On the diffuse interface method using a dual-resolution Cartesian grid

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Abstract

We investigate the applicability and performance of diffuse interface methods on a dual-resolution grid in solving two-phase flows. In the diffuse interface methods, the interface thickness represents a cut-off length scale in resolving the interfacial dynamics, and it was found that an apparent loss of mass occurs when the interface thickness is comparable to the length scale of flows [24]. From the accuracy and mass conservation point of view, it is desirable to have a thin interface in simulations. We propose to use a dual-resolution Cartesian grid, on which a finer resolution is applied to the volume fraction $C$ than that for the velocity and pressure fields. Because the computation of $C$ field is rather inexpensive compared to that required by velocity and pressure fields, dual-resolution grids can significantly increase the resolution of the interface with only a slight increase of computational cost, as compared to the single-resolution grid. The solution couplings between the fine grid for $C$ and the coarse grid (for velocity and pressure) are delicately designed, to make sure that the interpolated velocity is divergence-free at a discrete level and that the mass and surface tension force are conserved. A variety of numerical tests have been performed to validate the method and check its performance. The dual-resolution grid appears to save nearly 70% of the computational time in two-dimensional simulations and 80% in three-dimensional simulations, and produces nearly the same results as the single-resolution grid. Quantitative comparisons are made with previous studies, including Rayleigh Taylor instability, steadily rising bubble, and partial coalescence of a drop into a pool, and good agreement has been achieved. Finally, results are presented for the deformation and breakup of three-dimensional drops in simple shear flows.

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1. Introduction

 Appropriately representing an interface and accurately tracking its evolution are crucial in simulating multiphase flows. A variety of approaches have been proposed in the past decades for interface description, among which volume-of-fluid (VOF), level set (LS) and front tracking (FT) methods are the most popular ones. To geometrically define an interface, VOF and LS methods use a scalar field, while FT methods use a set of linked markers. In the presence of surface tension, a smoothed delta function or equivalent is often used to transform the singular surface forces into continuous body forces localized in the interface region [1]. Despite of first-order accuracy in dealing with the jump conditions at the interface,
the concept of continuous surface tension has been widely adopted by VOF [2-4], LS [5-8] and FT methods [9,10] in solving two-phase flows, due to its simplicity of coding and high effectiveness. The interface thickness in these methods is prescribed by the specific Heaviside function and varies from two to four grid spacings. It also represents a cut-off length scale in resolving the interfacial fluid dynamics, such as waves and topological changes. In principle, the thinner the interface thickness, the more accurate the numerical results. To reach a balance between the computational costs and interface resolution, one may consider to use the technique of adaptive grid refinement [11,12], which allows to put the dense grid locally at the place of interest, e.g. interface region. In the present paper, we resort to an alternative way of improving the computational efficiency, namely dual-resolution grid, on which the two different resolutions are used for the scalar field and the velocity (and pressure), respectively.

We use a diffuse interface (DI) method, precisely the convective Cahn–Hilliard model, to track the time evolution of an interface [13,14]. The mathematically sharp interface is replaced by a thin layer or diffuse interface, across which the jumps in flow properties such as viscosity and density are smeared to some extent and so does the tangential velocity gradient (see [15] for an extensive review). Because of easy implementation and the ability of maintaining mass conservation and accurate computation of surface tension, the DI method enjoys increasing popularity in the simulation of two-phase flows; so far it has been used for a wide range of applications including non-Newtonian fluid [16], Hele–Shaw flows [17], droplet ejection [18] and moving contact lines [19-22].

The interface can be described by the volume fraction of one fluid \( C \) \((0 \leq C \leq 1)\) [23,14]. The interface thickness is determined by an artificial parameter \( \epsilon \), which is normally proportional to the grid size \( h \). If the interface region is defined by \( 0.1 \leq C \leq 0.9 \), which contains 98.5\% of the surface tension force [13], the interface thickness (the distance between the contours \( C = 0.1 \) and \( 0.9 \)) is about 8.26\( \epsilon \). In order to maintain the interfacial profile as the equilibrium state and accurately compute the interface tension force, the value of \( \epsilon \) cannot be arbitrarily small and normally ranges from 0.5\( h \) to \( h \), corresponding to the range of interface thickness from 4.13\( h \) to 8.26\( h \). This suggests that the interface thickness in the DI method is generally larger than those in the VOF, LS and FT methods on the same grid. On the other hand, it was found when the interface thickness becomes comparable to the characteristic length scale of the flow, e.g. droplet radius, the volume fraction \( C \) tends to deviate from the expected value in the bulk phases, leading to an apparent loss of mass [24]. Therefore, it is rather desirable for the DI method to use a dual-resolution grid, which allows for a finer resolution for the C field.

