COUPLING OF IMPLICIT-EXPLICIT METHODS FOR TWO-PHASE FLOW WITH A FULLY VOLUME PRESERVING METHOD

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SUMMARY

The SIMPLE-based Finite Volume Method is combined with the Volume of Fluid (VOF) method to solve the two-phase flow field. Interface conditions are satisfied by means of the continuous surface force (CSF) methodology. A geometrical Eulerian interface reconstruction method is presented, where the volume fraction field is fully conserved. In addition, while the momentum equations are solved implicitly, an explicit time split scheme is used for the volume fraction equation. The preconditioning matrix solver ILUT-GMRES is used to solve the algebraic system. Computational results presented for dam break and sloshing tank problems are shown to be in good agreement with other results reported in the open literature.

1 INTRODUCTION

Today the computer has become a powerful tool for the prediction of fluid flow. The acronym CFD (Computational Fluid Dynamics) represents numerical solutions to fluid problems by solving some form of the governing equations. However, simulations of flows with interface (free-surface) effects have been of interest to the numerical community both for their real-world engineering applications and for the challenges which moving-boundary problems present. If numerical simulation of non-interface flows seems to reach a certain maturity and robustness, the simulation of interface flow requires more improvements such as volume preserving, determination of interface normal, slowing down of convergence due to high density ratio…

Regardless of the numerical approach employed the essential features needed to properly model free surfaces are; a scheme to describe the movement of the surface and a means to implement the boundary conditions at the surface. There are two broad classes of methods: interface capturing method where the equations are solved upon a fixed mesh, with the free surface being found within the solution domain (marker-and-cell (MAC) method \cite{1, 2, 3}, Volume-Of-Fluid method \cite{4, 5, 6, 7}, Level-Set method \cite{8, 9, 10, 11, 28}), and interface tracking methods , where the free surface is located at one boundary of the mesh , and the mesh deforms as the free surface moves. The marker-and-cell (MAC) method introduces massless marker particles in all cells initially containing the fluid. A Lagrangian approach is used to determine the later position of these particles and hence the location of the free surface. The VOF method modifies the MAC method by replacing the discrete marker particles with a continuous field variable (colour function). The basic principle is as follows: for each computational cell, the fraction of the cell which is filled by a particular fluid, say fluid 1, is defined. These volume fractions are then advected using the underlying velocity field. The interface is contained in those cells which have volume fraction other than one or zero. Level set methods imbed the interface in a distance function such that the zero-level of the distance is the interface. The distance is then advected using the velocity field. There are several numerical issues that must be taken into consideration when computing the motion of the interface. The high density ratio (about 1000:1) may cause slow convergence and the modelling of the surface tension force may lead to accuracy problems. Another important issue is the global mass conservation during the computation. Since the investigation of the solution requires several time steps integration, all schemes that do not guarantee mass conservation will sooner or later, result in unacceptable mass losses. In other words, the main disadvantage of the VOF method is that it suffers from the numerical errors typical of Eulerian schemes such as the level set method. The imposition of a preservation constraint does not eliminate these errors, but instead changes their symptoms replacing mass loss with inaccurate mass motion leading to small pieces of fluid non physically being ejected as flotsam and jetsam artificial surface tension forces that cause parasitic currents, and an inability to accurately calculate geometric information such as normal vector and curvature \cite{16}. Gerrits et al. use local height function to avoid the “flotsam and jetsam”. For more details see \cite{15, 17, 18, 26, and 27}.

