ is the surface tension coefficient. $\alpha = \frac{3\sqrt{2}}{4}$ is a constant derived by the property of the Dirac delta function. The order parameter ϕ needs to be locally in the equilibrium state. Hence, to match the surface tension of the sharp-interface description, α must satisfy the following condition

$$\epsilon\alpha \int_{-\infty}^{+\infty} \left(\frac{d\phi}{dR}\right)^2 dR = 1 \tag{11}$$

which leads to $\alpha = \frac{3\sqrt{2}}{4}$. R is the coordinate normal to the interface.

4 Two-dimensional rising bubble

We simulate two benchmarks proposed by [9] (case A and case B). The task of the proposed benchmarks is to track the evolution of a two-dimensional bubble rising in a liquid column, with the initial configuration described in Fig. 1.

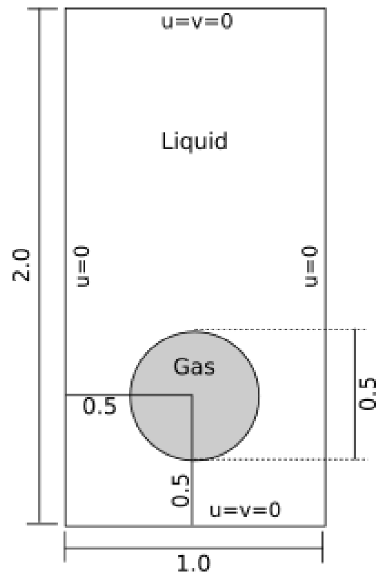


Figure 1. 2D rising bubble: Initial configuration and boundary conditions for the test cases.

The initial configuration is identical for both test cases and consists of a circular bubble of radius $R = 0.25$ m centered at $[0.5, 0.5]$ m in a $[1 \times 2]$ m rectangular domain. The no-slip boundary condition is used at the top and bottom boundaries, whereas the free-slip condition is imposed on the vertical walls. Table 1 lists the parameters used for this simulation.

Table 1. 2D rising bubble: Data.

Computational domain	1×2		(m)
Grid sizes	0.05 to 0.00625		(m)
Number of time steps	960		(-)
Time-step	0.01		s
Bubble radius	0.25		m
Initial bubble position	$(x, y) = (0.5, 0.5)$		m
Liquid density	(A) 1000	(B) 1000	kg/m^3
Liquid viscosity	(A) 10	(B) 10	kg/(ms)
Gas density	(A) 100	(B) 1	kg/m^3
Gas viscosity	(A) 1	(B) 0.1	kg/(ms)
Surface tension	(A) 24.5	(B) 1.96	N/m
Gravity	(A) 0.98	(B) 0.98	m/s^2

We use an adapted mesh, initially with 20×40 bilinear quadrilateral elements, and after the refinement, the smallest element has size 0.00625 m. We initially refine the region where the bubble is located in three levels. The adaptive mesh refinement is based on the flux jump of the phase-field function error. We apply the adaptive mesh refinement every two time-steps. The interface is modeled with $\epsilon = 0.00625$. We define $\eta = 0.05$;

In Fig. 2a, we present the bubble shape at the final time $(t = 3)$ for the test case A. We compare our results with the obtained by [3]. Our prediction is in good agreement with the reference (Fig. 2a). However, the final shape is not sufficient to validate the code. Therefore, we introduce the following quantities of interest, which will be used to assist in describing the temporal evolution of the bubbles quantitatively:

Center of mass. To track the translation of bubbles, it is common to use the center of mass,

$$\mathbf{X_c} = \frac{\int_{\Omega^-} \mathbf{x} dx}{\int_{\Omega^-} 1 dx} \tag{12}$$

where Ω^- denotes the region that the bubble occupies.

Circularity. The "degree of circularity", $\not{c}$, introduced by [10], can be defined as,

$$\not{c} = \frac{P_a}{P_b} = \frac{\text{perimeter of a area-equivalent circle}}{\text{perimeter of the bubble}} = \frac{2\pi R}{P_b}. \tag{13}$$

Here, P_a denotes the perimeter or circumference of a circle with radii R which has an area equal to that of a bubble with perimeter P_b. The perimeter and the area of the bubbles are calculated post-processing the simulation results.

Rise Velocity. The mean velocity, $\mathbf{U_{mean}}$, with which a bubble is rising or moving, is a particularly interesting quantity since it does not only measure how the interface tracking algorithm behaves but also the quality of the overall solution. We define the mean bubble velocity as,

$$\mathbf{U_{mean}} = \frac{\int_{\Omega^-} \mathbf{u} dx}{\int_{\Omega^-} 1 dx}. \tag{14}$$

In Figures 2b, 2c, 2d we compare the circularity, center of mass position, and rise velocity for test case A. All groups have a good agreement for the quantities of interest.

