A novel consistent momentum-conserving subgrid method for high density-ratio liquid-gas flows using the Volume-of-Fluid method for staggered grids

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Abstract
In this study we present a numerical method for the simulation of high density-ratio interfacial flows using a VOF methodology. We use the conservative formulation of the Navier-Stokes equations in order to ensure consistency between the discrete transport of mass and momentum. This strategy is implemented on a uniform cartesian grid, with a staggered configuration, where mass advection is carried out on a grid twice finer than that for momentum(velocity). Implementation is in the spirit of Rudman (1998) [1], coupled with the Weymouth-Yue [9] algorithm for direction-split time integration, resulting in discrete mass and momentum conservation to machine accuracy in 3D. Several flow configurations are presented which demonstrate the robustness and stability of the solver, coupled with qualitative and quantitative comparisons with respect to certain benchmarks.

Keywords
Momentum-conserving advection, dual-grid method, Weymouth-Yue advection, subgrid advection, VOF, Volume-Of-Fluid, staggered grids, direction-split advection, 3D flow simulation, multiphase flow simulation.

Introduction

The development of numerical methods to simulate liquid-gas flows involving interfaces faces several key challenges, particularly for flows with high density-ratios, which are ubiquitous in nature. Several studies in current literature have demonstrated that the use of a conservative formulation for the discrete momentum transport coupled with the momentum transport made consistent with discrete mass transport allows us to alleviate many of the issues which usually lead to loss of stability of numerical methods, which are generally adapted from techniques developed for single-phase flows. The primary challenge in dealing with such flows is the transport of a spatial discontinuity of considerable magnitude (proportional to the contrast in the densities and viscosities of the two fluids), where small errors made in the estimation and transport of momentum in the lighter phase can lead to catastrophic results due to complex non-linear interactions of the interface with the advection operator itself, or through a coupling with surface tension,viscosity and other body forces. In the past two decades, considerable progress has been made in the design of numerical methods, in an effort to alleviate such issues. The underlying principle behind these efforts is that the governing equations are modeled using a conservative formulation (divergence of fluxes), instead of the standard non-conservative forms regularly employed in single-phase flow formulations. This enables us to render the discrete transport of momentum consistent with respect to the discrete transport of mass (which governs the transport of the interface). As demonstrated in the literature [1][3][4][5][6][8][7][2]), adoption of the above mentioned framework does lead to significant improvements in terms of code stability and robustness, therefore enabling the methods to simulate flows with more realistic density and viscosity ratios compared to the standard non-conservative formulations. In this study, we present our attempt at developing such momentum-mass consistent methods, combining influential strategies from past literature in a novel manner.

Numerical Methodology

In this section, we describe in detail the functionality of our free flow solver 'PARIS Simulator' [11], which deals with incompressible multiphase interfacial flows. The solver is based on finite volume discretization on uniform cartesian grids in 3D, utilizing state of the art methods in interfacial reconstruction, interface tracking, curvature computation and surface tension modeling.

Governing Equations

We use the one-fluid formulation for our system of governing equations, thus solving the Navier-Stokes equations throughout the whole domain with regions of variable density and viscosity depending on the explicit location of the interface between the two fluids.

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

$$\partial(\rho \boldsymbol{u}) + \nabla(\rho \boldsymbol{u} \otimes \boldsymbol{u}) = -\nabla p + \nabla \cdot (2\mu \boldsymbol{D}) + \sigma \kappa \delta_s \boldsymbol{n} + \rho \boldsymbol{g} \tag{2}$$

where $\boldsymbol{D}$ represents the deformation rate tensor, σ is the surface tension coefficient, κ is the local interface curvature and δ_s is the Dirac delta function which governs the distribution of the interfacial surface forces into their volumetric

equivalents for our control volumes, $\boldsymbol{n}$ being the normal vector of the interface. In terms of interfacial tracking, we use a Volume-of-Fluid method, the evolution of the volume fraction field given by :

$$\frac{\partial C}{\partial t} + \nabla \cdot (C\boldsymbol{u}) = C\left(\nabla \cdot \boldsymbol{u}\right) \tag{3}$$

As one can observe, we choose to express the transport of the volume fraction function C in the conservative form. The reasoning behind this shall be covered in more detail where we discuss the momentum consistent advection.The variable densities and viscosities are derived from the volume fraction field :

$$\rho = \rho_1 C + (1 - C)\,\rho_2 \tag{4}$$
$$\mu = \mu_1 C + (1 - C)\,\mu_2 \tag{5}$$

where ρ_1, ρ_2 are the densities of fluids 1 and 2 respectively, likewise for viscosities μ_1 and μ_2.

