

THETIS is a numerical simulation tool developed by University of Bordeaux. It is a versatile code to solve different problems: fluid flows, heat transfers, scalar transports or porous mediums. The potential of the code in the field of fluid flow is relatively large, it allows to solve incompressible or slightly compressible problems (laminar flow or turbulent flow), as well as multi-phasic problems. It has also been validated and further developed in numerous studies related to water waves (references [1] to [6]).

1. Governing equations

We consider an incompressible flow composed of two unmiscible phases : water and air. If we assume continuity of fluid velocity through the interface and neglect surface tension effects, the governing equations are simply the incompressible Navier-Stokes equations (NS) obviously valid in each phase to which an interface evolution equation is added ([1],[2],[3]). The system of equations, also called one-fluid model, is then the following:

$$\begin{aligned} \nabla \cdot \mathbf{u} &= 0 \\ \rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) &= \rho \mathbf{g} - \nabla p + \nabla \cdot [\mu (\nabla \mathbf{u} + \nabla^t \mathbf{u})] \end{aligned} \quad (1)$$

$$\frac{\partial \chi}{\partial t} + \mathbf{u} \cdot \nabla \chi = 0 \quad (2)$$

In which, ρ and μ , respectively density and viscosity of the fluids, are spatially varying variables and $\chi(x, y, t)$ is a phase characteristic function equal to 1 in water and 0 in air.

2. Numerical method for NS equations

The NS equations are discretized on a fixed Cartesian grid using a finite volume formulation. Following [7], the finite volumes formulation is solved using staggered mesh known as the Marker And Cells (MAC) method from [8]. For this reason, in THETIS we find a mesh of two grids: the pressure grid and the velocity grid. The coupling between velocity and pressure can be solved using the augmented Lagrangian method or Projection method.

- Augmented Lagrangian method

This is a minimization method under the constraint of the continuity equation, where the pressure which is decoupled to the speed, appears as a Lagrange multiplier. The incompressibility constraint is directly introduced into the equation of motion as a penalty term $r_u \nabla(\nabla \cdot \mathbf{u})$, that couples the components of speed. Writing k the iteration of the method, the system is written by:

$$\begin{aligned} \rho^n \left(\frac{\mathbf{u}^{k+1}}{\Delta t^n} + (\mathbf{u}^k \cdot \nabla) \mathbf{u}^{k+1} \right) + B_u (\mathbf{u}^{k+1} - \mathbf{u}_\infty) + \frac{\mu^n \mathbf{u}^{k+1}}{K} - \rho^n \mathbf{g} - \nabla p^k - \nabla \cdot (\mu^n [\nabla \mathbf{u}^{k+1} + \nabla^t \mathbf{u}^{k+1}]) \\ - r_u \nabla(\nabla \cdot \mathbf{u}) = \rho^n \frac{\mathbf{u}^n}{\Delta t^n} \end{aligned} \quad (3)$$

$$p^{k+1} = p^k - r_p \nabla \cdot \mathbf{u}^{k+1}$$

The advantage of such a formulation is the explicit calculation of the pressure. It uses only the pressure in the previous temporal iteration and the divergence of speed, no

boundary condition in the pressure is required.

- Projection method

This method comprises two steps:

1. From the pair (u^n, p^n) , a velocity field \tilde{u} is calculated using the expression

$$\tilde{u} - u^n = \frac{\Delta t^n}{\rho^n} (\rho^n g - \nabla p^n + \nabla(\mu^n [\nabla u^n + \nabla^t u^n]) - \nabla \cdot (\rho^n u^n \otimes u^n)) \quad (4)$$

2. The velocity u is calculated by projection of \tilde{u} on a field with no divergence

$$u^{n+1} = \tilde{u} - \frac{\Delta t^n}{\rho^n} \nabla (p^{n+1} - p^n) \quad (5)$$

This second step (projection step) involves determining the pressure p^{n+1} . We use the Poisson equation:

$$\nabla \cdot \left(\frac{\Delta t^n}{\rho^n} \nabla (p^{n+1} - p^n) \right) = \nabla \cdot \tilde{u} \quad (6)$$

This method is relatively simple to program and easy to solve because it's not an iterative method (contrary to the previous method). However, the boundary conditions on the pressure must be imposed to allow the resolution of (6).

3. Interface tracking and transport

The equation (2) is solved by introducing a color function F defined as the average of the phase characteristic function $\chi(x, y, t)$ over the mesh cell. With this definition, F indicates the volume fraction occupied by water in a mesh cell and the interface position is defined as the iso-line $F = 0.5$.

