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THREE DIMENSIONAL FINITE ELEMENT TWO-PHASE FLOW SIMULATION USING A FRONT TRACKING METHOD

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Abstract. *This research aims to accurately simulate two-phase flow using the Finite Element Method along with a Front Tracking method for capturing the fluid interface. This is achieved by solving the Navier-Stokes equations with varying properties over the fluid domain, using two meshes, one representing both phases of the fluid and one representing the fluid interface. The fluid mesh is fixed, and it is not altered during the simulations. The interface mesh is advected by the velocity fields, and is subjected to remeshing to maintain the same node density in all areas. Since the interface mesh has considerably less nodes compared to the fixed fluid mesh, the remeshing operation does not increase the computational cost significantly. The two meshes are decoupled, they do not share any nodes. The surface tension force is calculated by evaluation of the interface mesh curvature by the Laplace-Beltrami operator. This term is added to the Navier-Stokes equation, and the velocity fields obtained from the FEM solution on the fixed fluid mesh are used to advect the interface mesh. The surface tension term is treated explicitly using the continuum surface force model, and calculated using the curvature obtained by the application of a finite element discretization of the Laplace-Beltrami operator to the interface mesh. The chosen finite element is the Mini element, in order to respect the LBB condition, avoiding the addition of artificial stabilization terms. The convective term in the Navier-Stokes equation is discretized through a first order semi-Lagrangian method. Fluid properties at the interface are smoothed through a Heaviside function to avoid numerical instability, over an artificial thickness of the fluid interface. To validate the method discussed, some test cases are proposed. The first test is the static droplet, where surface tension forces are balanced by the pressure gradient. In this test no velocities should appear, any velocity values are due to numerical errors, therefore the lower, the better. The second test is the oscillating droplet, where a droplet of fluid with a slight perturbation in its diameter is released with no gravity forces. The droplet should oscillate with a known frequency towards a spherical shape. Lastly, the rising bubble test case, where the gravity forces promote the bubble's ascension in quiescent fluid. The bubble shape evolution can be compared to experimental data.*

Keywords: *Laplace-Beltrami, Semi-Lagrangian Method, Front Tracking, 3-D CFD modelling*

1. INTRODUCTION

Two-phase flow is a frequent phenomena in many engineering applications. Air conditioning, heat exchangers, oil extraction and refinement and nuclear power generation all feature two-phase flow (Chirag R. Kharangate, 2017). With such a diverse array of applications, it's desirable that two-phase flow can be simulated in a diverse set of geometric configurations. For this reason, this work proposes the simulation of two-phase flow with the finite element method, which permits unstructured meshes with ease, which can conform to a multitude of geometries. For the fluid interface representation, a front-tracking algorithm with decoupled interface mesh was chosen, which allows the curvature to be evaluated easily, while avoiding the remeshing procedures associated with other front-tracking methods, such as the Arbitrary Lagrangian-Eulerian method (ALE) (Jean Donea, 2003).

Two-phase flow has been researched through many approaches, some more suitable for a different class of problem, without a clear best approach to all cases. Amongst the research accomplished on the topic, one can mention D.L. Sun (2010) who extended the VOSET method, which is a combination of the Level Set and Volume of Fluid, to three dimensions, using the Piecewise Linear Interface Construction (PLIC) to reconstruct the interface shape. Kong Ling (2015) who expanded on D.L. Sun (2010)'s work, extended PLIC to 3D cases and using a geometric approach to compute the level-set function, with the intent of simplifying the extension of VOSET from 2D to 3D. Andrea Ferrari (2017) proposed a method that combines both the Level Set (LS) and Volume of Fluid (VOF), called Flexible Coupled Level Set and Volume of Fluid (flexCLV), designed to benefit from the good interface topology offered by the Level Set method. Mathieu Labois (2017) presented a multi-phase formulation with a pressure-based approach, using the 4+-equation model, for compressible flows. Tong Qin (2013) investigated the interaction between a deformable bubble and a rigid wall, through direct numerical simulation, using the ALE method to simulate the bubble interface.

E. Gros (2018) simulates a two-phase fluid flow with heat and mass transfer, using the finite element method combined with the ALE framework. Baolin Tian (2020) developed an ALE method for the five-equation model. The ALE model used is two-stage, with a Lagrangian phase and a rezone-remap phase. Zekang Cheng (2020) solved the incompressible Navier-Stokes equations for a two dimensional domain by discretizing them by Taylor-Hood elements, using an ALE finite element method, where the mesh conforms to the fluid interface, and re-meshes when the interface suffers deformations, following its evolution. Anjos *et al.* (2020) presented an ALE finite element method for simulation of axisymmetric two-phase flows, with dynamic boundaries and interface tracking. In his work, the mesh points move to give a detailed description of the fluid interfaces while using adaptive mesh refining and re-meshing to guarantee high quality mesh elements.