The idea of dual-resolution was previously suggested by [13], however, it was not implemented. Furthermore, the way of refining the grid for the C field recommended in [13] may not ensure the interpolated velocity for the advection of C field satisfies the divergence-free constraint at a discrete level, which would eventually result in a loss of mass. We therefore investigate the performance of the DI method in simulating two-phase flows using the present configuration of dual-resolution grid (as shown in Fig. 1), in which the grid size for the C field is only half of that for the velocity and pressure field. It shows that the mass conservation can be well maintained on the present dual-resolution grid, which is confirmed theoretically and numerically. Because the computation of the C field is much less expensive than that of the velocities and pressure field, it is anticipated that the dual-resolution grid can double the resolution of the interface, with only a slight increase of computational cost, compared to a single-resolution grid.

The paper is organized as follows: We first introduce in Section 2 the present dual-resolution grid and the spatial arrangements of the flow variables. Then, we investigate the solution coupling between the grids of different resolutions, to ensure that mass and surface tension force are conserved in this process, and that the velocity field interpolated from the coarse grid to the fine one satisfies the discrete divergence-free constraint. In Section 3 we investigated numerically the convergence and mass conservation of the DI method on the dual-resolution grid, and check the efficiency improvement by comparing with the run on a single-resolution grid. A variety of test cases have been selected to validate the method. The effect of Peclet number in the Cahn–Hilliard equation is tested by studying the nonlinear evolution of Rayleigh–Taylor instability in the absence of surface tension. We compare the results of a steadily rising bubble in liquid and the partial coalescence of a drop into a pool against the benchmark solutions from previous studies. Finally, we apply the method to simulate the deformation and breakup of three-dimensional drops in simple shear flows.

2. Numerical methodology

2.1. Governing equations

We consider here the flow of two incompressible immiscible fluids, and the interface separating the two fluids is represented by a diffuse interface model [13,14]. In the diffuse interface model, the mathematically sharp interface is replaced by an interfacial region of finite thickness, represented by contours of the volume fraction \( C \) of one of the fluids \((0 \leq C \leq 1)\). The time evolution of \( C \) field is governed by the convective Cahn–Hilliard (CH) equation,

\[
\frac{\partial C}{\partial t} + \nabla \cdot (u C) = \frac{1}{Pe} \nabla^2 \phi,
\]

where \( u \) is the flow velocity, \( \phi \) \((= \phi'(C) - \phi''t^2v^2C)\) the chemical potential, and \( \phi = \phi' = C^2(1-C)^2/4 \) is the bulk energy density. \( Pe \) is the Peclet number, representing the relative significance of convective fluxes to the diffusive fluxes.
To achieve the sharp interface limit with continuous mesh refinement, $Pe = \alpha/Cn$ is recommended in [25], where $\alpha$ is a constant.

The viscosity $\mu$ and density $\rho$ of the fluid with $C = 1$ are used to define the dimensionless numbers, and the viscosity (density) of the other fluid is denoted by $\lambda\mu/\rho$ ($\lambda\rho/\rho$). The governing equations for flow motion are then the dimensionless Navier–Stokes (NS) equations,

$$
\frac{\partial \bar{u}}{\partial t} + \nabla \cdot (\bar{u} \bar{u}) = -\nabla p + \frac{1}{Re} \nabla \cdot [\bar{\mu} (\nabla \bar{u} + \nabla \bar{u}^T)] + \frac{f_s}{We} - \frac{\bar{\rho}}{Fr} j,
$$

$$
\nabla \cdot \bar{u} = 0,
$$

where $j$ denotes the vertical unit vector. The dimensionless viscosity $\bar{\mu}$, density $\bar{\rho}$ and surface tension force $f_s$ are respectively approximated by,

$$
\bar{\mu} = C + (1 - C)\lambda\mu,
$$

$$
\bar{\rho} = C + (1 - C)\lambda\rho,
$$

$$
f_s = 6\sqrt{2}\psi \nabla C/Cn.
$$

Dimensionless groups are the Reynolds number $Re = \rho UL/\mu$, Weber number $We = \rho U^2 L/\sigma$, and Froude number $Fr = U^2/(gL)$, where $g$ is gravitational acceleration, and $U$ the characteristic velocity. We shall also refer to the Ohnesorge number $Oh = \sqrt{We}/Re$. Unless otherwise mentioned, $Pe = 0.5/Cn$ is used in the present study.

2.2. Discretization on a dual-resolution grid

We use a dual-resolution grid, on which the flow variables are located at different positions, for the finite volume discretization of the governing equations (1)–(3) (Fig. 1). The pressure and velocity components are defined in a staggered manner, with the pressure at the cell center and the velocity components at the cell faces. The volume fraction field is only half of that for the other flow variables, and that CH equation is effectively solved on a finer grid than the equations of conservation of momentum and mass (i.e. Eq. (2) and Eq. (3)). For convenience, we shall refer to the grid with the pressure and velocity as coarse grid, and the grid with $C$ as fine grid thereafter.

