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MODELLING SURFACE TENSION DOMINATED MULTIPHASE FLOWS USING THE VOF APPROACH

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Abstract. This study considers enhancements to the volume-of-fluid (VOF) approach to allow for the accurate modelling of low capillary or surface tension dominated flows. Conservative VOF approaches tend to result in the formation of spurious or parasitic currents due to sharp changes in gradient over the interface. With the aim of reducing this imbalance between the fluid pressure and the surface tension forces an alternative pressure interpolation scheme is evaluated. Furthermore, the continuum surface forces (CSF) method is extended to use a smoothed volume fraction field which is computed using an implicit diffusion-type algorithm.

1 INTRODUCTION

Low-capillary number or surface tension dominated flows are found in a number applications, ranging from small scale microfluidics up to larger scale analysis of microgravity sloshing. This paper evaluates the possibility of modelling of surface tension dominated multiphase flows using an Eulerian volume-of-fluid (VOF) approach with high-resolution surface capturing. With the aim of improved stability and computational efficiency, a conservative formulation is implemented that ensures parasitic currents are negligibly small.

Level-set (LS) and VOF methods are extensively used in modelling multiphase flows as these approaches are easily extended to arbitrary unstructured three-dimensional meshes and allow for efficient scaling in parallel computation. When modelling surface tension dominated problems, LS methods allow for an accurate approximation of the curvature as it is based on a smooth, continuous approximation of the Heaviside equation. LS methods are, however, found to be non-conservative [2, 16] and require the reinitialisation of the distance function at regular time intervals to ensure a well maintained gradient [21]. It is noted that a number of studies suggested corrections to the LS approach to improve mass

conservation, but it is argued that these tend to become over complex and computationally inefficient.

Conservative VOF schemes [14, 5] tend to provide an inaccurate approximation of the interface curvature due to the sharp change in the volume fraction gradient. This subsequently results in the formation of spurious or parasitic currents [10], which stems from an imbalance between the pressure and surface tension forces. It is, however, found that through careful treatment of the numerical discontinuities over the interface a more accurate approximation can be achieved, which results in a reduction of the said parasitic currents.

Using the OpenFOAM® finite volume toolset, a new VOF solver was developed which aims to improve on the following:

- Pressure interpolation;
- Surface capturing; and
- Interface curvature.

By utilising the said open-source platform, it is possible to link and use an extensive set of existing libraries.

2 GOVERNING EQUATIONS

If an Eulerian volume-of-fluid approach is followed, a control volume partially filled with two fluids can be considered where the volume fractions of the fluids occupying a cell are denoted α and $1-\alpha$. Furthermore a homogeneous flow model, which assumes a cell-averaged velocity and pressure, is employed and it is assumed that the fluids can be treated as incompressible.

2.1 Volume-of-fluid approach

For a two-fluid system, the VOF approach involves the construction of an advection equation for the indicator volume fraction, α, to describe the evolution of the free-surface interface

$$\frac{\partial \alpha}{\partial t} + \frac{\partial (\alpha u_j)}{\partial x_j} = 0 \tag{1}$$

where time is denoted t and the velocity and spatial coordinate in direction i are u_i and x_i, respectively.

For incompressible flow, the continuity equation or divergence free velocity reads

$$\frac{\partial u_j}{\partial x_j} = 0 \tag{2}$$

and the averaged momentum equation for homogenous two-fluid flow follows

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} + \frac{\partial p}{\partial x_i} = S_i \tag{3}$$

where p is the pressure and the source term, $\mathbf{S}$, contains the hydro-static pressure term, the viscous term as well as the surface tension term. If Newtonian flow is assumed, the following holds

$$S_i = \rho g_i + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial u_i}{\partial x_j}\right) + f_\sigma^i \tag{4}$$

The mixture density and dynamic viscosity, expressed in terms of the volume fractions, are

$$\begin{aligned} \rho &= \alpha\rho_1 + (1-\alpha)\rho_2 \\ \mu &= \alpha\mu_1 + (1-\alpha)\mu_2 \end{aligned}$$

where 1 and 2 denote the respective fluids.