Configuration of Variables
In our implementation, pressure and velocity are defined in a staggered configuration, with pressures on the cell centers (centroids) and velocities on the cell face centers. The volume fraction C (i.e. density field) is defined on a grid that is twice finer than that of the pressure/velocity grid. Therefore in 3D, each cubic control volume is divided into eight constituent smaller cubic volumes, at the centroids of which the volume fraction is centered. The variables dependent on the volume fraction field such as density and viscosity are defined at the centroids of the coarse grid control volumes.

Interface Tracking: Mass Advection
In our Volume-of-Fluid method, we employ geometric reconstruction of the interface in the PLIC framework (piece-wise linear segments), followed by geometric construction of fluxes in order to integrate in time. We shall not go into the details for the geometric computation of the volume fraction (mass) fluxes. In terms of temporal integration, we use the algorithm described by Weymouth & Yue [9], which is basically an explicit forward Euler method in a direction-split manner. The advantages of using this particular method are :

- Exact (to machine precision) conservation of mass (VOF) in 3D, which is non-trivial in direction-split algorithms.
- The algorithm can be extended to the direction-split advection of momentum to render it fully conservative.

The numerical implementation of the method for each individual direction sweep is as follows :

$$\rho_{i,j,k}^{n,d+1} = \rho_{i,j,k}^{n,d} - F_{d+}^{n}\left(\rho\right) - F_{d-}^{n}\left(\rho\right) + C_{d}^{n}\left(\rho\right) \triangle t \tag{6}$$

where

$$\rho^{n,0} = \rho^{n} \tag{7}$$
$$\rho^{n+1} = \rho^{n,3} \tag{8}$$
$$F_{f}^{n} = \rho_1 F_{f}^{n}\left(C\right) + \rho_2 F_{f}^{n}\left(1 - C\right) \tag{9}$$
$$C_{d}^{n}\left(\rho\right) = \left[\rho_1 c_{i,j,k}^{n,d} + \rho_2\left(1 - c_{i,j,k}^{n,d}\right)\right]\frac{\partial u_d}{\partial x_d} \tag{10}$$

with the coefficients $c_{i,j,k}^{n,d}$ being defined according to the Weymouth-Yue method [9] as :

$$c_{i,j,k}^{n,d} = 0 \quad if \quad C_{i,j,k}^{n} < \frac{1}{2} \tag{11}$$
$$c_{i,j,k}^{n,d} = 1 \quad if \quad C_{i,j,k}^{n} \geq \frac{1}{2} \tag{12}$$

This enables us to maintain the prefactor for the directional divergence term on the right hand side of equation (6) as a constant throughout all three directional sweeps, as it depends only on the values of the volume fraction of the cell at the start of the entire time-step. Thus, we ensure that the sum of the directional divergences over all three direction sweeps turn out to be equal to zero, therefore leading to conservation of mass to machine accuracy as we integrate in time.

Consistent Momentum Advection

The development of the present method is motivated by two governing principles :

- The discontinuity of the mass (volume fraction derived density field) should propagate at exactly the same speed as that of the discontinuity of the momentum field.
- The transport of momentum should be performed in a manner consistent with the transport of mass, which basically implies that the momentum fluxes should be computed directly from mass fluxes.

This essentially boils down to how we construct the fluxes of momentum using the mass fluxes which were already computed geometrically for the time integration of the density function (volume fraction). In our approach :

$$F_f^n\left(\rho u\right) = \bar{u}_d \cdot F_f^n\left(\rho\right) \tag{13}$$

Equation (13) states that the momentum flux is directly proportional to the mass flux for each directional sweep, and the factor $\bar{u}_d$ is a velocity which represents the quantity of a particular component of momentum per unit mass, at the start of the time-step. This is computed using standard flux limiters such as QUICK, Upwind, Superbee etc, and in geometric terms it is quite simply an estimate of the velocity (corresponding to the component of momentum) at the centroid of the flux polygon, which in turn represents the mass flux leaving or entering the cell boundary.