It is known that solving the pressure Poisson equation in the projection method normally consumes most of the computational time in unsteady flow simulations. Comparatively, the computational time required in the advection of $C$ field is much less expensive. Therefore, it is reasonably expected that the use of the dual-resolution grid can considerably improve the interface resolution at the expense of only slight increase in computational effort. We use here an over-relaxation acceleration technique such as multigrid schemes, which are compatible with the dual-resolution grid, can also be employed.

In time the $C$ field is defined at the time levels $t^{n+1/2}$, while the velocity and pressure are defined at $t^n, n = 1, 2, 3, \ldots$. The discretization of CH and NS equations are also performed in a temporally staggered manner. Eq. (1) is discretized at the time level $n$,

$$
\frac{C^{n+1/2} - C^{n-1/2}}{\Delta t} = \left\{ -\nabla \cdot (u^F C) + \frac{1}{2Pe} \nabla^2 (C - 3C^2 + 2C^3) \right\}^{AB} - \frac{Cn^2}{Pe} (\nabla^4 C)^{CN},
$$

where $\Delta t = t^{n+1} - t^n$ is the time step, and the superscripts $AB$ and $CN$ denote the second-order Adams–Bashforth scheme and Crank–Nicolson scheme, respectively. For a function $f(C)$, $f^{AB}(C^n) = [3f(C^{n-1/2}) - f(C^{n-3/2})]/2$ and $f^{CN}(C^n) = [f(C^{n+1/2}) + f(C^{n-1/2})]/2$. To start this scheme, both $C^{-1/2}$ and $C^{1/2}$ are set to the initial condition of the $C$ field. $u^F$ is the
velocity defined at the faces of the control volume of \( C \) on the fine grid (Fig. 2(left)), and is required to be interpolated from \( \mathbf{u}^C \) on the coarse grid, which are the solutions of NS solver; details of the interpolation scheme are provided in Section 2.3. In the finite volume formulation, the values of \( C \) at these cell faces in Fig. 2(left) are also required; they are evaluated with a fifth-order weighted essentially non-oscillatory (WENO) scheme, using the local flow velocity to determine the upwind direction. The time step has a scale of \( h^2 \) for stable computation.

The momentum equation (2) is discretized at the time level \( n + \frac{1}{2} \) as follows:

\[
\rho^{n+\frac{1}{2}} \left( \mathbf{u}_i^{n+1} - \mathbf{u}_i^n \right) = -\nabla p^{n+\frac{1}{2}} - \mathbf{H}^{AB} + \mathbf{L}^{C} + \frac{\mathbf{f}_s^{n+\frac{1}{2}}}{We} - \frac{\rho^{n+\frac{1}{2}}}{Fr} \mathbf{j},
\]

where the advective term \( \mathbf{H} = \rho^{n+\frac{1}{2}} (\nabla \cdot \mathbf{u}) \) and the viscous term \( \mathbf{L} = \frac{1}{Re} \nabla \cdot [\mu^{n+\frac{1}{2}} (\nabla \mathbf{u} + \nabla \mathbf{u}^T)] \). \( \rho^{n+\frac{1}{2}}, \mu^{n+\frac{1}{2}} \) and \( \mathbf{f}_s^{n+\frac{1}{2}} \) are the respective functions of \( C^{n+\frac{1}{2}} \). The coupling of Eqs. (2) and (3) is achieved by using a standard projection method. Unless otherwise mentioned, central difference schemes are used for the spatial discretization of the governing equations.

### 2.3. Solution coupling between the coarse and fine grids

Appropriate coupling of solutions between the coarse and fine grids is crucial for accurate computation of the interface evolution. On the coarse grid, solving the momentum equations (6) requires the calculations of the averaged density, viscosity and surface tension force, which are explicitly related to an integration of \( C \) field over the respective control volume on the fine grid. A two-dimensional example of integrating a function \( f(C) \) is shown in Fig. 3. Clearly, the integral of \( f \) over a control volume \( \Omega_{i,j} \) can be approximated with second-order accuracy by,

\[
\int_{\Omega_{i,j}} f^C d\Omega \approx h^2 \left\{ f_{i,j}^f + \frac{1}{2} (f_{i-1,j}^f + f_{i+1,j}^f + f_{i,j-1}^f + f_{i,j+1}^f) + \frac{1}{4} (f_{i-1,j-1}^f + f_{i-1,j+1}^f + f_{i+1,j-1}^f + f_{i+1,j+1}^f) \right\},
\]

where the superscripts \( F \) and \( C \) denote \( f \) values on the fine and coarse grids, respectively. Then, it is easy to obtain

\[
f_{i,j}^C = \frac{1}{16} (4f_{i,j}^F + 2f_{i-1,j}^F + 2f_{i+1,j}^F + 2f_{i-1,j}^F + 2f_{i,j-1}^F + f_{i,j+1}^F + f_{i+1,j-1}^F + f_{i+1,j+1}^F).
\]

