Performance Evaluation of a 2D Front Tracking Method – a Direct Numerical Simulation Method for Multiphase Flows

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Abstract

This paper evaluates the performance of a direct numerical simulation (DNS) method called "front-tracking" for multiphase flows. The interface separating two fluids or two phases is represented by connected elements that move on a fixed rectangular grid used for solving the Navier-Stokes equations. The phase's values of material properties are specified by an indicator function that is reconstructed from the interface point location. The interface points are updated by the velocities, which are interpolated from the velocities on the fixed grid. The method is evaluated through a thorough investigation of the performance using a variety of verification and validation test cases including advection of the interface, computations of the surface tension, and interplay of the viscous and interfacial tension terms. The method is then used to simulate the evolution of the Rayleigh–Taylor instability. Good agreement in comparison of the present method with the previous literature proved the accuracy and capability of the method.

Keywords: DNS, Front-tracking, Performance evaluation, Multiphase flow, Rayleigh-Taylor instability

1. Introduction

Multiphase flows play an important role in the workings of nature and engineering problems. In terms of mathematics, multiphase problems are very difficult. Therefore, exact analytical solutions are available only for the simplest problems. In addition, experimental studies of multiphase flows are not easy to carried out. Accordingly, computational fluid dynamics, including direct numerical simulations (DNS), becomes a standard tool in multiphase flow research.

For DNS, it is necessary to solve the full Navier-Stokes equations, and a number of different approaches have been developed and applied. One of the pioneering works calls back to Harlow and Welch [1], in which the authors distributed marker particles throughout the fluid region. They solved the governing equations on a regular grid that covers the fluid-filled and the empty part of the domain. Accordingly, the method is called "marker-and-cell" (MAC) method. The next generation of methods for multiphase flows was developed gradually from the MAC method. One of the most known methods is the volume of fluid (VOF) method that was introduced and discussed by Hirt and Nichols [2]. In the VOF method, the different fluids are identified by a marker function that takes different values in the different fluids. Other maker function methods include the level set (LS) method, the phase field method, and the cubic interpolated pseudo-particle (CIP) method. For further discussions of these methods, the reader is referred to Sussman et al. [3] for the LS method, [4] for the phase field method, and Takewaki et al. [5] for the CIP method. Instead of advecting the marker function directly, the interface between the different fluids can be tracked using marker points, and then the marker function is reconstructed from the information of the interface points. These methods are referred to as "front-tracking" (FT) methods. One of the most popular FT method is that introduced by Unverdi and Tryggvason [6]. Detailed description of the method and its applications can be found in [7]. In the above-mentioned approaches, only one single field governing equations are used, and the boundary conditions, e.g., the surface tension force, at the interface are introduced to the equations as the source terms. Accordingly, these methods are called "one-fluid" approaches. A long with development of the one-fluid formulation methods, other techniques were also explored, such as the boundary-fitted lagrangian method

The front-tracking method introduced in [6] has been widely used in multifluid and multiphase problems [7], and recently in our works [10–12]. Despite the wide use of the front-tracking method, its evaluation has been confined to validation problems specific to the particular applications of interest to the respective authors. This calls to question the performance of the method for the various multiphase flow problems. Accordingly, this paper presents a detailed analysis of the behavior of the method over a wide range of verification and validation problems

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including advection of the interface, computations of the interfacial tension, and interplay of the viscous and interfacial tension terms. These problems are commonly used to verify and validate the accuracy and capability of the DNS methods for multiphase flows. We focus here only 2D problems.[8], and the lattice-Boltzmann method [9].

