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A mass-conserving volume-of-fluid method: Volume tracking and droplet surface-tension in incompressible isotropic turbulence

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ABSTRACT

We have developed a volume of fluid (VoF)/projection method for simulating droplet-laden incompressible turbulent flows with uniform density and viscosity. The method is mass-conserving, wisp-free, and consistent (i.e., the VoF function, C, satisfies the condition $0 \leqslant C \leqslant 1$).

First, we present the results of the VoF method for tracking volumes of initially spherical shape and with zero surface tension in analytical velocity fields (linear translation, solid-body rotation, single-vortex flow, and Taylor–Green vortex) and in incompressible isotropic turbulence at $Re_{\lambda 0} = 75$ and 190. These numerical tests show that (i) our VoF method is mass-conserving, consistent, and wisp-free; (ii) for a CFL number of 0.1, the VoF geometrical error has almost a second-order convergence rate for a mesh resolution with more than 10 grid points per diameter; (iii) in the isotropic turbulence case, a resolution of about 32 grid points per diameter of the sphere is required in order to limit the VoF geometrical error below 1%. Then, in order to simulate droplet-laden flows, we have adopted the continuum surface force (CSF) model to compute the surface tension force. We have modified the sequence of the VoF advection sweeps, and show that, in the case of droplet in a translating reference frame, the r.m.s. of the spurious currents is about 1% of the translating velocity. Finally, we present DNS results of fully-resolved droplet-laden incompressible isotropic turbulence at $Re_{\lambda 0} = 75$ using a computational mesh of 1024^3 grid points and 7000 droplets of Weber number $We_{rms} = 0.5$, and initial droplet diameter equal to the Taylor length-scale of turbulence.

1. Introduction

The computational methods to perform fully-resolved simulations of multiphase flows fall into two main categories: 1. interface capturing methods (ICM), such as the volume of fluid (VoF) [1] and the level-set [2] methods; 2. interface tracking methods (ITM), such as the front tracking [3] and the immersed boundary [4] methods. Both ICM and ITM are designed to compute (capture or track) sharp interfaces, and can be used on a fixed Cartesian mesh. Mass conservation, the ability to compute strong deformations of the interface, and interface topology changes due to break-up and coalescence are highly desirable features in the simulations of multiphase flows, e.g. gas–liquid and liquid–liquid. Interface topology changes need *ad hoc* modeling in ITM [3], whereas they are directly captured by the ICM [5].

Among the ICM, the level-set is a widely used method where a distance function to the interface is advected with the flow throughout the computational domain in place of the interface itself, thus avoiding the need to advect a discontinuous function. The drawback of the level-set method is that it does not conserve mass even when coupled with a particle tracking method [6]. In the VoF method, instead, the advection equation of the volume fraction is directly solved for, thus, the VoF method could potentially conserve mass exactly. Limits to this potential may only come from the numerics adopted. A color function representing the volume fraction of the reference phase is advected geometrically and the interface is reconstructed from this function typically with a piecewise linear representation.

VoF advection schemes can be broadly classified as either direction split or unsplit schemes. Split advection schemes consist of a sequence of one-dimensional advection and reconstruction steps in each coordinate direction, thus they are algorithmically straightforward to implement compared to multidimensional (unsplit) schemes. On the other hand, unsplit methods have the advantage of only requiring one advection and reconstruction step per time step, however the advection step is often algorithmically complex. This is because unsplit methods require either the computation of a flux polyhedron for each cell face [7] or calculation of polyhedra

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volumes with non-planar surfaces requiring triangulation [8]. In our experience, these geometric calculations are the computational bottleneck of the VoF advection scheme. Thus, the computational savings of the unsplit versus the split method (if any) are likely to be small. Furthermore, unsplit methods do not necessarily conserve mass to zero machine precision [8]. For these reasons, we chose to adopt a split mass-conserving VoF advection approach.

This paper presents a numerical methodology to perform DNS of droplet-laden incompressible turbulent flows with uniform density and viscosity. This is a necessary step to verify that the numerical method is accurately simulating the motion of finite-size droplets, i.e., volume tracking and surface tension computations, before we can develop a coupled flow solver where density and viscosity variations occur between the droplet and the surrounding fluid (such a flow solver has been developed in Ref. [9]). We adopted the volume of fluid (VoF) method because of its potential to conserve mass with zero-machine accuracy. The VoF advection is performed through a spatially split approach, i.e., the Eulerian implicit - Eulerian algebraic - Lagrangian explicit (EI-EA-LE) algorithm which was originally proposed by Scardovelli et al. [10]. We chose EI-EA-LE over the EILE-3D algorithm [11] because EI-EA-LE requires half the number of advection and reconstruction steps and does not require the calculation of three two-dimensional divergence-free velocity fields. Thus, EI-EA-LE is at least two times computationally faster than EILE-3D. The original EI-EA-LE algorithm [10] is globally mass-conserving but generates wisps, and does not conserve the mass of the individual volumes tracked in the flow. We have improved this method with the addition of a redistribution and a wisp suppression algorithm. Our method is consistent (i.e., the volume of fluid function, C, satisfies the condition $0 \leqslant C \leqslant 1$) and wisps-free and, thus, conserves mass both globally and locally within each volume tracked. We also present and analyze the numerical treatment of the surface tension force within a projection method combined with our VoF method. The surface tension effects are treated with the continuum surface force (CSF) approach proposed by Brackbill et al. [12] and adapted to the VoF method by Francois et al. [13].