Thus in order to ensure consistency in the discrete transport of mass and momentum for each cell along each directional sweep, we have to use a numerical stencil identical to that for the mass advection (eqn. 6). For each component of momentum, we have the directional update using the mass fluxes for the same direction, expressed as :

$$\left(\rho u\right)_{i,j,k}^{n,d+1} = \left(\rho u\right)_{i,j,k}^{n,d} - \bar{u}_{d+} F_{d+}^n\left(\rho\right) - \bar{u}_{d-} F_{d-}^n\left(\rho\right) + C_d^n\left(\rho u\right) \triangle t \tag{14}$$

where, $C_d^n\left(\rho u\right) = u_d^n C_d^n\left(\rho\right)$, thus estabilishing the discrete conservation of momentum within the framework of the Weymouth-Yue algorithm. At the end of the three direction sweeps for equations (6) and (14), we obtain an intermediate velocity field given by :

$$u^* = \frac{\left(\rho u\right)^{n+1}}{\rho^{n+1}} \tag{15}$$

We can subsequently apply other operators such as surface tension, viscous diffusion or body forces in an explicit manner on the intermediate field u^*, before finally passing it on to the pressure-poisson solver in order to project the solution onto a solenoidal field.

Implementing a numerical method for the consistent discrete transport of mass and momentum on a staggered configuration such as in this case, poses the additional challenge of reconstructing the density and momentum fields on the staggered control volumes (on which the velocities are centered), and the subsequent transport of those quantities using equations 6 and 14 in order to obtain the intermediate field u^* centered on the staggered cells. We resolve this using information from our subgrid, in the spirit of Rudman [1]. The important operations involved in the coupling of subgrid information with the coarse grid are:

- Prolongation of the coarse grid velocity field onto the subgrid in order to transport the volume fraction function centered on the subgrid control volumes
- Restriction of the subgrid volume fraction (mass) field to reconstruct the coarse grid mass and momentum fields on the staggered control volumes
- Restriction of the subgrid mass fluxes (geometric) to reconstruct the coarse grid momentum fluxes for the staggered control volumes.

To summarize the numerical algorithm, we present fig. 1 , which demonstrates the 2D version (for sake of brevity) of the consistent momentum and mass transport we have described, illustrating the interaction between the variables defined on the different grids. The variables in red are all defined on the coarse level, and those in green are at the subgrid level. The operators R and P denote the restriction and prolongation operations respectively. The tilde's on top of the variables (e.g. $\tilde{\rho}^n$) signify that they are centered with respect to the staggered control volumes at the coarse grid level. The fine grid velocities $\bar{u}^n$ and $\bar{v}^n$ represent the velocities which are staggered with respect to the fine grid density field. The variables with known values at the start of the advection are surrounded by black elliptical borders, and the variables we obtain at the end of all the directional sweeps are u^* and ρ^{n+1}, as we have explained in the earlier sections. Looking at the algorithm globally, the key differences between our method and the strategies adopted from Rudman[1] and Weymouth-Yue[9] are respectively :

- The use of a geometric framework instead of an algebraic one for the volume fraction field reconstruction and subsequent flux computations required for the VOF method on the subgrid.
- The extension of the transport algorithm to momentum, culminating in the discrete conservation of mass and momentum in a consistent manner for direction-split time integration in 3D.