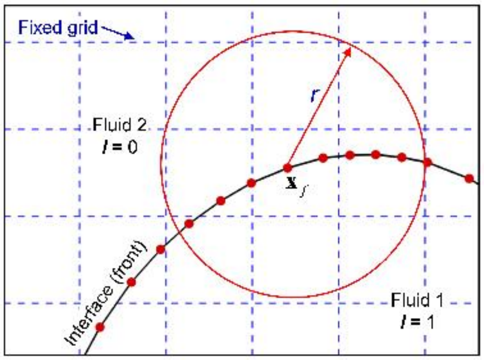

Fig. 1. An interface represented by connected elements on a fixed grid. Information is passed between the front points and the fixed grid

2. Numerical method

The fluids are assumed incompressible, immiscible and Newtonian. All phases are treated as one fluid with variable density ρ and viscosity μ. In terms of the one-fluid formulation, the governing equations include:

$$\partial(\rho\mathbf{u})/\partial t+\nabla\cdot(\rho\mathbf{uu})=-\nabla p+\nabla\cdot\mu\left(\nabla\mathbf{u}+\nabla\mathbf{u}^{T}\right)$$

$$+\rho\mathbf{g}+\int_{f}\sigma\kappa\mathbf{n}_{f}\delta(\mathbf{x}-\mathbf{x}_{f})dS \quad (1)$$

$$\nabla\cdot\mathbf{u}=0 \quad (2)$$

Here, $\mathbf{u}$ is the velocity vector, p is the pressure, $\mathbf{g}$ is the gravitational acceleration, and t is time. The superscript T denotes the transpose. The last term in Eq. (1) accounts for the interfacial tension force at the interface. At the interface, denoted by f, σ is the interfacial tension coefficient, κ is twice the mean curvature, and $\mathbf{n}_f$ is the unit normal vector to the interface. The Dirac delta function $\delta(\mathbf{x}-\mathbf{x}_f)$ is zero everywhere except a unit impulse at the interfaces $\mathbf{x}_f$. The above equations are discretized using a second-order centered difference approximation for the spatial derivatives and an explicit predictor-corrector method for time integration. The discretized equations are solved on a fixed, staggered grid using the MAC method [1].

The interface separating two fluids is represented by connected points on a fixed grid (Fig. 1). The movement of the interface points is given as

$$\mathbf{x}_f^{n+1}=\mathbf{x}_f^{n}+\mathbf{V}\Delta t \quad (3)$$

where $\mathbf{V}$ is the velocity at the front point, which is interpolated from the fixed grid points using a smooth weighting function [13]

$$\mathbf{V}=\sum w_{ij}\mathbf{u}_{ij} \quad (4)$$

$$w_{ij}=d\left(x_f-ih\right)d\left(y_f-jh\right) \quad (5)$$

$$d(r)=\begin{cases}1/(4h)\left[1+\cos(\pi r/2h)\right], & |r|<2h\\ 0 \quad , & |r|\geq 2h\end{cases} \quad (6)$$

where h is the grid spacing (Fig. 1), and i and j is the indices of the fixed grid point. The information of the front points is used to reconstruct an indicator that has a value of one in one fluid and zero in the other:

$$\nabla I=\int_{f}\delta\left(\mathbf{x}-\mathbf{x}_f\right)\mathbf{n}_f dS \quad (7)$$

Then the density and viscosity fields are updated:

$$\rho=\rho_1 I+(1-I)\rho_2\ ;\qquad \mu=\mu_1 I+(1-I)\mu_2 \quad (8)$$

To calculate the interfacial tension force, we first calculate the net force on each front element:

$$\delta\mathbf{F}_l=\int_{\Delta s}\sigma\kappa\mathbf{n}ds=\int_{\Delta s}\sigma\ \partial\mathbf{t}/\partial s\, ds=\sigma\ \left(\mathbf{t}_2-\mathbf{t}_1\right) \quad (9)$$

where $\mathbf{t}$ is the tangents of the end points of each element. After that, this force is transferred to the fixed grid (so that it is included in the solution of the Navier-Stokes equations) using the same smooth weighting function, i.e. Eq. (6),

$$\mathbf{F}_{ij}=\sum_{l}\delta\mathbf{F}_l w_{ij}\Delta s_l/h^2 \quad (10)$$

Here Δs_l is the length of the element. In the following, we briefly describe the solution procedures.