2.2 Surface tension or capillary forces

As noted previously, in this work the continuum surface force (CSF) method [1] is employed. However, to reduce the numerical inaccuracies associated with the approximation of the curvature a smoothed volume fraction field, which display the same characteristics as the Heaviside equation, is computed. As with Level-set methods, this approach provides a more reasonable approximation of the interface normal vectors and subsequently the interface curvature, curbing the effect of the parasitic currents as discussed by Lafaurie et al. [10]. Although various smoothing methods have been presented in literature [3, 19, 17], an implicit diffusion-type smoothing is implemented which can be solved efficiently using an iterative solver while still providing the necessary flexibility. The semi-discrete form of the diffusive equation reads

$$\frac{\alpha^* - \alpha}{\Delta\tau} - \frac{\partial}{\partial x}\left(\Gamma_\alpha \frac{\partial \alpha^*}{\partial x}\right) = 0 \tag{5}$$

where α^* is the computed smoothed volume fraction and τ denotes the artificial or pseudo time which is scaled according to the cell size, $\mathcal{V}$, to ensure a mesh independent solution. The diffusive coefficient, Γ_α, can be adjusted according to the problem to ensure adequate smoothing for an accurate approximation of the the curvature.

Following the CSF approach, the surface tension source term in the average momentum equation can be expressed as

$$f_\sigma^j = \sigma\kappa\frac{\partial \alpha}{\partial x_j} \tag{6}$$

where σ is the surface tension constant, which is positive for immiscible fluids.

For large density ratio systems, Brackbill et al. [1] suggest an alternative to compute the surface tension. Using this expression, they note the fluid acceleration due to the surface tension is only dependent on the density gradients and not the density itself.

$$f_\sigma^j = \sigma\kappa \frac{\nabla\rho}{(\rho_l - \rho_g)} \frac{2\rho}{(\rho_l + \rho_g)} \tag{7}$$

Martinez et al. [11] explain the first fraction is equivalent to Eq. 6, but the second provides a local density correction. This ensures an equal approximation of the acceleration within each cell independent of the density.

To recover the correct force when the curvature radius approaches zero, a normalised curvature value is used. The curvature of the interface is described as the divergence of the unit vector normal to the interface

$$\kappa = -\frac{\partial n_i}{\partial x_i} = -\frac{\partial}{\partial x_i}\left(\frac{\partial\alpha^*/\partial x_i}{\left|\partial\alpha^*/\partial x_i\right|}\right) = -\nabla\cdot\left(\frac{\nabla\alpha^*}{|\nabla\alpha^*|}\right) \tag{8}$$

where the smoothed volume fraction, α^*, is calculated as per Equation 5.

To compute the curvature, Saha et al. [15] and Martinez et al. [11] recommend the correlation

$$\kappa = \frac{1}{|\nabla\alpha^*|}\left(\left(\frac{\nabla\alpha^*}{|\nabla\alpha^*|}\cdot\nabla\right)|\nabla\alpha^*| - \nabla\cdot\nabla\alpha^*\right) \tag{9}$$

which simply follows from the expansion of Equation 8 using the quotient rule.

3 NUMERICAL IMPLEMENTATION

The proposed VOF solver accounting for surface tension is implemented in the open source CFD toolset OpenFOAM®. The said toolset employs an arbitrary unstructured, finite volume approach [8, 17] to numerically describe the partial differential equations, where the unknown variables are solved for each non-overlapping subdomain or control volume using a colocated or non-structured approach [4].

3.1 Pressure-velocity coupling

The continuity and momentum equations are coupled using a pressure projection/correction approach similar to the one originally proposed by Patankar and Spalding [13]. The system of equations is solved in segregated manner, where they are coupled explicitly by linearising the non-linear terms. Start by considering the semi-discrete form of the momentum equation (3)

$$\frac{\rho u_j|^{n+1}}{\Delta t} = \frac{\rho u_j|^n}{\Delta t} - \frac{\partial}{\partial x_i}\left(\rho u_i u_j\right) - \frac{\partial p}{\partial x_j} + S_i \tag{10}$$

