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Detailed comparisons of front-capturing methods for turbulent two-phase flow simulations

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SUMMARY

In the framework of numerical study of multiphase flows, different front-capturing methods are compared. Two different approaches dealing with the incompressibility constraint will be compared, too. Then, every technique is tested on several relevant test cases in order to make a comparison. The surface tension treatment is evaluated for each method and every front-capturing method is tested on a case where interface deformations have something in common with turbulent behaviour. Finally, every method is studied through a phase inversion problem, which is an unsteady test case. Front-capturing methods are tested on physical cases where Navier–Stokes and advection equations are coupled in a non-linear way.

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1. INTRODUCTION

The objectives of the present work are to evaluate Navier–Stokes discretization and solvers as well as interface tracking methods dedicated to unsteady incompressible multiphase flows. This work aims at providing a synthetic and critical work on two-phase flow simulations in order to develop in the near future an original large eddy simulation (LES) numerical modelling of incompressible free surface flows. In the numerical study of multiphase flows, the way the interface is treated has crucial importance. Indeed, the understanding of local phenomena near the interface is impossible without an interface, which has been properly located in the flow field. Let $\mathbf{u}$ be the velocity, t the

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time, ρ the density, μ the dynamic viscosity, p the pressure, $\mathbf{g}$ the gravity vector, $\mathbf{S}_D = \frac{1}{2}(\nabla\mathbf{u} + \nabla^t\mathbf{u})$ the deformation rate, χ a function that represents the position of the interface and $\mathbf{T}$ the surface tension force. Multiphase flows were calculated on a fixed Eulerian mesh in order to deal with unsteady, three-dimensional flows, with fragmentations and re-connections of the interface. A one-fluid model is obtained [1], in which an advection equation for χ is introduced to describe the interface evolutions:

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

$$\rho\left[\frac{\partial\mathbf{u}}{\partial t} + \nabla\cdot(\mathbf{u}\otimes\mathbf{u})\right] + \nabla\cdot(p\mathbf{Id} - 2\mu\mathbf{S}_D) - \rho\mathbf{g} + \mathbf{T} = 0 \tag{1b}$$

$$\frac{\partial\chi}{\partial t} + \mathbf{u}\cdot\nabla\chi = 0 \tag{1c}$$

In order to accomplish the purpose of this research, two home-made computational fluid dynamics libraries are used to solve the system (1a)–(1c). The first one, named Aquilon, is based on finite volumes with an augmented Lagrangian method for the treatment of incompressibility. The interface tracking is achieved by volume of fluid (VOF)–piecewise linear interface construction (PLIC) [2], VOF–total variation diminishing (TVD) [3] and Front Tracking [4] methods. The surface tension is modelled by a CSF method of Brackbill [5]. Concerning the second library called Dyjeat, the incompressible flow solver is based on classical projection methods [6, 7] to verify the incompressibility constraint. In Dyjeat, the ghost-fluid method [8] was used to deal with surface tension forces as well as density and viscosity jumps. The application of the ghost-fluid method is represented in Equation (1b) by the function $\mathbf{T}$. To capture the interface level-set methods [9] are used in Dyjeat. In this work, every front-capturing method and every technique used to solve Navier–Stokes equations are taken from the literature. Each method passed the classical tests successfully (Zalesak rotating disk [10], streamer test case [11], parasitic currents [12], etc.), and the drawbacks of every technique are well known. The originality of our approach is to test every front-capturing method on physical cases where Navier–Stokes and advection equations are coupled in a non-linear way. Front-capturing methods coupled with Navier–Stokes solvers will be studied on stiff unsteady physical problems.

2. NUMERICAL METHODS

The techniques dedicated to solve the Navier–Stokes equations are first considered. The velocity–pressure uncoupling can be computed with the augmented Lagrangian method. The standard augmented Lagrangian method was first introduced by Fortin and Glowinski [13]. This predictor/corrector iterative method optimizes the solution by solving a velocity–pressure saddle point with an Uzawa algorithm [14]. A flexible version of the augmented Lagrangian method is proposed in [15]. On the other hand, the velocity–pressure uncoupling can be carried out by a classical projection method, in its fully explicit formulation, as it has been accomplished by [6, 7].