Therefore, these flow variables related to \( C \) field, e.g. as in Eq. (4), can be calculated accordingly on the coarse grid. It is easy to confirm that the mass and surface tension force, of which the potential form is used here, are conserved.
On the other hand, the interface motion is tightly coupled with the velocity field governed by the NS equations, i.e. $u^C$ on the coarse grid. However, the velocity $u^F$ on the fine grid is needed for the advection of the $C$ field. A velocity interpolation scheme is thus required for this purpose, to associate $u^F$ with $u^C$. It is worthwhile to note that the interpolated $u^F$ must satisfy the divergence-free constraint at the discrete level, in order to conserve the mass. Taking the cell $I$ in Fig. 2(left) as an example, the velocity components of $u^F$ should obey,

$$u^F_{i+1/2,j} - u^F_{i-1/2,j} + v^F_{i,j+1/2} - v^F_{i,j-1/2} = 0. \tag{9}$$

A bilinear interpolation scheme with second-order accuracy is selected in this regard, and the interpolation schemes for the velocity components of $u^F$ at various positions are listed below,

$$u^F_{i+1/2,j} = \frac{1}{4}(u^C_{i-1,j} + 3u^C_{i+1,j}),$$

$$u^F_{i+1/2,j-1} = \frac{1}{8}(u^C_{i-1,j} + 3u^C_{i+1,j} + 3u^C_{i+1,j-2} + u^C_{i-1,j-2}),$$

$$v^F_{i,j-1/2} = \frac{1}{4}(v^C_{i,j+1} + 3v^C_{i,j-1}),$$

$$v^F_{i+1,j-1/2} = \frac{1}{8}(v^C_{i,j+1} + 3v^C_{i,j-1} + 3v^C_{i+2,j-1} + v^C_{i+2,j+1}). \tag{10}$$

The interpolation scheme (10) ensures that the interpolated $u^F$ satisfies the discrete continuity equation like Eq. (9), if the velocity $u^C$ satisfies the discrete continuity equation (see Appendix A). Since the velocity $u^F$ is the solution of NS equations and has been made divergence-free in the projection step, it justifies the selection of the scheme (10). Higher order interpolation methods may provide more accurate prediction of $u^F$, however, our numerical experiments showed that they appear to result in mass loss. For non-uniform meshes we do not find a linear interpolation similar to Eq. (10) to obtain a divergence-free $u^F$, mainly due to the asymmetry of the mesh cells.

Although only two-dimensional examples are presented here, an extension of Eq. (10) to three-dimensional cases is straightforward. However, the interpolation scheme in Eq. (10) cannot be directly applied to axisymmetric simulations, in which the discretization of the continuity equation is different from the two-dimensional cases. An alternative interpolation scheme is proposed in this regard; details are provided in Appendix A.

3. Results and discussion

Three axisymmetric and one three-dimensional cases are deliberately chosen to test the performance of the diffuse interface model on the dual-resolution grid, including rising bubbles, Rayleigh–Taylor instability, partial coalescence of a drop into a pool, and drop deformation in shear flows. The case of a rising gas bubble in water is primarily used to investigate the convergence and mass conservation of the method on the dual-resolution grid, as well as the improvement of the computational efficiency compared to uniform Cartesian grids. Rayleigh–Taylor instability is used to validate the model, particularly in the absence of surface tension force. The case of partial coalescence of a drop into a pool, is selected to examine the performance of the dual-resolution grid in the presence of topological changes of the interface. The last case, drop deformation in shear flows, is used to show the performance of the method in the three-dimensional applications.

For the purpose of illustration, the interface location is represented by the contour of $C = 0.5$. Unless otherwise mentioned, the value of $Cn$ is set to 0.5$h_C$, where $h_C$ is the grid size for the $C$ field.

3.1. Convergence and mass conservation tests

We consider here a rising gas bubble in liquid within a cylindrical container, in order to test the convergence and mass conservation of the diffuse interface methods on a dual-resolution grid. The liquid properties and the diameter of the initial bubble $D$ are selected to define the Bond number $Bo = \rho_L g D^2/\sigma$ and Reynolds number $Re = \rho_L g^{0.5} D^{1.5}/\mu_L$, in which the subscript $L$ denotes the liquid. The corresponding time scale is $\sqrt{D/\rho_L}$, and the density and viscosity ratio of the gas to the liquid are 0.001 and 0.01, respectively. The computational domain is set to $(0.2D) \times (0.4D)$ in the cylindrical coordinates, with symmetric condition at the left boundary and slip boundary conditions at the other boundaries. The bubble initially rests at a distance of 0.5D to the bottom wall, and then moves upwards due to the buoyancy force.