In this paper, we propose a new method which can preserve not only the volume but also remove the flotsam and jetsam problem. In addition, an algorithm which can combine an implicit time integration of momentum equations and explicit time integration of the volume fraction equation is proposed. The mean advantage of this coupling is the reduction of computation time in comparison with fully explicit scheme.
2 NUMERICAL FORMULATION

2.1 GOVERNING EQUATIONS

The motion of the unsteady, viscous, incompressible two-phase flow is described by the Navier-Stokes equations:

- Continuity equation
  \[ \frac{\partial u_i}{\partial x_i} = 0 \]  

- Momentum equations
  \[ \frac{\partial}{\partial t} \left( \rho u_i \right) + \frac{\partial}{\partial x_j} \left( \rho u_i u_j \right) = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + \frac{1}{\rho} \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] + f_i + \frac{1}{\rho} \nabla \cdot \mathbf{F} \]  

with
  \[ \rho = \rho_i + (1 - F) \rho_e \]  

\[ \mu = \mu_i + (1 - F) \mu_e \]  

- Volume fraction equation
  \[ \frac{\partial F}{\partial t} + \frac{\partial (Fu_i)}{\partial x_i} = 0 \]  

In the above equations, \( u_i \) and \( g_i \) are the Cartesian velocity and the gravity components in i-direction respectively. \( p \) is the pressure. \( \mu_k \) and \( \rho_k \) are the viscosity and density respectively, of the fluid \( k \), where \( k=\text{g} \) for gas and \( k=\text{l} \) for liquid.

The last term \( f_i \) is the surface tension force obtained via the continuum surface force CSF approach [10, 24, 28, and 29] which is active only on liquid-gas interface. The properties (density and viscosity coefficients) appearing in the momentum equation are determined by the presence of the component phase (volume fraction) \( F \) in each control volume, which is bounded by zero and one.

2.2 DISCRETISATION

The finite volume discretisation of \( u_i \)-momentum equation is based on the integration over the control volume and time step. Quadratic Upwind Interpolation of Convective Kinetics (QUICK) scheme of Hayase et al. is used for convective terms and central difference for diffusive terms and fully implicit time scheme. In order to avoid the numerical instability, often known as the “checkerboard problem, an improved Rhie-Chow interpolation is used to calculate the convective flux [19, 20, and 21]. The spatial and temporal discretisation leads to

\[ \sum_{nb} A_{nb} u_i|_{nb} = B_i \]  

where

\[ A_{nb} = A_E u_i + A_W u_i + A_N u_i + A_S u_i + \Delta F + \frac{J}{\Delta t} \]  

\[ A_W = D_w + H(F_w)F_w \]  

\[ A_S = D_s + H(F_s)F_s \]  

\[ A_N = D_n - H(-F_n)F_n \]  

\[ A_E = D_e - H(-F_e)F_e \]  

\[ A_F = \frac{1}{\rho} \left( \frac{\mu \Delta x}{\Delta y} \right), \quad D_n = \frac{1}{\rho} \left( \frac{\mu \Delta x}{\Delta y} \right), \text{ etc.} \]  

\[ F_e = (u \Delta y), \quad F_n = (v \Delta x), \text{ etc.} \]  

\[ B_i = \left( \frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{f_i}{\rho} + g_i \right) \Delta x \Delta y + S_{\text{conv}} \]  

\[ S_{\text{conv}} = \frac{1}{8} \left[ H(F_e)F_e(3 \phi_e - 2 \phi_e - \phi_N) + H(-F_e)F_e(3 \phi_e - 2 \phi_e - \phi_N) \right] \]
\[ + \frac{1}{8} \left[ H(F_w)F_w(3 \phi_w - 2 \phi_w - \phi_N) + H(-F_w)F_w(3 \phi_w - 2 \phi_w - \phi_N) \right] \]
\[ + \frac{1}{8} \left[ H(F_s)F_s(3 \phi_s - 2 \phi_s - \phi_N) + H(-F_s)F_s(3 \phi_s - 2 \phi_s - \phi_N) \right] \]
\[ + \frac{1}{8} \left[ H(F_n)F_n(3 \phi_n - 2 \phi_n - \phi_W) + H(-F_n)F_n(3 \phi_n - 2 \phi_n - \phi_W) \right] \]

The Heveaside function is defined by

\[ H(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x > 0 \end{cases} \]  