In Fig. 3a, we present the bubble shape at the final time $(t = 3)$ for the test case B. Again, we compare our results with [3]. As shown in [3], although different codes predict a similar shape for the main bulk of the bubble, there is no agreement concerning the thin filamentary regions. There are discrepancies when we compare all quantities of interest. The circularity (Fig. 3b) agrees very well until about $t = 1.75$ seconds, and for later times significant differences start to appear, that is, when the thin filaments are present. The center of mass, shown in Fig. 3c, is predicted similarly despite the shape differences, and the mean rise velocity also presents a quite good agreement between the different codes (Fig. 3d).

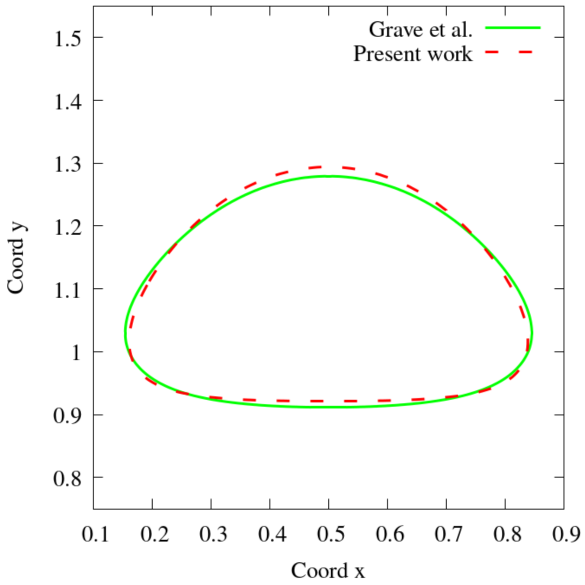
In Figure 4, we show the influence of the mobility coefficient. We show the final phase-field considering a fixed mobility parameter $\gamma = 1$ and the time-dependent one with $\eta = 0.05$. When $\gamma = 1$, the interface preserving capability is insufficient to keep the interface profile against the convective distortion. Therefore, at the bottom of the bubble, the interface is subjected to an observable extensional distortion, which leads to an excessively low Laplace pressure. This distortion changes the bubble shape, decreases the buoyancy force, and further reduces the rise velocity. On the contrary, when the time-dependent mobility model with $\eta = 0.05$ is used, the interface profile is preserved well, which gives a correct bubble shape and surface tension force calculation.

5 Conclusions

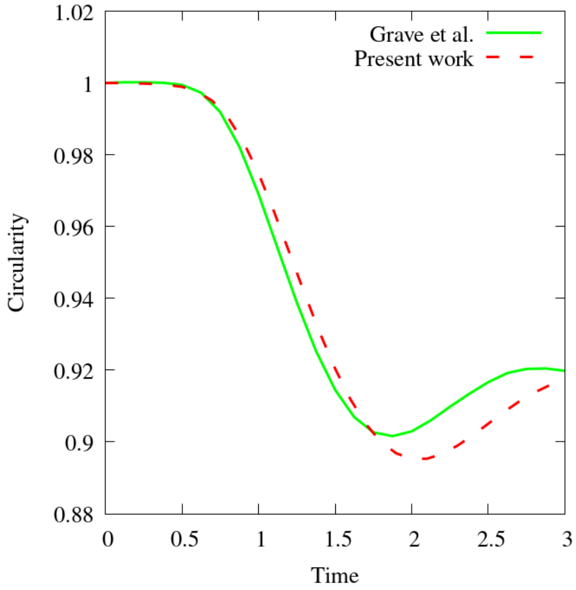
In this work, we develop a procedure capable of predicting two-phase flows, and thus, represent bubbles rising in viscous liquids. To do so, we implement the Allen-Cahn phase-field model with a Lagrange multiplier coupled with the Navier-Stokes equations. We apply the method to solve the 2D rising bubble benchmark, a well-known test case to validate two-phase flow models.

The model provides for each simulation bubbles' quantities of interest very similar to the ones found with the convected level-set, presented in [3]. As the convected level-set model, which is very sensitive to a penalty parameter, the Allen-Cahn phase-field model is very sensitive to the mobility coefficient, which is inversely proportional to the RMS convective distortion parameter η. This sensibility was pointed in [11] and also verified in our simulations.