Regarding the computation of the surface tension force (represented by $\mathbf{T}$ in (1b)) and the jump conditions at the interface, different methods were performed. One of the choices to calculate this force is by using the CSF method of BrackBill [5]. The method is based on the regularization of the surface tension force thanks to a regularized volume formulation, which gives an approximation

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to the original formulation of this surface tension force. The force per unit volume is spread on several mesh cells around the interface. To take into consideration the jumping behaviour at the interface directly and to remain closer to physics reality, there is the alternative of using ghost-fluid approach [8]: it is a simple boundary treatment, which allows the incorporation of jump conditions into the discretization of the momentum equations.

To deal with the interface Equation (1c), three front-capturing (Eulerian) methods were applied: the VOF technique with a PLIC [2], the TVD VOF approach [3] (without geometric reconstruction) and the level-set method [9]. In addition, a Lagrangian front-tracking method [4] is presented in some cases. Hirt and Nichols [16] were the first to propose the VOF technique in which, for each medium, a phase function or colour function is used to locate the different fluids and solids standing $C=0$ in the outer media, $C=1$ in the considered medium. The colour function is advected depending on the fluid velocity. With VOF–PLIC method the interface is defined by its slope and unit normal. The slope is calculated thanks to the colour function C gradients, and the position of the piecewise interface elements is determined in the normal direction to ensure the conservation of volume fraction in each cell. When analyzing the TVD schemes, they belong to VOF methods and are still based on the colour function C advected in the flow. Contrary to VOF–PLIC methods, there is no explicit interface reconstruction, and the colour function is calculated directly. With this intention, the TVD schemes [17] were used to deal with non-continuous aspects of the colour function and to solve the hyperbolic equation (1c). A technique dedicated to front-capturing approach is the level-set method, introduced by Osher and Sethian [9] and refined by Sussman *et al*. [18]. A level-set function ϕ is defined as the normal distance function from the interface with its original value set to zero at the interface. This function is advected thanks to Equation (1c). The interface is associated with $\phi=0$. ϕ is a smooth function and provides a natural way to calculate the unit normal vectors at the interface and curvatures of the interface.

3. VALIDATIONS

To deal with Equations (1a) and (1b), two different techniques were used to compute the velocity–pressure uncoupling: the augmented Lagrangian method and the classical projection method. Studies are made on the inviscid Taylor–Green vortex. Here, only the two-dimensional case was carried out [19]. Periodic boundary conditions on a square domain, with a $[0,2\pi]^2$ side length, were chosen. Numerical dissipation is studied: the error between the theoretical value of kinetic energy (π^2) and the one calculated is represented in Figure 1 for several mesh sizes. When using refined grids, both augmented Lagrangian method and projection method are equivalent and of second order. Hence, when capillary terms are not taken into consideration, both methods give the same results and will not be at the origin of the differences observed in the solutions when capillary terms will be taken into account. For the projection method a distinction is made about the way spatial discretization is carried out: fifth order weighted essentially non-oscillatory (WENO) schemes [20] can be used in a conservative form [21] (weno-c) or not (weno-nc).

Several test cases were performed to compare different techniques to solve Equation (1c). Firstly, two-dimensional Rayleigh–Taylor instability [22] in its linear form is studied. A heavy fluid is over a lighter one (density ratio$=1000$), the two phases being separated by an interface. A small sinusoidal disturbance is initiated at the interface, and the resulting growing instability is studied. For each front-capturing method and for several surface tension forces, the growth