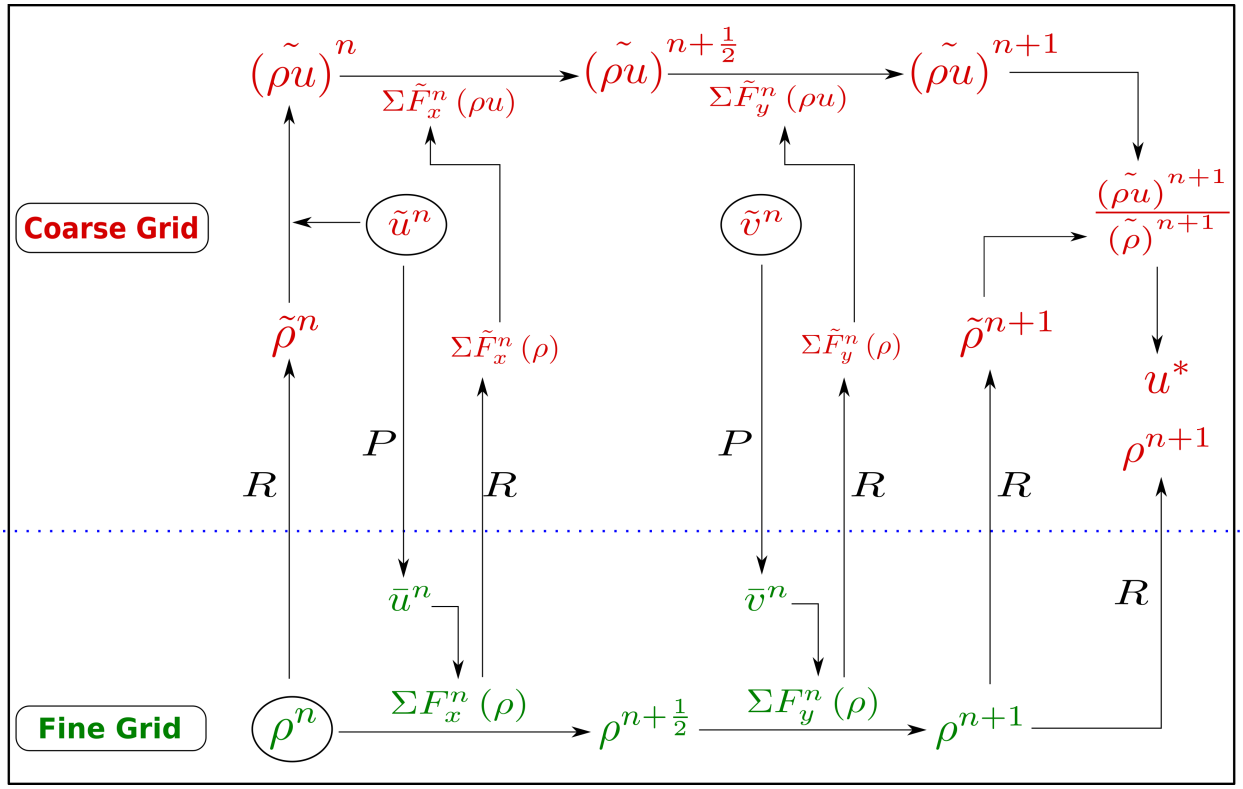

Figure 1. Global view of the numerical algorithm showing the coupling between the grids at two different levels. The figure refers to a 2D situation for simplicity, with the advection first along the x direction, and then along y. Extension of the algorithm to 3D is trivial.

Surface Tension & Viscous Diffusion

We use the Continuum Surface Force method (CSF) for the numerical approximation of surface tension, coupled with mixed height functions for curvature computation. In areas of interfacial regions which are poorly resolved, the method reverts to polynomial fitting instead of height functions, based on the algorithm described by Popinet [10]. We also couple this with a well-balanced discretization with respect to the pressure gradient. The discretization of the viscous diffusion operator is second order in space, using standard central differences. We shall not be describing in detail the algorithms implemented for the surface tension and diffusion as they are not the focus of the present study. The key takeaway from this section is that both of these operators are centered on the staggered control volumes at the coarse grid level, so that they can add their contributions in an explicit manner to the intermediate field u^* that we obtained after the consistent mass and momentum transport (application of the advection operator).

Pressure-Poisson Solver

The discrete variable coefficient pressure-poisson problem is solved using either a simple SOR solver based on Gauss-Seidel iterations, or a V-cycle multigrid solver. Further details regarding the algorithm are not within the scope of the present study, and are therefore skipped.

Results and Conclusions

The results and subsequently, the conclusions shall be presented at the conference during the full presentation.

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