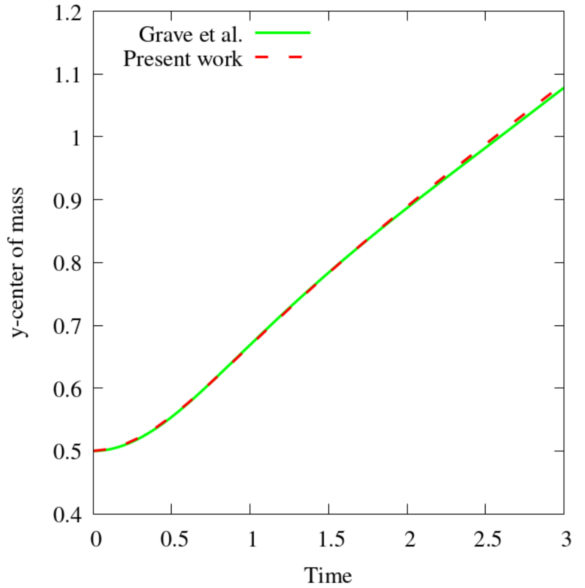
Another fact about the mobility coefficient highlighted in this work is the importance of its being time-dependent. For a fixed mobility coefficient, the phase-field may not be recovered, and, consequently, the surface



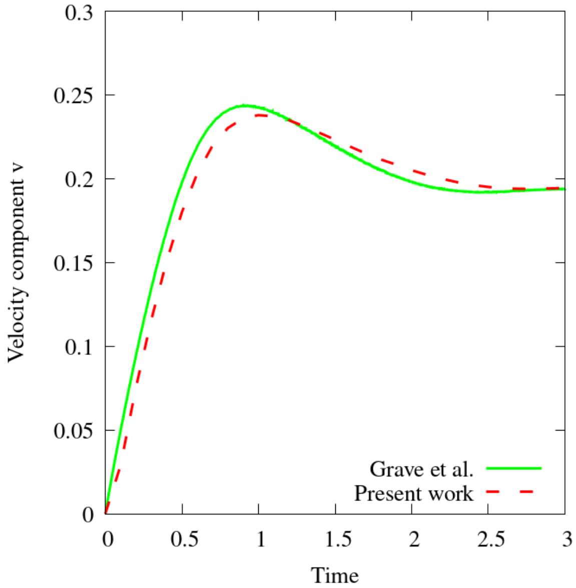
(a) Bubble shape at $t = 3$.



(b) Circularity.



(c) Center of mass.



(d) Rise velocity.

Figure 2. 2D rising bubble: Test A results.

tension is not well evaluated. This lack of accuracy in the surface tension evaluation is similar to what happens when using the convected level-set and a bad choice of the penalty constant.

The use of adaptive mesh refinement based on the flux jump of the phase-field function worked well for the simulations. It is important to point out that the criteria used for the adaptive mesh refinement may change depending on the problem. It is possible to consider the error based on the flux jump of the velocity field together with the phase-field function, for example. The AMR/C procedure may save much computational effort, especially for two-phase flows simulations, in which we need a large refinement near the interface between fluids.

For future works, we would like to extend the simulations to 3D problems and more complex geometries, as splashing and coalescence of bubbles.