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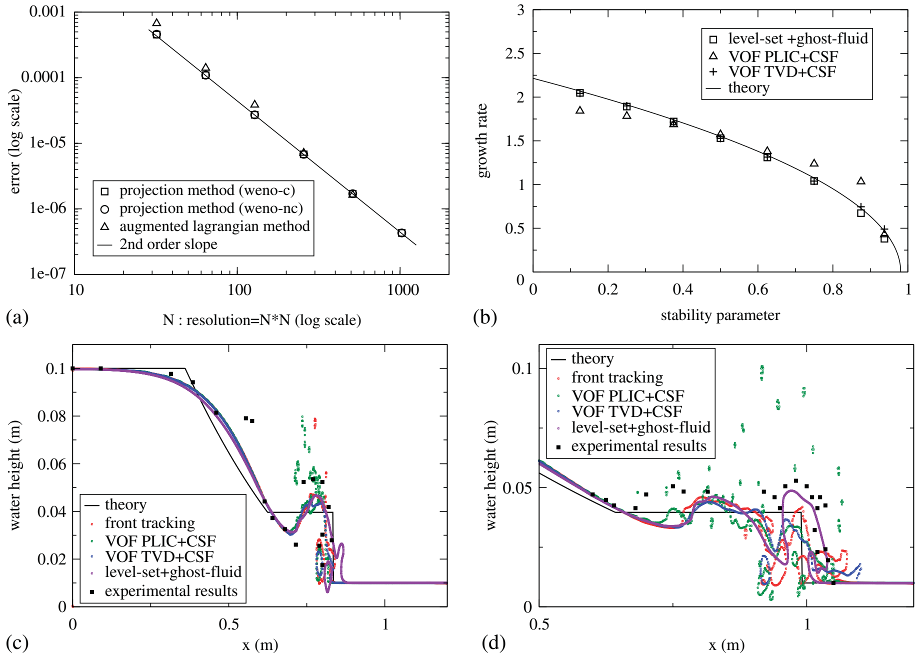

Figure 1. From left to right: (a) Taylor–Green test case; (b) Rayleigh–Taylor test case; (c) dam break $t=0.24$ s; and (d) dam break $t=0.42$ s.

rate n is calculated. The stability parameter ϕ represents the intensity of surface tension forces. This test case allows one to understand how the different front-capturing techniques behave when surface tension forces are the main driving forces. The results are presented in Figure 1. For the ghost-fluid level-set method, the growth rates calculated are very close to those given by the theory. However, differences can be observed for high ϕ corresponding to high surface tension forces, which can make calculations unstable. VOF–TVD schemes seem to be very efficient to deal with the capillary terms. With VOF–TVD schemes the interface is spread over two or three cells of the mesh. This is the reason behind the greater accuracy of VOF–TVD schemes with the CSF model. With VOF–PLIC methods the issue is stiff on the interface and the CSF model requires an artificial spreading of the interface, which can explain coarser results in Figure 1.

Another test case is the surface wave test case of Prosperetti [23]: an initial sinusoidal perturbation is created in an interface separating two viscous fluids. The simulation is carried out without gravity. The surface tension force tends to make the interface oscillate. This oscillation is damped because of the viscosity diffusion. Results are shown in Figure 2. When using insufficiently refined grids, none of the front-capturing methods are able to capture the interface accurately. When using enough refined grids, the ghost-fluid level-set techniques appear to be very accurate to capture the interface. In contrast, several interface smoothing iterations are needed to obtain good results when using VOF techniques. VOF methods tend to be less efficient, when high surface tension forces are at stake and when fine meshes are used. The Rayleigh–Taylor and Prosperetti test cases evaluate the surface tension treatment more than the interface tracking. However, for the same

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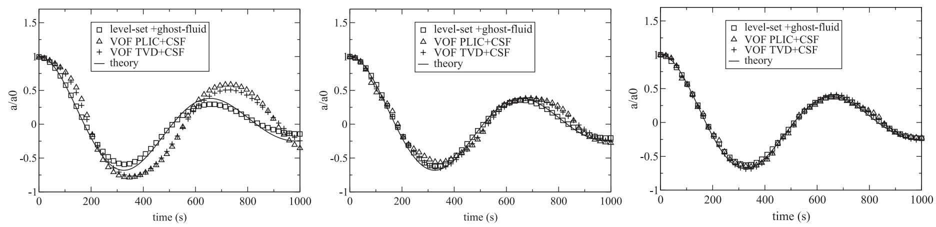

Figure 2. Prosperetti test case. Left = 32 × 32 mesh; middle = 64 × 64 mesh; and right = 128 × 128 mesh.

CSF model, it has been demonstrated that the utilization of the TVD or the PLIC technique can induce significant differences.