2.3 INTERFACE MODELLING

The interface is treated as a shift in the fluid properties. Along the interface, the surface tension arises as the result of attractive forces between molecules in a fluid. Here, we use the Continuum Surface Force (CSF) Approach proposed in [10, 24, 28, 29], which
incorporates the surface tension as a volume force \( f_i \) included in the momentum equations;

\[
f_i = \sigma \kappa \nabla F_i
\]  
(18)

where

\[
\kappa = \nabla \left( \frac{n}{|n|} - (\nabla \cdot n) \right)
\]  
(19)

The volume fractions transition abruptly across the interface, causing problem of accuracy when calculating the normal and the curvature. A solution to this problem is to first convolve \( F \) with a smooth kernel \( K \) to construct a smoothed or mollified interface point \( F \);

\[
\tilde{F}(x) = K \ast F(x) = \int_{\Omega} F(x')K(x - x')dx'
\]

\[
= \sum F(x')K(x - x')\Delta x'
\]  
(20)

where \( \Omega \) denotes the support of the kernel \( K \) (i.e., those points \( x \) for which \( K(x) \neq 0 \)) which is typically compact (i.e., of finite extent).

Many types of kernels have been used in the past, such as Gaussians, B-Spline and polynomials. Some of these kernels are radially-symmetric while others are products of one dimensional function. In this paper, we have chosen the Peskin function which is given by

\[
K(\vec{x} - \vec{x}_k) = \prod_{\text{dim}} \left\{ \begin{array}{ll}
1 & \text{if} |\vec{x} - \vec{x}_k| \leq d \\
1 + \cos \frac{\pi}{d} - \frac{|\vec{x} - \vec{x}_k|}{d} & \text{otherwise}
\end{array} \right.
\]  
(21)

where \( \text{dim} \) is the partial dimension, \( d = 2h \) with \( h \) the grid spacing, \( \vec{x} \) the grid coordinates, \( \vec{x}_k \) interface point coordinates. In this paper, the grid spacing is not uniform, so we have

\[
h = \max(dx, dy)
\]  
(22)

2.4 PRESSURE CORRECTION

The coupling between velocity and pressure is implicitly implemented by an auxiliary pressure correction equation [18, 19, and 20]. First, given a guessed pressure field, one can obtain a velocity field by solving equations (6). This resulting velocity field may not satisfy the continuity equation.

\[
A^*_P u^*_i P - \sum_{nb} A_{nb} u^*_i nb = B^*_i
\]  
(23)

To enforce the continuity conservation, a correction procedure is needed. The pressure and velocities are corrected by

\[
p = p + p'
\]  
(24)

\[
u = u^* + u', \quad v = v^* + v'
\]  
(25)

The relation between the velocity and pressure corrections is obtained by subtracting equation (6) from (23) that yields

\[
u'_P = -\frac{A_p^*}{A_p'} p'_x, \quad v'_P = -\frac{\Delta x}{A_p'} p'_y
\]  
(26)

Finally, substituting the corrected velocities into the continuity equation and integrating over the control volume, yields the pressure correction equation

\[
A^*_P p'_P - \sum_{nb} A_{nb} p'_nb = B^*_P
\]  
(27)

where

\[
A_{E/W} = \left( \frac{\Delta x^2}{A_p^*} \right), \quad A_{N/S} = \left( \frac{\Delta x^2}{A_p'} \right)
\]

\[
A_P = A_E + A_W + A_N + A_S, \quad B_P' = (u_w^* - u_e^*) dy + (v_n^* - v_s^*) dx
\]

2.5 VOLUME TRACKING ALGORITHM

In this paper, the geometric reconstruction PLIC scheme is employed because of its accuracy, compared to the other methods such as donor acceptor, Euler explicit method.