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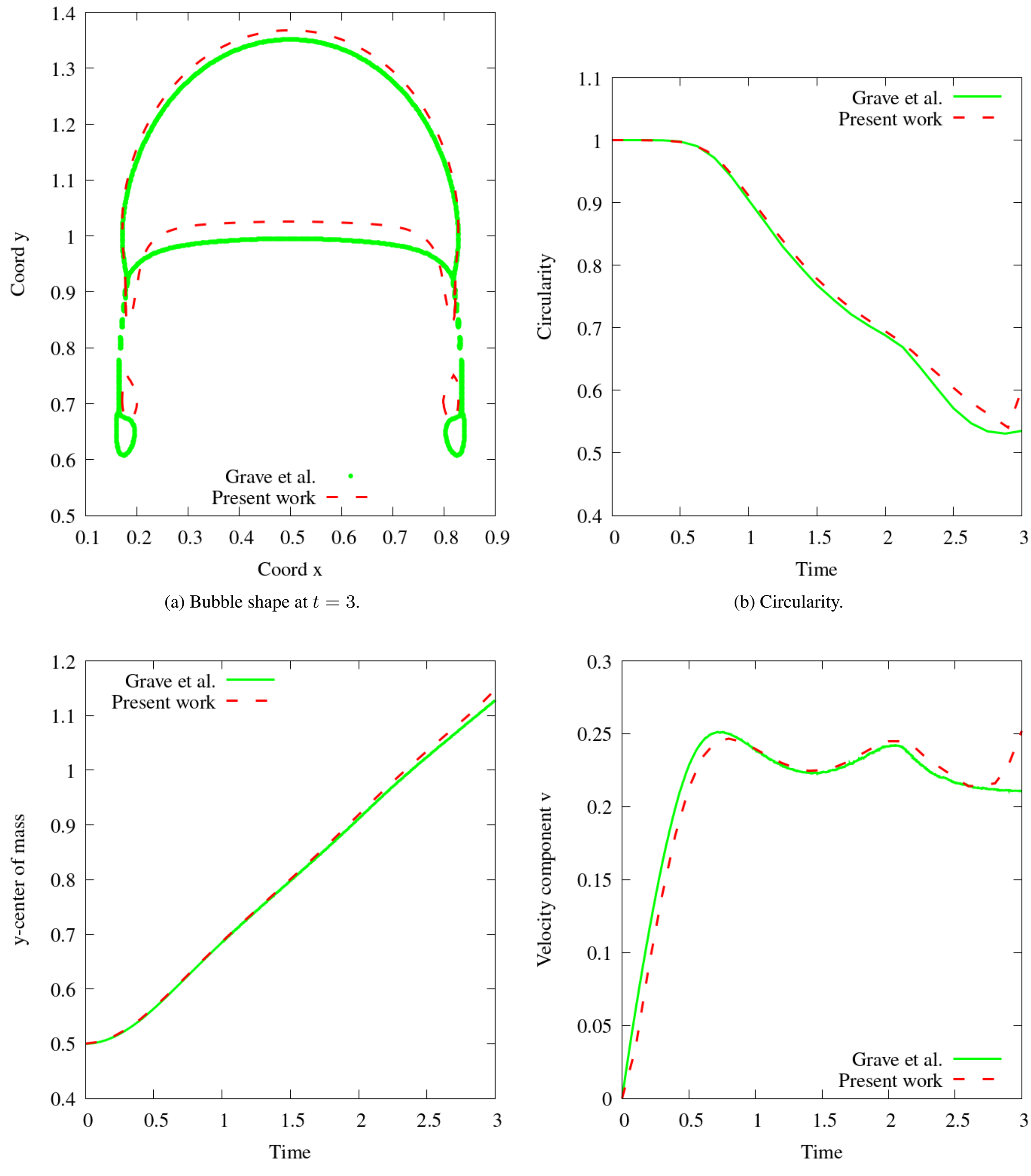

(a) Bubble shape at $t = 3$.

(b) Circularity.

(c) Center of mass.

(d) Rise velocity.

Figure 3. 2D rising bubble: Test B results.

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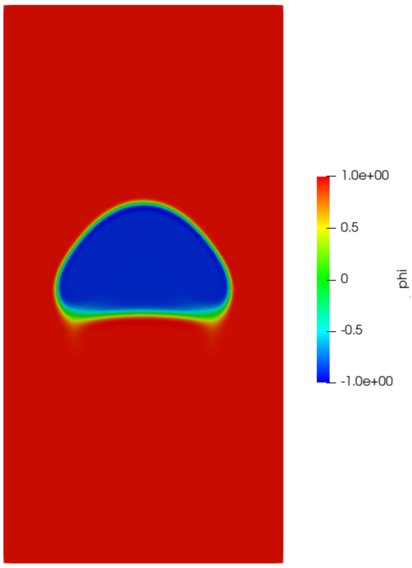
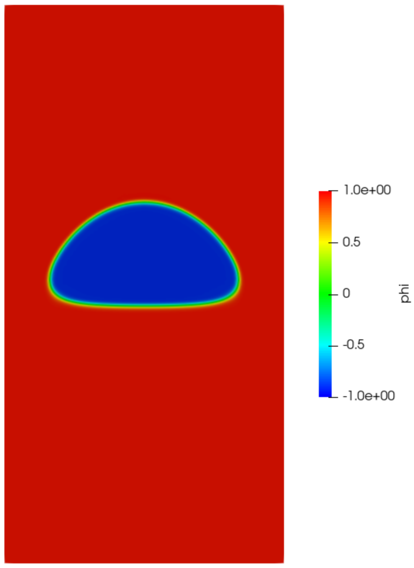


(a) Constant mobility coefficient $\gamma = 1$.



(b) Time-dependent mobility model at $\eta = 0.05$.

Figure 4. 2D rising bubble: Mobility coefficient.

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