Three values of $h_C$ have been used for the convergence study, i.e. 0.025, 0.0125 and 0.00625, and the results at $t = 1.5$ are shown in Fig. 4 in terms of bubble shapes, for both the dual-resolution grids and the single-resolution staggered grids. We see that the bubble shapes obtained on the dual-resolution grids are in good agreement with those on the single-resolution staggered grids with the same $h_C$, and in fact they are nearly identical with $h_C = 0.00625$. On the other hand, the results on the dual-resolution grid also appear to converge with the successive refinement of $h_C$. The inset of Fig. 4 shows that with increasing resolution the bubble shapes converge to the solution with the finest resolution, i.e.
Fig. 4. Comparison of rising-bubble shapes at $t = 1.5$ obtained on single-resolution staggered grids and dual-resolution grids, with $Re = 3.57$, $We = 19.47$ and $Fr = 0.17$. Three values of $h_C$ have been used, i.e. 0.025, 0.0125 and 0.00625, and the corresponding results on the dual-resolution grid and the single-resolution staggered grids are represented by the solid and dash-dotted lines, respectively. The dashed line represents the results on the dual-resolution grid, with $h_C = 0.00313$. The arrow indicates the direction of decrease in the grid size.

Fig. 5. Bubble shapes in terms of $C$ contours of 0.1 and 0.9 on the dual-resolution grid with $h_C = 0.0125$ (dash-dotted), 0.00625 (solid) and 0.00313 (dashed). These are the same cases as in Fig. 4.

Table 1

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<th>Percentage (%)</th>
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of 0.00313. The variation of bubble shapes on the different meshes, notably at the bottom, results from the numerical difficulty of the physical problem. The significant density contrast between the liquid and the gas leads to a big difference in flow acceleration across the interface. Particularly, the resulting straining flow at the bubble bottom tends to stretch the interface, and consequently increases the local thickness of the diffuse interface. Such local deviation of interface profile from the equilibrium becomes insignificant when the value of $Cn$ is sufficiently small, and as a result, the interface thickness is nearly uniform along the bubble surface as shown in Fig. 5. Mass conservation is an important issue in multiphase flow simulations. We check the total volume of the bubble by integration of the $C$ field over the whole domain (see [14] for details), and find that the mass loss is in the order of $10^{-6}$ of the initial bubble volume. This suggests the mass loss is negligible during the computation.

Table 1 shows the efficiency improvement of the diffuse interface method using a dual-resolution grid as compared against that using a single-resolution grid with the same resolution of $C$ field. Computations are performed on a single thread of an Intel CPU (Xeon 5660, 2.8 GHz) with 32 GB memories. It is shown that a running up to 100 time steps on the dual-resolution grid requires less than one third of the CPU time needed on the single-resolution grid in axisymmetric (two-dimensional) simulations, and nearly one-fifth of the CPU time in three-dimensional simulations. Therefore, we can say that the dual-resolution grid is able to achieve an equivalent accuracy as the single-resolution grid, and more importantly, significantly improves the computational efficiency.
3.2. Validations and applications

3.2.1. Rayleigh–Taylor instability

When a heavy fluid $A$ is placed on a light fluid $B$, it is anticipated that any perturbation at the fluid–fluid interface would lead to the occurrence of Rayleigh–Taylor instability subject to the gravitational acceleration. The characteristic parameter in this phenomenon is the Atwood ratio

$$At = (\rho_A - \rho_B)/(\rho_A + \rho_B).$$

The growth of Rayleigh–Taylor instability has been widely investigated, including inviscid flows [26], viscous flows [27] and flows with surface tensions [28]. We consider here a two-dimensional test case at $At = 0.50$, $Re = 3000$ and with no surface tension. The fluids are assumed to have the same dynamic viscosity $\mu$. Computations are performed in a rectangular domain $[0, d] \times [0, 4d]$, with the interface initially being located at $y(x) = 2d + 0.1d \cos(2\pi x/d)$, which corresponds to a planar interface superimposed by a perturbation of wave number $k = 1$ and amplitude $0.1d$. In the absence of surface tension, the CH equation can be viewed as a passive interface tracker.

A dual-resolution grid is used here with the resolutions of $hC = 0.005$ and $Cn = 0.0025$. The comparison between results for two different values of $Pe$ is presented in Fig. 6, in terms of the variations of the $y$-coordinate of the top of the rising fluid and the bottom of the falling fluid with time. The results at $Pe = 0.1Cn^{-1}$ are in good agreement with the benchmark solutions [27], however, at $Pe = 0.5Cn^{-1}$ the top of the rising fluid gradually deviates from the benchmark solutions. Fig. 7 shows the snapshots of these results at two different times, superimposed by the solutions obtained on a uniform grid with the same resolution of the $C$ field. At $Pe = 0.5Cn^{-1}$ some perturbations occur at the early stage of Rayleigh–Taylor instability, propagating towards the top of the interface and growing with time. It appears that these unphysical perturbations arise from the velocity interpolation, and can be removed by using a smaller $Pe$, e.g. $Pe = 0.1Cn^{-1}$. On the other hand, some fine features of fluid interface (e.g., the cusp and satellite drop), of which the scale is comparable to the interface thickness, are different between the single-resolution and dual-resolution simulations in Fig. 7. These generally under-resolved interface features will gradually mix with the outer bulk fluid, resulting in an apparent loss of mass (in terms of the area enclosed by the contour of $C = 0.5$) [24]. The use of a smaller $Pe$ in the dual-resolution simulation clearly accelerates this process.