Suppose n time steps have been completed, to calculate the solution at time level n+1 carry out the following steps:

1. Update the position of the interface points [Eq. (3)]

2. Reconstruct the indicator function, update the material properties, and calculate the interfacial tension force

3. Calculate an intermediate velocity field:

$$\mathbf{u}^{*}=\left(\Delta t\mathbf{A}^{n}+\rho^{n}\mathbf{u}^{n}\right)/\rho^{n+1} \quad (11)$$

where the advection, the diffusion, the gravitational body force and the interfacial tension force in Eq. (1) are denoted by $\mathbf{A}$

4. Find the pressure field by solving the Poisson equation:

$$\left(\nabla\cdot\mathbf{u}^{n+1}-\nabla\cdot\mathbf{u}^{*}\right)\big/\Delta t=-\nabla\cdot\frac{1}{\rho^{n+1}}\nabla p \tag{12}$$

where $\nabla\cdot\mathbf{u}^{n+1}=0$

5. Compute the divergence-free time level n+1 fluid velocity field

$$\mathbf{u}^{n+1}=\mathbf{u}^{*}-\Delta t\,\nabla p/\rho^{n+1} \tag{13}$$

This solution procedure for time integration is first order, to produce a second-order scheme, the technique described by Esmaeeli and Tryggvason [14] is used. More detailed description of the method can be found in [7].

3. Performance tests

The following, we present the verification and validation of the method. The configurations to be adopted in these tests follow directly from the respective references, including dimensions and velocity fields.

3.1. A notched disc in rotating flow

Solid body rotation of a notched disc introduced by Zalesak [15] (Fig. 2) is a test commonly used for evaluating the accuracy of a method in maintaining a sharp corners. The initial data is a slotted circle centered at (50,75) with a radius of 15, a slot width of 5, and a slot length of 25. The domain is 100×100.

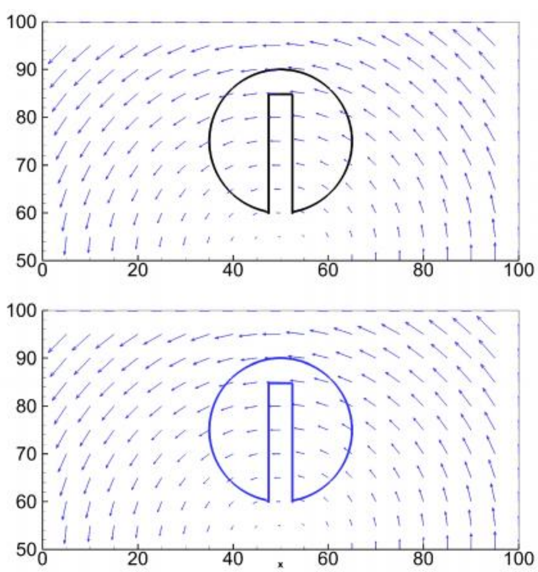

Fig. 2. Comparison of the Zalesak disk interface before (top) and after one rotation (bottom)

The velocity field is given as:

$$(u,v)=\left[\pi(50-y)/314,\pi(x-50)/314\right] \tag{14}$$

The grid resolution is 100×100. Fig. 2 indicates that after one revolution, the interface of Zalesak's disk is almost identical to the initial shape.

3.2. A circular drop in a vortical flow field

This accuracy test introduced by Bell et al. [16] is to test how well a method to resolve thin filaments on the scale of the mesh which can occur in stretching and tearing flows. A circular drop with a radius of 0.15 is initially located at (0.5, 0.75) in a box of 1.0×1.0 (Fig. 3a). The velocity field is given as:

$$\begin{cases}u=2\cos(\pi t/T)\sin^2(\pi x)\sin(\pi y)\cos(\pi y)\\ v=-2\cos(\pi t/T)\sin^2(\pi y)\sin(\pi x)\cos(\pi x)\end{cases} \tag{15}$$

where T is the period. This velocity field first stretches the drop into a thinner filament that is wrapped around the center of the box, then slowly reverses and pulls the filament back into the initial circular shape, i.e. at the end of the period T, the shape should be the same as the initial one (Fig. 3a). The grid resolution is 32×32 with T = 8. Fig. 3b shows the drop shape at time $t = T$ computed by the present front-tracking method (FT) – the dash line in Fig. 3b – in comparison with the initial shape. Obviously, the difference is barely visible. In contrast, the level set method (LS) [17] produced remarkable difference (the dash-dot line in Fig. 3b) even though a much finer grid 256×256 was used.