In PLIC method, the interface is approximated by a straight line of appropriate inclination in each cell. A typical reconstruction of the interface with a straight line in cell \((i,j)\), which yields an unambiguous solution, is perpendicular to an interface normal vector \( \vec{n} \) and delimits a fluid volume matching the given \( F_{i,j} \) for the cell. The normal vector \( \vec{n} \) is defined by

\[
\vec{n} = \nabla F
\]  
(28)

Initially, a cell-corner value of the normal vector \( n_{i,j} \) is computed, as is illustrated for the corner at \( i+1/2, j+1/2 \)

\[
n_{x,e} = \frac{F_{NE} + F_{E} - F_{P} - F_{N}}{2(x_E - x_P)}
\]  
(29)
The cell-centred value is given by
\[ n_{s,c} = \frac{F_{sE} + F_{N} - F_{P} - F_{E}}{2(y_{N} - y_{P})} \]  
(30)

The cell-centred value is given by
\[ n_{c} = \frac{\bar{n}_{E} + \bar{n}_{N} + \bar{n}_{P} + \bar{n}_{E}}{4} \]  
(31)

In VOF/PLIC method, the interface is approximated in each cut cell by a portion of a straight line in 2D (plane in 3D), defined by the equation
\[ n_{x}x + n_{y}y = \lambda \]  
(32)

where \( \lambda \) is the interface constant (parameter which is related to the smallest distance between the interface and the origin.

The volume fluxes are calculated geometrically. The flux estimation is based on the interface configuration inside the surface cell. The liquid volume \( \delta V \), which flows through a face of a cell during a time step, \( \delta \) may be found using the interface parameter \( \lambda_{c} \) via the relation (33). For instance the volume flux advected \( \delta V \) during time \( \delta \) through the east face of the donor cell can be found as follows; since the position of the interface is known in the donor cell, that is, \( \lambda_{c} \) is known, then we can apply the relation (33) to the sub-region with lengths \( dx - |u_{a}| \delta \) and \( dy \)
\[ F_{c} = \frac{\lambda_{c} - \max(0,(\lambda_{c} - dy)^{2})}{2dx,dy_{c}} \]  
(42)

and
when \( \lambda \leq 0.5 \lambda_{m} \) and \( n_{x}u_{c} < 0 \)
\[ \delta V_{c} = F_{c}dy - F_{c}dy(dx - |u_{a}| \delta) \]  
(43)
when \( \lambda > 0.5 \lambda_{m} \) and \( n_{x}u_{c} < 0 \)
\[ \delta V_{c} = F_{c}dy - (1 - F_{c})dy(dx - |u_{a}| \delta) \]  
(44)

\[ F_{c} = \max(0,(\lambda_{c} - dy)^{2}) \]  
(45)

when \( \lambda \leq 0.5 \lambda_{m} \) and \( n_{x}u_{c} \geq 0 \)
\[ \delta V = F_{c}dy|u_{a}| \delta \]  
(46)
when \( \lambda > 0.5 \lambda_{m} \) and \( n_{x}u_{c} \geq 0 \)
\[ \delta V = (1 - F_{c})dy|u_{a}| \delta \]  
(47)

The volume of liquid inside the cell is deduced as
\[ \lambda_{c} = \sqrt{\frac{2F_{c}dx_{c}dy_{c}}{F_{c}dx_{c} + \frac{dy_{c}}{2}}} \text{ if } \lambda_{c} < dy_{c} \]  
(41)
\[ \lambda_{c} = \sqrt{\frac{F_{c}dx_{c} + \frac{dy_{c}}{2}}{F_{c}dx_{c}} \text{ if } \lambda_{c} \geq dy_{c}} \text{ if } \lambda_{c} \]  
(42)