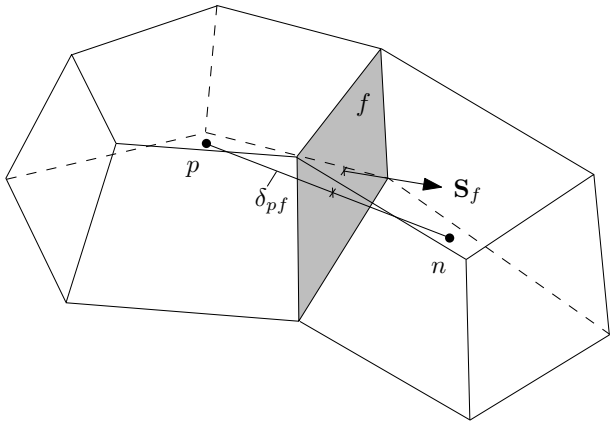


Figure 1: Unstructured mesh with an edge connecting node p and n.

which, when using a similar form as proposed by Jasak [8], can be written as

$$Au_j^{n+1} = H - \frac{\partial p}{\partial x_j} + S_i \tag{11}$$

To couple pressure and velocity, Equation 11 is substituted into the continuity equation (2) which can be re-arranged to obtain the pressure Poison equation

$$\frac{\partial}{\partial x_i}\left(\frac{1}{A}\frac{\partial p^{n+1}}{\partial x_j}\right) = \frac{\partial}{\partial x_i}\left(\frac{1}{A}\left(H + S_i\right)\right) \tag{12}$$

Subsequently, the latest pressure is employed to update velocity using the corrected momentum equation

$$u_j^{n+1} = \frac{1}{A}\left[H - \frac{\partial p^{n+1}}{\partial x_j} + S_i\right] \tag{13}$$

3.2 Pressure interpolation

To allow for a large variation in fluid densities over the free-surface interface, the spatial pressure derivative is discretised in a piecewise linear manner [12]. Figure 1 shows an edge connecting node p and n of an arbitrary unstructured mesh. The cell face is a distance δ_{pf} from node p an edge ratio can be defined as $w = \delta_{pf}/L$ where L is the edge length. It is noted that for incompressible free-surface flow the velocity field is continuous throughout the domain, so that for a given edge,

$$\frac{1}{\rho}\left[\frac{\partial p^{n+1}}{\partial x_j} - S_i\right] = c \tag{14}$$

The interpolated pressure is computed using a piecewise linear approximation, while the density, ρ, and source term, S_i, are treated as nodal values and approximated as

piecewise constant. Equation 14 is integrated from node, p, to the edge face, f, to find an expression for p_f in terms of the values at node p

$$\int_p^f \frac{1}{\rho}\frac{\partial p}{\partial x_j} - \frac{S_i}{\rho} dx = \int_p^f c\, dx \tag{15}$$

which yields

$$\frac{1}{\rho_p}(p_f - p_p) - \frac{S_i^p}{\rho_p}\delta_{pf} = c\delta_{pf} \tag{16}$$

In a similar fashion, by integrating from the edge face, f, to node n an expression for face pressure in terms of the values at node n is obtained

$$\frac{1}{\rho_n}(p_n - p_f) - \frac{S_i^n}{\rho_n}\delta_{fn} = c\delta_{fn} \tag{17}$$

To find an expression for the face pressure, the equations given above are substituted and manipulated

$$p_f = \frac{(1-w)\rho_n p_p + w\rho_p p_n}{(1-w)\rho_n + w\rho_p} - \frac{\rho_p\rho_n L}{\rho_p/(1-w) + \rho_n/w}\left(\frac{S_i^n}{\rho_n} - \frac{S_i^p}{\rho_p}\right) \tag{18}$$

where the first term is the piecewise linear interpolation of the pressure and the second is a correction for the discontinuous source.