3.3. Stationary drop

This accuracy test is to test how well a method to predict the pressure difference between the inside and outside of the drop. This pressure difference is induced by the surface tension force acting on the interface, as given by Laplace's law. For a circular droplet in equilibrium the velocity should be exactly zero. However, because of numerical errors, the velocity field is not zero, and is referred to "spurious currents" (Fig. 4). A good method should produce the accurate pressure difference with spurious currents as small as possible. There are three dimensionless numbers that characterize the flow: the Laplace number $La=\rho_d D\sigma/\mu_d^2$ where D is the drop diameter, and density and viscosity ratios ρ_d/ρ_c and μ_d/μ_c. The subscripts d and c respectively represent the fluids inside and outside the drop. The maximum nondimensional velocity, i.e., the capillary number Ca, is defined as $Ca=\mu_d U_{\max}/\sigma$.

We consider a circular drop with a radius of 0.5 placed at the center of a box of 2×2 with all other properties set to unity except for σ (Fig. 4a). The grid resolution is 64×64. Accordingly, the value of σ is equal to the value of *La*. For instance, La = 0.12 yields σ = 0.12, and according to the Young–Laplace equation the pressure difference is $\Delta p_{exact} = \sigma / R$ = 0.24. Fig. 4 indicates that the method predicts the pressure rise reasonable well with $Ca = 2.65\times10^{-4}$. In comparison with the VOF method implemented with

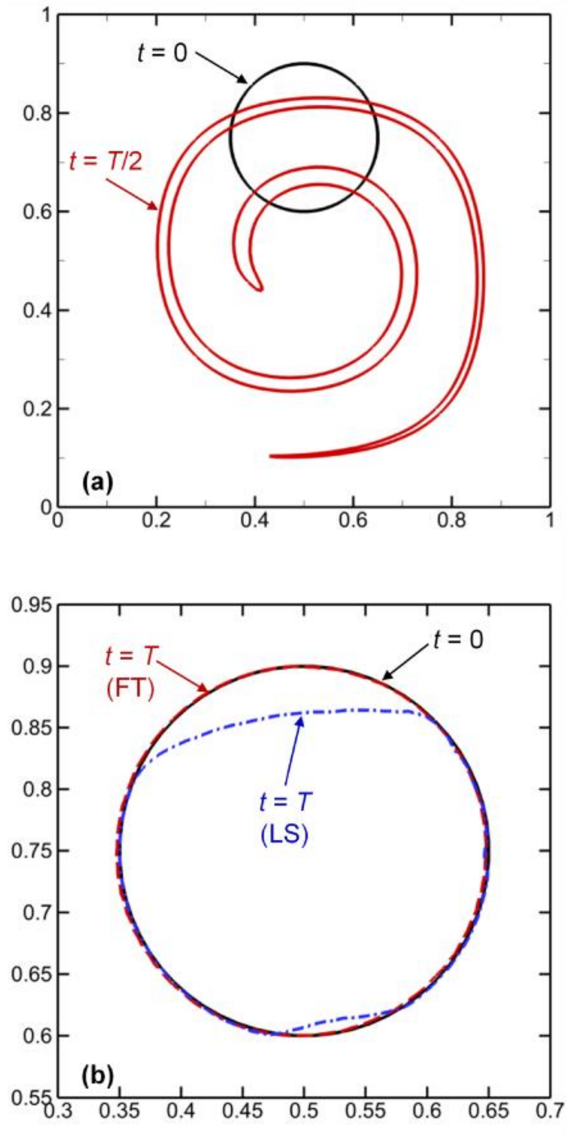

Fig. 3. Accuracy test for the advection of the interface points. (a) The initial shape (t = 0) and the shape at half period (t = T/2). (b) The shape of the drop at the end of the period (t = T) computed by the FT method, i.e. the dash-line, compared with that computed by the LS method [17], i.e. the dash-dot line (the solid line representing the initial shape). The LS method was used with a 256×256 grid resolution

different techniques for computing surface tension, e.g., the continuous surface force (CSF) and the continuous surface stress (CSS) [18], the magnitude of the spurious currents produced by the front-tracking is much smaller as shown in Table 1.