At the end of each time step, the local cell water volume fraction is used to recalculate local values of density and viscosity necessary to solve the NS equations. For cells containing a fraction of water and air, equivalent density and viscosity are calculated by linear interpolation based on the water fraction F . This type of interpolation allows for a mass conservation due to the presence of two fluid in mix cells. A correct physical justification can not be given for this calculation of the equivalent viscosity. But the use of other type of approximations (e.g. harmonic average) does not show any significant effect on the results witnessing the weakness of the viscosity influence on the impact physics. Different VOF methods are implemented in the model THETIS to solve equation (2).

- VOF-TVD method

This first method consists in solving equation (2) directly using a suitable numerical scheme. Writing the convective term of equation (2) in the conservative form and using a first order discretization in time, the discretization in space over the volume control (i,j) reads :

$$\frac{F_{i,j}^{n+1} - F_{i,j}^n}{\Delta t^n} \Delta X \Delta Y + \phi_X \Delta Y + \phi_Y \Delta X = 0 \quad (7)$$

With

$$\phi_X = F_{i+\frac{1}{2},j}^{n+1} u_{i+\frac{1}{2},j}^{n+1} - F_{i-\frac{1}{2},j}^{n+1} u_{i-\frac{1}{2},j}^{n+1}$$

$$\phi_Y = F_{i,j+\frac{1}{2}}^{n+1} u_{i,j+\frac{1}{2}}^{n+1} - F_{i,j-\frac{1}{2}}^{n+1} u_{i,j-\frac{1}{2}}^{n+1}$$

ΔX (respectively ΔY) represents the horizontal space step (respectively vertical). At this stage, a good approximation of the fluxes ϕ_X and ϕ_Y is required to obtain an accurate representation of the interface. A TVD scheme typically has two main properties : in the parts of the domain where the solutions are regular, it is equivalent to a high-order scheme that reduces diffusion. And in the parts where there are strong discontinuities it is a first order scheme that prevents oscillations.

- VOF-PLIC method

The Piecewise Linear Interface Calculation (PLIC) method is also employed. One of the great advantage of this Eulerian/Lagrangian method is to keep the discontinuous nature of the interface between water and air thanks to the Lagrangian character of the transport method. The five successive steps of the PLIC method are the followings:

- Mixed cells (i.e. $0 < F < 1$) identification.
- In each cell containing air and water, calculation of the interface normal direction using a finite difference approximation on nine points.
- Piecewise linear interface reconstruction, knowing the normal direction in each cell and the volume fraction.
- Lagrangian advection of the interface segments using a linear interpolation of velocities calculated on the staggered mesh.
- Calculation of the new volume fraction distribution.

To ensure the conservative or stability nature of the PLIC method, a sufficient condition is that the segments are not advected over more than half of a cell size during a time step Δt ([1]).

- SVOF-PLIC method

The SVOF-PLIC method consists in slightly smoothing the volume fraction function by introducing a controlled diffusion zone around the interface. This is performed by using an analogy with the thermal diffusion whose governing equation equation reads:

$$\frac{\partial T}{\partial t} - \nabla \cdot (a \nabla T) = 0 \quad (8)$$

$a > 0$ being the thermal diffusivity coefficient. The smoothed volume fraction function F^S is built from equation (9) discretized in time :

$$- \nabla \cdot a \nabla F^{S,n+1} + F^{S,n+1} = F^{S,n} \quad (9)$$

In which the equivalent diffusion coefficient a is expressed upon the interface thickness L_i and the local dimension of the considered cell ΔX by :

$$a = L_i \Delta X^2 \quad (10)$$

Equation (10) is discretized in space by using the finite volume method and a centered scheme. The final smoothed function F^S is obtained iteratively by applying the following algorithm :

$$L^1 = F \quad (11)$$

For $k=1 \dots N-1$, solve

$$-\nabla \cdot \tau_d^* \nabla F^{S,k+1} + F^{S,k+1} = L^k \quad (12)$$

$$L^{k+1} = F^{S,k+1} \quad (13)$$

with τ_d^* defined by $\tau_d^* = \frac{L_i \Delta h^2}{N}$. After resolution of (9) - (13), the condition $F^S = F^{S,N}$ is verified.

The function F^S includes a narrow diffusion zone that represents the interface more regularly. By this way, the discontinuities which may appear with the PLIC algorithm are smeared and the interface is more stable while being a little less accurate. The model can then describe high interface distortions occurring during the impact without diverging. Practically, the parameters L_i and the number of internal iterations are adjusted to limit the interface fractioning while keeping an accurate description of the interface.

References

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