2.5.1 VOLUME FLUXES CALCULATION

In PLIC method, the volume fluxes are calculated geometrically. The flux estimation is based on the interface configuration inside the surface cell. The liquid volume \( \delta V \), which flows through a face of a cell during a time step, \( \delta \) may be found using the interface parameter \( \lambda_{c} \), via the relation (33). For instance the volume flux advected \( \delta V \) during time \( \delta \) through the east face of the donor cell can be found as follows; since the position of the interface is known in the donor cell, that is, \( \lambda_{c} \) is known, then we can apply the relation (33) to the sub-region with lengths \( dx - |u_{a}| \delta \) and \( dy \)
\[ F_{c} = \frac{\lambda_{c} - \max(0,(\lambda_{c} - dy)^{2})}{2dx,dy_{c}} \]  
(42)

and
when \( \lambda \leq 0.5 \lambda_{m} \) and \( n_{x}u_{c} < 0 \)
\[ \delta V_{c} = F_{c}dy - F_{c}dy(dx - |u_{a}| \delta) \]  
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when \( \lambda > 0.5 \lambda_{m} \) and \( n_{x}u_{c} < 0 \)
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(44)

\[ F_{c} = \max(0,(\lambda_{c} - dy)^{2}) \]  
(45)

when \( \lambda \leq 0.5 \lambda_{m} \) and \( n_{x}u_{c} \geq 0 \)
\[ \delta V = F_{c}dy|u_{a}| \delta \]  
(46)
when \( \lambda > 0.5 \lambda_{m} \) and \( n_{x}u_{c} \geq 0 \)
\[ \delta V = (1 - F_{c})dy|u_{a}| \delta \]  
(47)

Lagrangian approach is used in [11] to advance the old, reconstructed interface with interpolated velocities to a new position and the new \( \phi \)-field is deduced from the new interface locations. Here, we apply Eulerian techniques which are mainly divided in two categories:
multidimensional or unsplit schemes and one-dimensional or operator split schemes. Multidimensional schemes require only one reconstruction per time step, i.e., a full multidimensional solution is updated in a single time step. They are more complex because boundary fluxes depend on fluxes calculated along each coordinate direction. Examples of multidimensional algorithms can be found in [147], [176], and [41]. Split schemes, on the other hand, construct the multidimensional solution as a series of sequential, one-dimensional sweeps.

\[
\frac{F_{n+1}^* - F_n^*}{\Delta t} + \frac{\partial u F_n^*}{\partial x} = F_n^* \frac{\partial u}{\partial x} \quad (47)
\]

\[
\frac{F_{n+1}^* - F_n^*}{\Delta t} + \frac{\partial v F_n^*}{\partial y} = F_n^* \frac{\partial v}{\partial y} \quad (48)
\]

where the advected volume fractions during a time step are given by:

\[
F_{e/w} = \frac{\delta V_{e/w}}{|\delta d/dy|_{e/w}} \quad (49)
\]

\[
F_{n/s} = \frac{\delta V_{n/s}}{|\delta d/dx|_{n/s}} \quad (50)
\]

### 2.5.2 IMPLICIT EXPLICIT SCHEMES COUPLING

In this paper, the momentum equations are solved implicitly. It is well known that time step for implicit is unconstrained, that is the scheme is unconditionally stable for reasonable large value of time step. Usually, the same time step is used to solve the interface function equation. In this paper, we propose a scheme in which the momentum equations are solved implicitly while the evolution equation of the interface is solved explicitly, so we use two different time steps such that

\[
\delta t_m \propto k \delta t_i \quad \text{with} \quad k \gg 1
\]

where \(\delta t_m\) and \(\delta t_i\) represent time step for momentum and interface evolution equations respectively.

### 2.5.3 VOLUME PRESERVING METHOD

Volume conserving is guaranteed when the total volume of fluid remains constant during resolution process, that is the volume at initial state is equal to the volume of final state. Consider \(V_0\), as the sum of volume fractions over the domain at initial time, and \(V_n\) the sum of volume fractions at time \(t_n\) over the domain. Then, if \(V_n < V_0\) volume is lost, if \(V_n > V_0\) volume is added, if \(V_n = V_0\) volume is preserved. In order to ensure total volume preserving, we correct only the value of volume fraction in each interface cell, but not over all cells as is done usually in literature [13, 14].