We present the governing equations for droplet-laden flows in Section 2, the projection method in Section 3, the VoF interface reconstruction and advection algorithms in Section 4, and the method to compute the interface curvature in Section 5. In Section 6, we present the numerical results for the volume-tracking test-cases (zero surface tension), and for the coupled droplet-flow cases (non-zero surface tension). In Section 7, we give the concluding remarks.

2. Governing equations

The non-dimensional governing equations for a droplet-laden incompressible flow are the continuity and momentum (Navier–Stokes) equations,

$$\nabla \cdot \boldsymbol{u} = 0, \tag{1}$$

$$\partial_t \boldsymbol{u} + \nabla \cdot (\boldsymbol{u}\boldsymbol{u}) = \frac{1}{\rho}\left[-\nabla p + \frac{1}{\mathrm{Re}}\nabla \cdot \left[\mu\left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right)\right] + \frac{1}{\mathrm{We}}\boldsymbol{f}_\sigma\right], \tag{2}$$

where $\boldsymbol{u}(\boldsymbol{x},t)$ is the fluid velocity, $p(\boldsymbol{x},t)$ is the pressure, $\rho(\boldsymbol{x},t)$ is the density, $\mu(\boldsymbol{x},t)$ is the viscosity, and $\boldsymbol{f}_\sigma(\boldsymbol{x},t)$ is the force per unit volume due to the surface tension,

$$\boldsymbol{f}_\sigma = \sigma\kappa\boldsymbol{n}\delta(\boldsymbol{x}-\boldsymbol{x}_s). \tag{3}$$

In Eq. (3), σ is the surface tension coefficient, κ is the curvature of the interface between the two fluids (i.e., droplet and surrounding fluid), $\boldsymbol{n}$ is the unit vector normal to the interface whose position is $\boldsymbol{x}_s$, and δ is the Dirac δ-function that is needed such to impose the force only at the interface between the two fluids. Note that for droplet-laden flow with a uniform surface tension, the non-dimensional σ is equal to unity. $\boldsymbol{f}_\sigma$ is directed towards the fluid respect to which the interface is concave. Fig. 1 shows the direction of the interface normal $\boldsymbol{n}$ and the sign of the interface curvature κ. The interface normal is oriented such that it always points into fluid 2 and the curvature is positive (negative) if the interface is concave (convex) with respect to fluid 2.

In Eq. (2), the Reynolds and Weber numbers are defined as

$$\mathrm{Re} = \frac{\widetilde{U}\widetilde{L}}{\widetilde{\nu}}, \tag{4}$$

$$\mathrm{We} = \frac{\widetilde{\rho}\widetilde{U}^2\widetilde{L}}{\widetilde{\sigma}}, \tag{5}$$

where $\widetilde{U}$, $\widetilde{L}$, $\widetilde{\nu}$, $\widetilde{\rho}$ and $\widetilde{\sigma}$ denote respectively the reference dimensional velocity, length, kinematic viscosity, density, and surface tension coefficient used to normalize the Navier–Stokes equations, (1) and (2). Throughout the paper all variables are dimensionless unless they are written with $\widetilde{\ }$, as in (4) and (5).

In the present paper, uniform density and viscosity ($\rho = 1$ and $\mu = 1$) are imposed such to focus the study on the accuracy of the volume tracking and surface-tension force algorithms. Thus, the Navier–Stokes equations, (1) and (2), we solve are written as

$$\nabla \cdot \boldsymbol{u} = 0, \tag{6}$$

$$\partial_t \boldsymbol{u} + \nabla \cdot (\boldsymbol{u}\boldsymbol{u}) = -\nabla p + \frac{1}{\mathrm{Re}}\nabla^2 \boldsymbol{u} + \frac{1}{\mathrm{We}}\boldsymbol{f}_\sigma. \tag{7}$$

3. Projection method

The Navier–Stokes equations, (6) and (7), are solved numerically using the projection method. Time integration of (7) from time t^n to t^{n+1} ($t^{n+1} = t^n + \Delta t$) is performed using the second-order Adams–Bashforth scheme,

$$\frac{\boldsymbol{u}^* - \boldsymbol{u}^n}{\Delta t} = \frac{3}{2}\mathbf{RU}^n - \frac{1}{2}\mathbf{RU}^{n-1}. \tag{8}$$

In Eq. 8, $\boldsymbol{u}^*$ is a non-divergence-free fluid velocity approximating $\boldsymbol{u}^{n+1}$, and

$$\mathbf{RU}^n = -\nabla \cdot (\boldsymbol{u}^n\boldsymbol{u}^n) + \frac{1}{\mathrm{Re}}\nabla^2\boldsymbol{u}^n + \frac{1}{\mathrm{We}}\boldsymbol{f}_\sigma^{n+1}. \tag{9}$$

The divergence-free condition on the updated fluid velocity is imposed by solving the Poisson equation for pressure,

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t}\nabla \cdot \boldsymbol{u}^*, \tag{10}$$

and by updating the fluid velocity as

$$\boldsymbol{u}^{n+1} = \boldsymbol{u}^* - \Delta t \nabla p^{n+1}. \tag{11}$$

Eqs. (9)–(11) are discretized in space on a uniform staggered mesh using second-order central difference schemes. The velocity and surface tension force components (u_i and $f_{\sigma i}$) are staggered, and all the other field variables are co-located. The Poisson Eq. (10) in finite-difference form is solved using a combination of a two-dimensional fast Fourier transform (FFT) in the x–y plane, and Gauss elimination in the z direction [14]. Periodic boundary conditions are imposed in the three spatial directions.

3.1. Surface tension force

In the continuous surface force (CSF) approach by Brackbill et al. [12], the surface tension force, $\boldsymbol{f}_\sigma$, is computed, after replacing