3.2.2. Steadily rising bubble

Driven by the buoyancy force, a bubble of sufficiently small size may eventually reach a quasi-steady state, rising at a constant speed $V$ and maintaining a shape at equilibrium. The steady state of the rising bubble can be described by the

![Fig. 6. Rayleigh–Taylor instability at $At = 0.50$ and $Re = 3000$: Positions of the top of the rising fluid and the bottom of the falling fluid as a function of time.](image)

![Fig. 7. Comparison of snapshots at $t = 1.41$ (left) and 2.48 (right). Red dashed lines denote the results on dual-resolution grid at $Pe = 0.5Cn^{-1}$, blue dash-dotted lines the results on the dual-resolution grid at $Pe = 0.1Cn^{-1}$, and solid lines the results on a single-resolution grid with the same $hC$ as the dual-resolution grid. Note that the dash-dotted lines virtually overlap with the solid lines. This is the same case as in Fig. 6. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)](image)
Reynolds number $Re = \frac{\rho g V D}{\mu L}$ and Weber number $We = \frac{\rho g V^2 D}{\sigma}$, where $D$ is the diameter of the initial bubble. The setup of the simulation is similar to that in Section 3.1, except that a larger computational domain is employed, i.e., $[12D] \times [9D]$, and that periodic boundary conditions are enforced at the upper and lower boundaries. The computations are performed on the dual-resolution grid with $h_C = 0.0075$ and $Cn = 0.00375$, and the runs stop until the bubble reaches the quasi-steady state. Results at two different sets of $We$ and $Re$ are shown in Fig. 8, in terms of equilibrium bubble shapes, and are compared with the experimental results from [39] and numerical results from [40], respectively. It can be seen that our results are virtually overlapped with the results from literatures. It is noteworthy that the velocities of the rising bubble are 1.015 (at $Re = 3.57$ and $We = 19.47$) and 0.983 (at $Re = 11.65$ and $We = 13.56$), indicating that the rising speed of the bubble is also in good agreement with the previous results.

### 3.2.3. Partial coalescence of a drop into a pool

Droplet coalescing with a pool of the same fluid has been receiving attentions of researchers in fluid mechanics, because it is not only commonly seen in nature and engineering applications [29,30], but also involved with complex flow phenomena [31,32]. We consider here a small droplet initially resting on the interface and subsequently coalescing with the pool due to surface tension force. The droplet radius is assumed to be smaller than the capillary length $\lambda_c = \sqrt{\frac{\sigma}{\rho g}}$, and therefore the effect of the gravitational force is neglected. The process is then characterized by the Ohnesorge number $Oh = \frac{\mu L}{\sqrt{\rho g \sigma R}}$, where $\mu L$ and $\rho L$ are the viscosity and density of the liquid, respectively; $R$ is the radius of the initial droplet and also the characteristic length. We choose the inertia-capillary time $T_{ic} = \frac{\sqrt{\rho g R^3}}{\sigma}$ as the characteristic time scale. The viscosity and density ratios of the gas to the liquid are set to be 0.01 and 0.001, respectively. The initial configuration of the computation is shown in Fig. 9. The computation is axisymmetric and performed in a domain of $6R \times 6R$ with $h_c = 0.006$ and $Cn = 0.003$.

A typical example of the partial coalescence of a droplet into the pool is shown in Fig. 10 at $Oh = 0.0053$, in which the droplet is deformed by the capillary waves generated by the coalescence, with its top gradually evolving into a cylindrical column higher than the initial droplet. A neck subsequently forms and eventually a daughter droplet is pinched off from the top, with a radius of 0.53. The size of the daughter drop is consistent with the experimental observations, ranging from 0.50 [33] to 0.55 [34]. The snapshots of the interface at $t = 1.26$ and 1.7 are shown in Fig. 11, together with the numerical results from [35]. It appears that our results are nearly overlapped with those from [35]. The pinch-off of the daughter droplet starts approximately at $t = 1.7$, also in good agreement with previous experiments [32].