3.4. A damped surface wave

To verify the interaction of the viscous term with the surface tension term, we perform a simulation a damped surface wave between two superposed immiscible fluids, as shown in Fig. 5, and compare the computational results with the initial value theory of Prosperetti [19]. In a [0, 2π]×[0, 2π] domain, two fluids are initially separated by an interface defined by

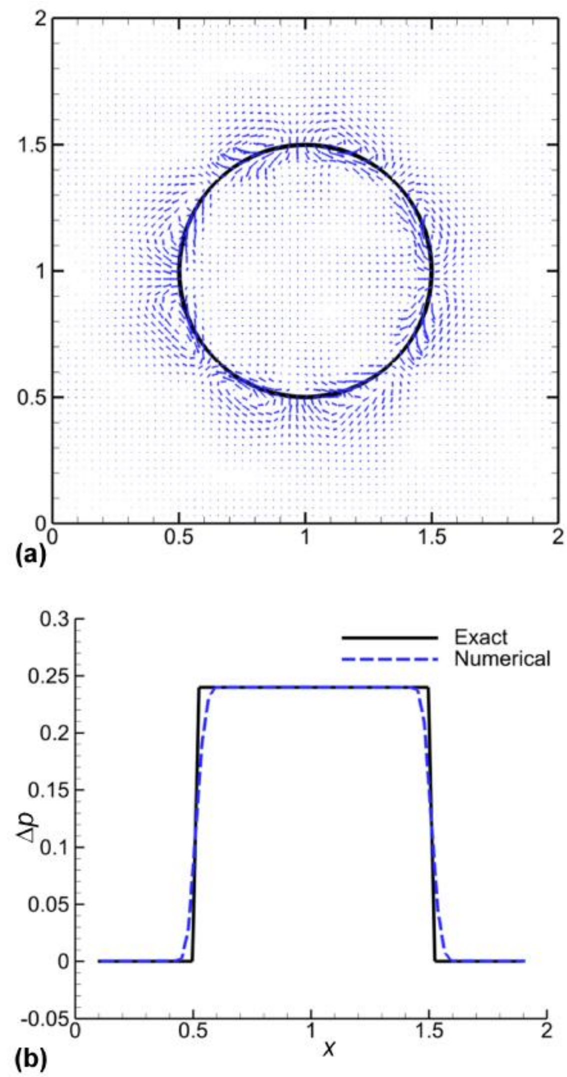

Fig. 4. (a) The spurious currents generated by a circular drop with La = 0.12 and (b) the distribution of the resulting pressure field along the line y = 1.0. The grid resolution is 64×64 with a domain of 2×2

Table 1. Measurements of spurious currents with three surface tension methods

La	ρ_d/ρ_c	μ_d/μ_c	Number of grid points/D		Ca		
			VOF	FT	CSS (VOF)	CSF (VOF)	FT
0.120	1	1	30	32	6×10^{-3}	1.4×10^{-2}	2.6×10^{-4}
0.357	1	1	32	32	3×10^{-3}	1.2×10^{-2}	2.7×10^{-4}

$$y = \pi + A_0 \cos(2x/\lambda) \tag{16}$$

where the wavelength λ is set to 2π, and the initial amplitude A_0 is set to 0.01λ. The boundary conditions are shown in Fig. 5a. Three grid resolutions are used: 32×32, 64×64 and 128×128. The surface tension coefficient σ is set to 2. The densities of two fluids are identical and set to $\rho_1 = \rho_2 = 1$. The kinematic viscosity ν of both fluids is set to 0.064720863. The time is non-dimensionalized by the inviscid oscillation frequency $\omega_0 = \sqrt{\sigma/(\rho_1+\rho_1)}$. Fig. 5b shows the temporal evolution of the wave amplitude normalized by λ in comparison with the theory of Prosperetti [19]. The figure shows that while 32×32 predicts an incorrect frequency the finner grid 128×128 produces a satisfactory result. This confirms that the method is capable of accurately predicting this flow.

