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A consistent mass and momentum flux computation method for two phase flows. Application to atomization process

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ABSTRACT

This paper presents a new computational method for consistent calculation of mass and momentum fluxes in a two-phase flow simulation. The problem of inconsistency of the mass and momentum transfers has been long known in the two-phase flow context. Once the density ratio between fluid phases becomes high, and/or the momentum of one phase differs significantly from that of the other, a decoupling phenomenon causes a non-physical transfer of momentum, rendering most codes unstable. Original works of Rudman [31] have addressed this by proposing a way to couple the mass and momentum flux transport. To ensure this consistency between both fluxes in a staggered configuration, Rudman introduces a finer sub-grid to transport the volume of fluid.

In our paper, we present a way to adopt Rudman's approach without this subgrid, but always in a stagerred grid. The method is presented along with validation test cases and example applications, including very demanding momentum-dominated 3D simulations.

1. Introduction

Many atomization processes are characterized by large density ratios coupled with large shear. A large velocity difference between fluid phases is required to destabilize the spray. For example, the fuel is injected at high velocity in Diesel engines but, in case of assisted atomization, found in cryotechnic applications, the liquid jet (ergol) is surrounded by a gas flow with quite high velocity to produce shear atomization. Numerical simulations of these configurations are known for becoming unstable . The main reason being insufficient coupling between mass and momentum numerical schemes.

In the VOF context, Rudman [31], in 1998, proposed an approach to ensure consistency between mass transport and momentum transport. This method allowed to perform two phase numerical simulations with high density ratio. The momentum flux calculations are directly obtained from VOF fluxes and require a finer sub-grid for the transport of the interface when using staggered grid. Many authors adapted this method to their numerical schemes. Among them, Bussman [22] adapted it to a collocated mesh and did not need subgrid strategy to transport the interface. This method is used by François et al. [9] and with an unsplit VOF algorithm by Le Chenadec et al. [18]. More recently, the method was modified for Level Set (LS) algorithms [7,12,28], in order to obtain the best approximation of flux momentum from the distance function. A simple LS approach was introduced by Raessi in 2009 [7,26] but the flux calculations were one-dimensional and so did not take into account the orientation of the interface passing through the control volume. Later, in 2010, a more sophisticated approach [27,28] for two-dimensional cases was developed. Ghods and Herrmann [12] and Desjardins et al. [6] succeeded in 2013 in proposing a three-dimensional discretization for flux calculation. Some of these methods were successfully applied to numerical simulation of liquid jet atomisation with high density ratio [6,18,28].

Sussman [33] introduced an extrapolated liquid velocity to provide stability in high speed flow with high density ratio, without previous treatment for the consistency between mass and momentum. The velocity field of the fluid with the largest density is extrapolated on some nodes in the lightest fluid, and introduced in the discretization of convective term. This method is also used by Li et al. [19] and Xiao et al. [36] to simulate the primary breakup of

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a liquid jet. The method is stable and gives good results. Desjardins and Moureau's approach [7] decouples gas and liquid velocities by introducing two distinct vector fields that are defined in all the domain. Velocity field of each phase is extended in the other phase thanks to the Aslam [2] method. Both fields are then advected and they are finally coupled through the pressure Poisson equation to obtain a single field.

Because our solver is a coupled levelset/VOF [3,25] on a staggered grid, the Rudman approach seems to be the best approach to ensure consistency between mass and momentum transport [35]. Nevertheless, the finer grid increases the computational cost of our CLSVOF method motivating the development of a single grid approach.

The structure of this paper is as follows: in the first section, we briefly present the numerical methods employed in our solver. Then the implementation of Rudman's method without a subgrid for the advection of the interface on a staggered formulation is detailled. Finally some test cases are presented validating the new method and showing the improvements when compare to previous results.

2. Two phase incompressible Navier–Stokes solver

2.1. Interface advection

The interface description is performed with a CLSVOF algorithm in which the Level Set function Φ describes geometric properties and the VOF function C ensures mass conservation. Both functions are simultaneously advected as presented in [25,34]. Because the advection of VOF is the key point for the conservative mass/momentum advection method, it is briefly recalled how it is performed.

The equation to solve is:

$$\frac{\partial C}{\partial t} + \nabla.(C\mathbf{U}) = C\nabla.\mathbf{U} \tag{1}$$

which is split in (2D description): for the x direction:

$$\tilde{C}_{i,j} = \frac{C^n_{i,j} + \frac{\Delta t}{\Delta x}(f^n_{i-1/2,j} - f^n_{i+1/2,j})}{1 - \frac{\Delta t}{\Delta x}(u^n_{i+1/2,j} - u^n_{i-1/2,j})} \tag{2}$$

and for y direction:

$$\hat{C}_{i,j} = \frac{\tilde{C}_{i,j} + \frac{\Delta t}{\Delta y}(\tilde{f}_{i,j-1/2} - \tilde{f}_{i,j+1/2})}{1 - \frac{\Delta t}{\Delta y}(v^n_{i,j+1/2} - v^n_{i,j-1/2})} \tag{3}$$

At each solver time step, x-y directions are switched.