The main idea behind our approach is that since the interface cells are used to define the interface, it has been reasonable to modify only the values inside those cells, by using a weighted method. Consider, \(I_e\) as the set of interface cells of which volume fraction are such that \(0 < F_P^* < 1\). The corrected value of volume fraction \(F_P\) inside an interface cell \(P\), is given by

\[
F_P = F_P^* \left( 1 + \frac{V_0 - V_n}{S} \text{sign}(V_0 - V_n) \right) \quad (52)
\]

Figure 3: Coupling of Implicit SIMPLE algorithm and Explicit VOF method.
\[ S_I = \sum_{r \in R} F_{IP}^* \]

3 NUMERICAL RESULTS

The impact loads are very important in designing offshore and coastal structures. Typical problems such as green water loads on ships, wave run-up on offshore structures, slam loads and sloshing loads in tanks are important in the area of naval hydrodynamics. The first test concerns a dam break problem as described below. The initial velocity field is set to zero, and wall boundary conditions where pressure gradient and velocities are set equal to zero are applied to all boundaries. The second test concerns a dam break problem with an obstacle. The pressure peak due to water impact on the right vertical wall will be analysed. Finally, the model is applied to a sloshing rectangular tank.

**Dam break without obstacle**

Figure 4: Initial geometry of dam break Problem

Figure 5: Visualisation of dam break solution.
Figure 6: Dam break Flow and impact against the Tank wall ($\tau = t\left(\frac{g}{H}\right)^{1/2}$).

(Obtained using Fluent)

Figure 7: impact pressure: (a) from our home code (b) from other works ($\rho g H \approx 4896.2$).

(c) impact pressure field at $t=0.704$ s when the front collapses on the wall.

Dam break with obstacle

Figure 8: pressure field at $t=0.045$ and impact fields at $t=0.145$ on an obstacle.
Sloshing Tank

The sloshing of the liquid can increase the dynamic pressure on the tank sides and bottom, so that the integrity of the tank is put at risk. An example is a ship carrying liquid cargo where sloshing can be critical in a partially filled tank. Another example is the case when the satellites start to accelerate for course corrections; the onboard fuel starts to slosh inducing a force and torque. This interaction between the motion of the satellite and the onboard sloshing liquid can have undesirable consequences as happened quite recently (in 1998) with NASA’s Near Earth Asteroid Rendezvous (NEAR) craft, which was on its way to the asteroid 433 Eros, Jeroen Gerrits [91]. The

In this test, a rectangular tank with fluid inside is initially at rest state [120]. An experimental test was performed in [72]. The tank is suddenly accelerated along the horizontal x-direction in a sinusoidal large-amplitude. The position of the tank is given by

\[ x = A \sin \left( \frac{2\pi}{T} t \right) \quad \text{and} \quad y = Cte \]

The inertial body force is given by \( F_i = -\rho V \ddot{x} \), \( \rho \) is the density of the fluid, \( V \) the volume of the liquid inside the control volume, and \( \ddot{x} \) the acceleration of the governing coordinate system which is given by

\[ \ddot{x} = -A w^2 \sin \left( \frac{2\pi}{T} t \right) \]

For the first test, we have chosen \( A = 0.1 \) and \( T = 2.5 \)

![Figure 9: Evolution of the interface due to horizontal excitation](image)

![Figure 10: movement of the interface point along the right vertical wall](image)
Figure 11: Sloshing in an octagonal tank excited by an horizontal acceleration with (Amplitude=0.5, T=4.0s)
Interface (left) and pressure fields (right)

CONCLUSION

A Coupling of SIMPLE algorithm with implicit algorithm for momentum equations and an explicit geometric VOF method with a fully volume preserving has been presented and evaluated. In this paper, the classical breaking dam and sloshing tank problems have been used to evaluate the computer code. The computational results presented for dam break and sloshing tank problems are shown to be in good agreement with other results reported in the open literature.

4 Reference