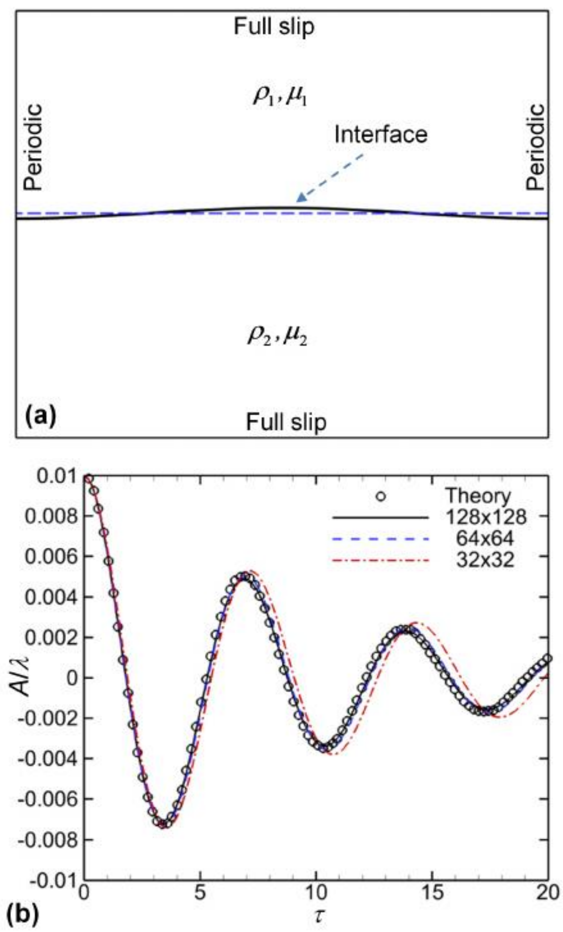

Fig. 5. Damped surface wave: (a) computational domain, and (b) evolution of the amplitude of the wave versus nondimensional time $\tau = \omega_0 t$

3.5. Rayleigh–Taylor instability

We consider the growth of a two-dimensional Rayleigh–Taylor instability that has been studied by numerous methods to characterize the quality of interface transport methods, see, for example [20], as shown in Fig. 6a. Two immiscible fluids with the denser one at the top are placed in a box of 1×4. The interface separating two fluids is defined as:

$$y = 2 + A_0 \cos(2\pi x) \tag{17}$$

where A_0 is taken to be 0.05. The top fluid has a density ρ_1 = 1.225, while the bottom fluid has a density of ρ_2 = 0.1694. Both fluids have the same