The final expression of VOF is given by:

$$C^{n+1}_{i,j} = \hat{C}_{i,j} - \hat{C}_{i,j}\frac{\Delta t}{\Delta y}(v^n_{i,j+1/2} - v^n_{i,j-1/2}) - \tilde{C}_{i,j}\frac{\Delta t}{\Delta x}(u^n_{i+1/2,j} - u^n_{i-1/2,j}) \tag{4}$$

In Eq. (2), $f_{i+1/2,j}$ denotes the VOF flux through the face $(i+1/2, j)$ between the cells (i, j) and $(i+1, j)$:

$$f_{i+1/2,j} = u_{i+1/2,j}c_{i+1/2,j}$$

and $c_{i+1/2,j}$ represents a volume fraction (Fig. 1) defined by:

$$c_{i+1/2,j} = \begin{cases} \dfrac{\int_{y_{j-1/2}}^{y_{j+1/2}}\int_{x_{i+1/2}-u_{i+1/2,j}\Delta t}^{x_{i+1/2}} H(\vec{n}_{i,j}.(\vec{r}-\vec{r}_{i,j}) + \alpha_{i,j})dxdy}{u_{i+1/2,j}\Delta t\Delta y} \\ \quad \Leftrightarrow u_{i+1/2,j} > 0 \\ \dfrac{\int_{y_{j-1/2}}^{y_{j+1/2}}\int_{x_{i+1/2}}^{x_{i+1/2}+|u_{i+1/2,j}|\Delta t} H(\vec{n}_{i+1,j}.(\vec{r}-\vec{r}_{i+1,j}) + \alpha_{i+1,j})dxdy}{|u_{i+1/2,j}|\Delta t\Delta y} \\ \quad \Leftrightarrow u_{i+1/2,j} < 0 \end{cases} \tag{5}$$

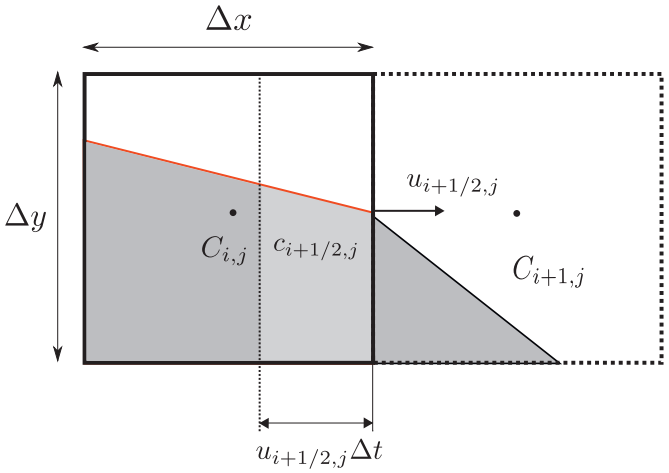

Fig. 1. Schematic representation of VOF advection on x-direction in the case of $u_{i+1/2} > 0$.

$H(.)$ is the Heaviside function, the interface is represented with a linear segment in 2D (plane in 3D) whose equation is derived from on a linear Level Set reconstruction $\Phi^R_{i,j}(\vec{r}) = \vec{n}_{i,j}.(\vec{r} - \vec{r}_{i,j}) + \alpha_{i,j}$. Here $\alpha_{i,j}$ represents the value of the reconstructed Level Set on the center point of the cell ($\vec{r}_{i,j} = (x_i, y_j)$). The integrals in both equations can be computed with geometrical computations, e.g. using the VOF tools of Lopez and Hernandez [21] or cube chopping method [13].

The density ρ in Navier–Stokes equations is computed using the volume fraction [13]:

$$\rho_{i+1/2,j} = C_{i+1/2,j}\rho_l + (1 - C_{i+1/2,j})\rho_g \tag{6}$$

where

$$\begin{aligned} C_{i+1/2,j} &= C_{i+1/4,j} + C_{i+3/4,j} \\ &= \frac{1}{\Delta x\Delta y}\left(\int_{y_{j-1/2}}^{y_{j+1/2}}\int_{x_i}^{x_{i+1/2}} H(\Phi^R_{i,j})dxdy \right. \\ &\quad \left. + \int_{y_{j-1/2}}^{y_{j+1/2}}\int_{x_{i+1/2}}^{x_{i+1}} H(\Phi^R_{i+1,j})dxdy\right) \end{aligned} \tag{7}$$

Note that, in our notation, $C_{i+1/4,j}$ and $C_{i+3/4,j}$ are between [0, 0.5].

2.2. Navier–Stokes equations resolution

To obtain the pressure and velocity fields, the incompressible Navier–Stokes equations are solved:

$$\begin{cases} \nabla.\mathbf{U} = 0 & \text{(8a)} \\ \dfrac{\partial \mathbf{U}}{\partial t} = -(\mathbf{U}.\nabla)\mathbf{U} + \dfrac{1}{\rho}(-\nabla P + \nabla.(2\mu\mathbf{D}) + \mathbf{F}) & \text{(8b)} \end{cases}$$

Where

- $\mathbf{U}$ is the velocity field (u, v, w).
- μ is the dynamic viscosity.
- ρ is the density.
- P is the pressure.
- $\mathbf{D}$ is the strain rate tensor $\mathbf{D} = \frac{1}{2}\left(\nabla(\mathbf{U}) + \nabla(\mathbf{U}^T)\right)$
- $\mathbf{F} = \mathbf{F}_V + \mathbf{F}_{ST}$ represents the body force and the surface tension force, $\mathbf{F}_{ST} = \sigma\kappa\delta_l\vec{n}$

σ is the surface tension, κ the curvature of the interface,$\vec{n}$ is the normal vector to the interface and δ_l is the Dirac function centered on it.