Next, through some manipulation the constant c can be expressed in terms of the known variables

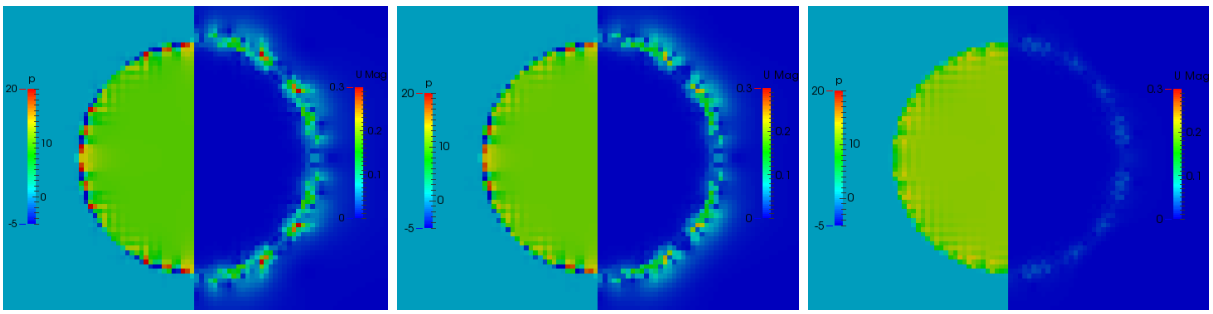
$$c = \frac{(p_p - p_n)}{(w\rho_p + (1-w)\rho_n)L} - \frac{wS_i^p + (1-w)S_i^n}{w\rho_p + (1-w)\rho_n} \tag{19}$$

where the previous two expressions are substituted into the projected pressure equation (12) and corrected momentum (13).

3.3 Interface capturing

The volume fraction equation (1) is numerically discretised using a higher-resolution artificial compressive (HiRAC) formulation [6]. HiRAC employes second-order Crank-Nicholson temporal discretision and the volume fraction face value, α_f, is discretised using a blended high-resolution scheme [18]. The higher resolution interpolation scheme switches between limiting schemes based on the alignment of the free surface interface and control volume face or surface vector. It also introduces an artificial compressive term [9] which is only activated in the interface to reduce the numerical smearing associated with the VOF method. To ensure consistency between the momentum and volume fraction equations, the semi-discrete from of the VOF equation reads

$$\frac{\alpha^{n+1} - \alpha^n}{\Delta t} = -\frac{1}{2}\left[\frac{\partial(u_i\alpha)}{\partial x_i}^{n+1} + \frac{\partial(u_i\alpha)}{\partial x_i}^{n}\right] - \frac{\partial}{\partial x_i}(u_c|_i\alpha(1-\alpha))^n \tag{20}$$



(a) *interFoam* (b) *interFoam* with smoothing (c) Current study

Figure 2: Two-dimensional drop subjected to surface tension

where u_c is the compressive velocity which acts normal to the free-surface interface. The combination of the higher-resolution spatial interpolation and the addition of an artificial term reduces numerical diffusivity, ensuring a sharp interface is maintained, while the integrity of the interface shape is preserved [6].

4 SURFACE TENSION

To evaluate the numerical implementation, the pressure distribution over a static two-dimensional drop subjected to surface tension is computed. The effect of gravity on the drop is neglected. White [20] gives the following relation to calculate the average internal pressure for a infinite cylinder.

$$p_{avg} = \sigma\kappa = \sigma/R \tag{21}$$

where R is the radius.

For this analysis drop with a 1 mm radius is modelled and a 100×100 structured mesh is used to describe the 4×4 mm^2 computational domain. The surface tension is set to 0.01 N/m for which the analytical solution is 10 N/m^2. In Figure 2 the pressure and velocities are shown for the *interFoam* solver. It is show that there is some reduction in the parasitic currents when a smoothed α field (Eq. 5) is used to compute the curvature compared to when using the volume fraction field directly. When considering the pressure and velocities, the proposed formulation provides a notable improvement in accuracy.

5 CONCLUSION

This paper considers the extension of the VOF approach to model low capillary or surface tension dominated flows. As part of the development an improved pressure interpolation formulation is implemented and the continuum surface forces method is extended to use a smoothed volume fraction field which is computed using an implicit diffusion-type smoothing algorithm. It is found that these extensions reduce the non-physical parasitic currents, providing a more accurate representation of the flow characteristics.

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