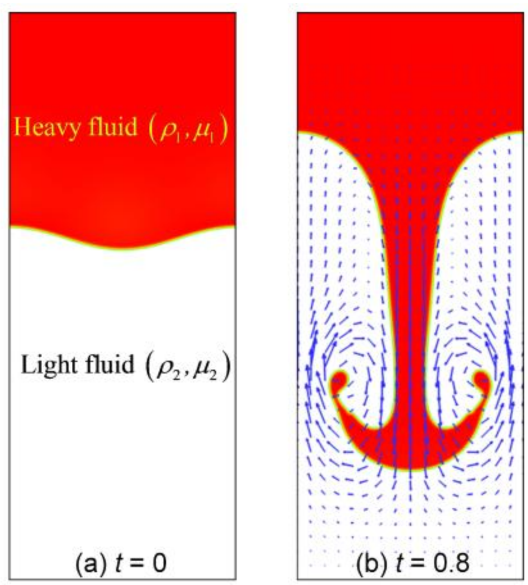

Fig. 6. Rayleigh–Taylor instability problem

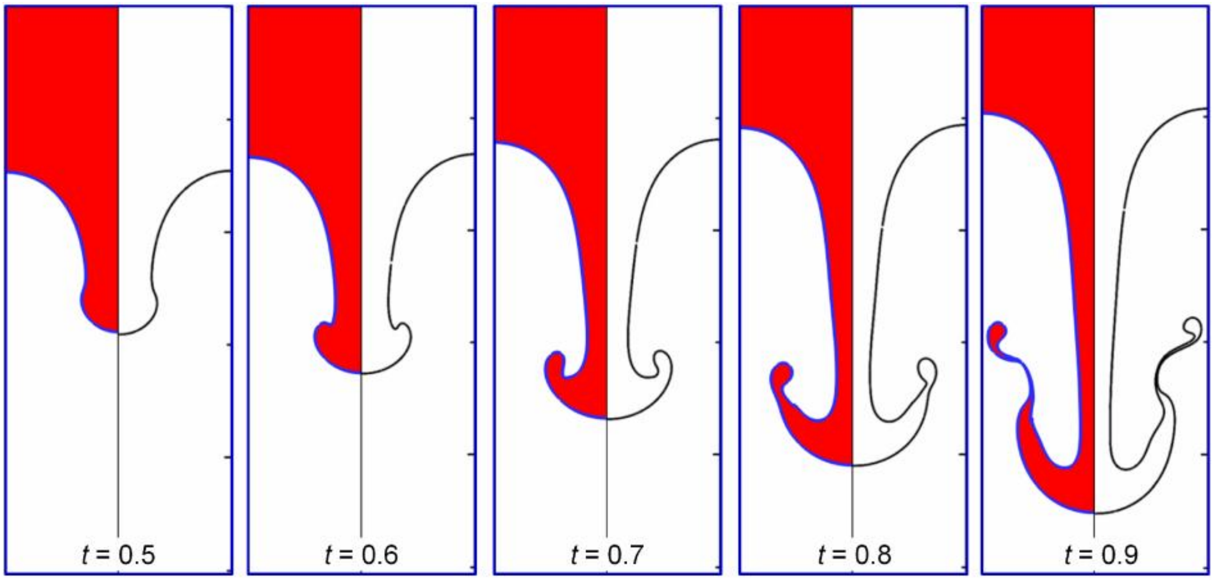

Fig. 7. Temporal evolution of the interface computed by the front-tracking method (left) in comparison with the results predicted by Herrmann [20] (right)

viscosity $\mu_1 = \mu_2 = 0.00313$. The gravity acceleration is set to 9.81. The boundary conditions are periodic at the left and right sides, and no-slip at the top and bottom. A grid resolution of 128×512 is used. As time progresses, the heavy fluid (top) falls into the lighter fluid (bottom) due to gravity, and rolls up into two counter-rotating vortices as shown in Fig. 6b.

Fig. 7 shows the evolution of the interface shape at different times in comparison with the results predicted by another numerical method of Herrmann [20] in which the author used a much finer grid of 512×2048. In each frame of Fig. 7, the left is the present result while the right is Herrmann's result. Excellent agreement has been archieved. This confirms that front-tracking method produces the accurate results for this multiphase problem.

5. Conclusion

We have presented the results of a number of verification and validation problems for the front-tracking method, which has been widely used for multiphase problems. The interface separating two phases or fluids is represented connected elements that are used to calculate the interfacial tension force. The discretized governing equations are solved by the second-order predictor-corrector method. The various problems have been solved: a notched disk in rotating flow, a circular drop in a vortical flow field, a stationary drop, and a damped surface wave. The method is then used to simulate the Rayleigh-Taylor problem. The numerical results produced by the method are reasonably accurate and satisfactory. This confirms and supports the accuracy of the method for numerous multiphase problems. In comparison with some other direct numerical simulation methods, e.g., level set method and volume of fluid method for the problems investigated in this study, with the similar grid resolutions the front-tracking method yielded the results which are more accurate, especially, in the case of calculating surface tension forces. In addition, the present 2D method is quite simple and very easy to be implemented. This facilitates computations of many multiphase problems.

However, the results presented in this paper are limited to the 2D cases. Therefore, in future research, we will investigate some 3D problems to evaluate the performance of the 3D front-tracking method.

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