The mechanism of the pinch-off process has been numerically studied by [36] and it appears not to be the Rayleigh instability. It was shown in [18] that the inviscid breakup dominates the pinch-off process, which exhibits a self-similar behavior when approaching the rupture and follows the theoretical analysis of [37]. Fig. 12 shows the interface shapes after the self-similar rescaling by the radius ($R_{min}$) and the vertical position ($z_{min}$) of the neck. We can see that the result of the theoretical analysis is approached asymptotically by the numerical results, which further validates the accuracy of the diffuse interface method on the dual-resolution grid.
Fig. 10. Time evolution of partial coalescence of a drip into a pool at $Oh = 0.0053$, at times $t = 0, 0.63, 1.26, 1.70, 1.80, 1.90$, respectively. Time increases from the left to the right, and from the upper to the lower.

Fig. 11. Comparison of interface shapes against the results in [35]. Left: Formation of a cylindrical column at the top ($t = 1.26$), and right: onset of pinch-off ($t = 1.7$). Solid lines represent the results from [35], and dashed lines the present results. This case is the same as in Fig. 10.

Fig. 12. Self-similar behavior of the pinch-off process. Dash-dotted line represents the theoretical analysis of [37], and solid lines represent the rescaled interface shapes from $t = 1.6$ to 1.7 with an interval of 0.01.
3.2.4. Three-dimensional drops in simple shear flows

We consider the deformation and breakup of a three-dimensional drop in simple shear flows with matched density and viscosity. The initially spherical drop of a radius $R$ is placed between two parallel plates which move at a speed of $U$ but in opposite directions. Due to the shear stress exerted by the surrounding fluid, the drop is elongated, and would break up if the shear rate is sufficiently large. The characteristic dimensionless parameters are the Reynolds number $Re (= \rho \dot{\gamma} R^2/\mu)$ and the capillary number $Ca (= \mu \dot{\gamma} R/\sigma)$, where the shear rate $\dot{\gamma} = U/H$ with $H$ being the half height of the channel. At low $Ca$, the drop ends up with an ellipsoidal shape, and its deformation can be measured by the parameter $D_f = (L - B)/(L + B)$, where $L$ and $B$ are the lengths of the major and minor axes of the deformed drop at equilibrium, respectively. When $Re \ll 1$ and $Ca \ll 1$, $D_f$ is expected to be linear in $Ca$, approximately $D_f = (35/32)Ca$ [38]. In the simulation, the following boundary conditions are enforced: periodic boundary conditions in the streamwise direction, symmetric boundary conditions in the transverse direction and no-slip wall boundary conditions in the vertical direction. In all cases, $h_C = 0.0333$ and $Cn = 0.0166$ are used. We simulate the drop deformation at small $Re$ and $Ca$, in a domain of $8R \times 4R \times 8R$. Fig. 13 shows the variation of $D_f$ as a function of $Ca$, and it can be seen that the results are in good agreement at $Ca \lesssim 0.1$. For $Ca > 0.15$ present results gradually deviate from the theoretical analysis with increasing $Ca$, and the drop at the steady state are more elongated than the theoretical prediction. We also investigate the case at $Ca = 0.39$, in a domain of $12R \times 4R \times 4R$. Since $Ca = 0.39$ exceeds the critical value for the onset of breakup at $Re = 1$ [3,41], the drop is elongated into a ligament, which eventually ruptures. Fig. 14 shows the snapshots of the drop at different times, and in the end the drop breaks up into three small droplets.
4. Conclusion

We propose to use a dual-resolution grid for the diffuse interface simulation of two-phase flows, with fine grid for the interface capturing and coarse grid for the variables of pressure and velocity. One of the most important steps in this approach is the coupling of solutions between the fine grid and the coarse grid. The schemes for the solution coupling in the present method can ensure that the interpolated velocity on the fine grid can be divergence-free at a discrete level, and that the mass and surface tension force are conserved on the coarse grid. The method appears to significantly improve the computational efficiency, saving nearly 70% of the computational time in two-dimension and 80% in three-dimension. From the accuracy point of view, it produces nearly the same results for the interface evolution as the single-resolution grid. A variety of numerical tests have been performed to validate the method and check its performance, including Rayleigh Taylor instability, steadily rising bubble, partial coalescence of a drop into a pool, and three-dimensional drops in simple shear flows. It is shown that good agreement has been achieved with previous studies.

In this article we only consider the resolution ratio of 2 between the coarse grid and the fine grid. Technically, it is rather easy to extend it to a resolution ratio of 4 or even more, with the proposed interpolation and integration schemes. However, it raises an issue of the optimal (or minimum) number of mesh points to accurately resolve the velocity and pressure across the interface, which is beyond the scope of the present study.

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Appendix A. Justification of divergence-free velocity \(\mathbf{u}^F\)

It is necessary to check whether the interpolated velocity \(\mathbf{u}^F\) complies with the divergence-free constraint at a discrete level, in order to make sure that the mass conservation is also maintained on the fine grid. The interpolations from the coarse grid to the fine grid can be generally classified into three types with respect to the positions of the variable \(C\) on the coarse grid (Fig. 2), i.e. cell centers (I), faces (II) and corners (III). In the following, we first check the two-dimensional case using the interpolation scheme in Eq. (10).