The last studied test case is the dam break flow over a wet bottom. Numerical results can be compared with experiments [24]. Here, the Reynolds number is 9000. The aim is to perform simulations on a test case where strong unsteady vortices of various scales interact with the interface, indeed mimic a pseudo-turbulent behaviour. The three front-capturing methods are compared with a Lagrangian front-tracking method [4]. In Figure 1, the air/water-free surfaces given by each technique are represented at two different times. The VOF–TVD technique is accurate to deal with problems, where strong deformations with little scales of turbulence occur, even if it has been shown that this method diffuses the interface when a strong local shearing occurs [3]. With VOF methods, filaments that fragment into droplets appear. Even if the mass conservation for VOF–PLIC methods is accurate, these droplets are not relevant to physical features as previously observed by [25]. Level-set methods give accurate results, as do VOF–TVD techniques.

4. THE CASE OF PHASE INVERSION

In a closed square box, a two-dimensional phase inversion is studied [26]. Initially a lighter phase (oil) is located in the lower left corner of the box (lower left quarter part of the box), the heavier one (water) filling the rest of the box. Under the action of gravity, the lighter phase moves upward, inducing complex stretching and tearing off the interface as well as strong unsteady vortex motions during the transient stage of the flow, looking like turbulent flows. Reynolds numbers are, respectively, 99 045 for the water phase and 891 for the oil phase. Strong deformations of the interface and instabilities appear. Such characteristics are found in turbulent flows. This problem is a stiff one and there is no reference solution. This test case offers a lot of configurations to study: varied interface structures, phenomena of coalescence, and break up. In Figure 3 are shown results about phase inversion on a 256 × 256 uniform Cartesian grid. Slight differences can be observed particularly near the left vertical wall, where VOF methods seem to generate unphysical small oil blobs. At a later time, as can be seen in Figure 3, larger differences are observed. Concerning the front-tracking method, the interface treatment on the wall seems different from the other methods. With VOF methods, filaments, which fragment into droplets, tend to appear. For level-set methods, problems of mass losses can appear. If macroscopic data are studied, Figure 3 (left) shows that every front-capturing method has the same behaviour in terms of kinetic energy with typical oscillations of 1 Hz.

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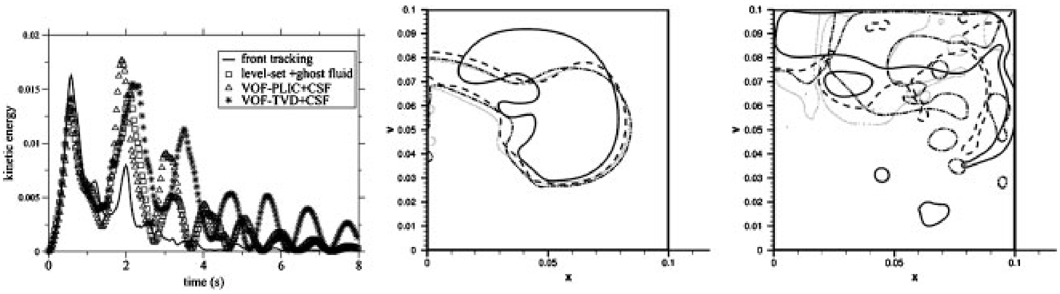

Figure 3. Left: time evolution of the kinetic energy of the oil phase; middle and right: interface locations at different times for several methods: front-tracking (solid), level set+ghost fluid (–), VOF–PLIC+CSF (..), VOF–TVD+CSF (-..-); middle: $t = 0.795$ s; and right: $t = 2.355$ s.

5. CONCLUSIONS AND PERSPECTIVES

The relevant coupling between a front-capturing method and the jump conditions treatment at the interface depends on the studied case. To capture mean effects (Prosperetti test case) and an instability (Rayleigh–Taylor test case), level-set methods coupled with ghost-fluid technique seem accurate. The same conclusion can be drawn when using VOF–TVD techniques with a CSF approach. Coupled with CSF method of Brackbill, VOF–PLIC technique is appropriate to capture mean effects. However, difficulties are encountered when computing problems with instabilities. Hence, when turbulence is taken into consideration, VOF–PLIC method coupled with CSF approach is not the more accurate technique to use. When strong deformations of the interface appear (dam break, phase inversion) each method has its own disadvantages, and conclusions are drawn to characterize the pros and cons of each method in the turbulent cases. Future works will be dedicated to introducing LES models, improving front-tracking results and testing other surface tension models for VOF methods [15].

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