At the fine cell I, the discretized divergence of the velocity \(\mathbf{u}^F\) yields,

\[
(\nabla_h \cdot \mathbf{u}^F)_{i,j} = \frac{1}{h} \left( u^F_{i+\frac{1}{2},j} - u^F_{i-\frac{1}{2},j} + v^F_{i,j+\frac{1}{2}} - v^F_{i,j-\frac{1}{2}} \right) = \frac{1}{2h} \left( u^C_{i+1,j} - u^C_{i-1,j} \right) + \frac{1}{2h} \left( v^C_{i,j+1} - v^C_{i,j-1} \right) = (\nabla_{2h} \cdot \mathbf{u}^C)_{i,j} \tag{A.1}
\]

Similarly, we can obtain at the fine cell II,

\[
(\nabla_h \cdot \mathbf{u}^F)_{i,j-1} = \frac{1}{2} \left[ (\nabla_{2h} \cdot \mathbf{u}^C)_{i,j} + (\nabla_{2h} \cdot \mathbf{u}^C)_{i,j-2} \right] \tag{A.2}
\]

and at the fine cell III,

\[
(\nabla_h \cdot \mathbf{u}^F)_{i+1,j-1} = \frac{1}{4h} \left[ (\nabla_{2h} \cdot \mathbf{u}^C)_{i,j} + (\nabla_{2h} \cdot \mathbf{u}^C)_{i,j-2} + (\nabla_{2h} \cdot \mathbf{u}^C)_{i+2,j} + (\nabla_{2h} \cdot \mathbf{u}^C)_{i+2,j-2} \right] \tag{A.3}
\]

Therefore, \(\mathbf{u}^F\) obtained from Eq. (10) satisfies the continuity equation at a discrete level if and only if the velocity field \(\mathbf{u}^C\) is divergence-free. Clearly, it is straightforward to extend this conclusion to three-dimensional cases.

On the other hand, we find that the interpolation scheme in Eq. (10) is not suitable for axisymmetric simulations, in which the discretized continuity equation is different from the two-dimensional case. For example, the divergence of \(\mathbf{u}^F\) at the fine cell II can be discretized in the axisymmetric coordinates \((r, z)\) as,

\[
(\nabla_h \cdot \mathbf{u}^F)_{i,j-1} = \frac{1}{hr_i} \left( r_i + \frac{1}{2} u^F_{i+\frac{1}{2},j-1} - r_i - \frac{1}{2} u^F_{i-\frac{1}{2},j-1} \right) + \frac{1}{hr_i} \left( v^F_{i,j-\frac{1}{2}} - v^F_{i,j-\frac{1}{2}} \right) \tag{A.4}
\]

where the grid spacings are assumed to uniformly have the same value, i.e. \(\Delta r = \Delta z = h\). The solution is to replace the velocity components \((u, v)\) in Eq. (10) by the product of the velocity times the respective radial positional. This gives

\[
(ru)^F_{i+\frac{1}{2},j-1} = \frac{1}{4} \left( r_{i-1}u^C_{i-1,j} + 3r_{i+1}u^C_{i+1,j} \right)
\]

\[
(ru)^F_{i+\frac{1}{2},j+\frac{1}{2}} = \frac{1}{8} \left( r_{i-1}u^C_{i-1,j} + 3r_{i+1}u^C_{i+1,j} + 3r_{i+1}u^C_{i+1,j-2} + r_{i-1}u^C_{i-1,j-2} \right)
\]
\[ (rv)_{i,j-1}^F = \frac{1}{4} (rv)_{i,j+1}^C + 3 (rv)_{i,j-1}^C, \]
\[ (rv)_{i+1,j-1}^F = \frac{8}{1} (rv)_{i+1,j+1}^C + 3 (rv)_{i+1,j-1}^C + (rv)_{i+1,j+1}^C. \]

(A.5)

Then, \( u^F (v^F) \) can be computed by \( (rv)^F = (rv)^C \). Substituting it into Eq. (A.4), it yields

\[ (\nabla_h \cdot u^i)^{i,j-1} = \frac{1}{4} r_i (u^i_{i+1,j+1} - u^i_{i-1,j+1} - u^i_{i+1,j-1} + u^i_{i-1,j-1}) + \frac{1}{4} (u^i_{i+1,j+1} - u^i_{i-1,j+1} - u^i_{i+1,j-1} + u^i_{i-1,j-1}) \]

(A.6)

suggesting that the relationship of velocity divergence between the fine grid and the coarse grid is as same as in Eq. (A.2). Similarly, the same results are obtained for the fine cells I and III as in Eqs. (A.1) and (A.3), respectively. In this way, the interpolated \( u^i \) in the axisymmetric simulations also satisfies the continuity equation at a discrete level, if and only if the velocity field \( u^i \) is divergence-free.

References