In this work, the uncoupled formulation proposed by Anjos (2021) is expanded to three dimensions. The non dimensional incompressible Navier-Stokes equations are written for varying properties in space, forming a single set of equations that represent both fluid phases. These equations are solved through the finite element method. The fluid domain is represented using the three dimensional mini tetrahedron element, while the interface is represented by a two dimensional triangular element. The surface tension force is obtained by a finite element discretization of the Laplace-Beltrami operator in two dimensions, applied to the interface mesh. A Heaviside function is utilized in order to identify the fluid phases, and a modification of the continuum surface force method of J. U. Brackbill (1992) is used to transform the surface tension force from an interfacial force into a body force. The static droplet, oscillating droplet and rising droplet test cases are executed and their results compared to exact values or experimental data.

2. METHODOLOGY

The methodology proposed employs the finite element method to numerically solve a single set of the non dimensional Navier-Stokes equations. This set of the Navier-Stokes equations represents both fluid phases, which are distinguished by their different properties, specific mass and viscosity. The equations presented below are written for non constant fluid properties:

$$\nabla \cdot \mathbf{v} = 0 \tag{1}$$

$$\rho(\mathbf{x})\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v}\right) = -\nabla p + \frac{1}{Re}\nabla \cdot \mu(\mathbf{x})[\nabla \mathbf{v} + (\nabla \mathbf{v})^T] + \frac{1}{Fr^2}\mathbf{g} + \frac{1}{We}\mathbf{f} \tag{2}$$

where $\rho(\mathbf{x})$ and $\mu(\mathbf{x})$ are the fluid phase's specific mass and viscosity, respectively. The last two terms on the right side represent the gravity force and the surface tension force, respectively, made non-dimensional by the Froude number and the Weber number.

The finite element discretization is done using the mini element (D. N. Arnold, 1984), in order to respect the Ladyzhenskaya–Babuška–Brezzi (LBB) condition. The discretization of the non-linear advective term of the Navier-Stokes equations is done through a first-order semi-Lagrangian method (Anjos *et al.*, 2022). The semi-Lagrangian method is unconditionally stable and conserves the stiffness matrix symmetry.

The surface tension term $\mathbf{f}$ is calculated through a finite element discretization of the Laplace-Beltrami operator applied to the interface mesh and transformed into a body force through the continuum surface force method. It is given by:

$$\mathbf{f_{st}} = \kappa \nabla H \tag{3}$$

and is a function of the interface curvature, κ. The other term in 3, ∇H, is the Heaviside function. The Heaviside function is a color function that serves to identify the fluid phases. It can also be used as a device to identify the interface region, since it's the only region of the fluid domain where the Heaviside function gradient is different from zero. It is used to give the interface an artificial thickness, over which the fluid properties, μ and ρ, transition smoothly. An abrupt fluid property transition over the interface can cause numerical instability, specially when property gradients are high. The Heaviside function is given by:

$$H(\mathbf{x}) = \begin{cases} 1, & \text{if } d(\mathbf{x}) > \epsilon \\ 0, & \text{if } d(\mathbf{x}) < -\epsilon \\ 1 - 0.5\left[1 + \dfrac{d(\mathbf{x})}{\epsilon} + \dfrac{1}{\pi} sin\big(\pi d(\mathbf{x})/\epsilon\big)\right], & \text{otherwise} \end{cases} \tag{4}$$

and the fluid properties are calculated by

$$\rho(\mathbf{x}) = \rho_1 H(\mathbf{x}) + \rho_2(1 - H(\mathbf{x})) \qquad \mu(\mathbf{x}) = \mu_1 H(\mathbf{x}) + \rho_2(1 - H(\mathbf{x})) \tag{5}$$

where ϵ is the interface thickness, d is the smallest distance from the interface to a given point evaluated by x.

Both fluid phases are represented by the tetrahedron mini element. This element has four nodes at its corners, and one extra node at its center of mass. To respect the LBB condition, the velocity is evaluated at all five nodes, while the pressure is evaluated only at the four corners. The interface is represented by a surface mesh composed of triangular elements, inserted in three dimensional space. The meshes representing the fluid phases and the interface separating them do not share any nodes. They are geometrically decoupled, and the interface mesh can move independently from the fluid mesh. The association between the interface and fluid meshes occurs through the calculation of curvature in the interface mesh, which subsequently generates the surface tension term that is distributed to the fluid mesh. After the Navier-Stokes equations are solved, the interface mesh is advected by the velocity fields obtained from the solution of the Navier-Stokes equations. The interface mesh, alongside the Heaviside function, is used to identify the fluid phases, and calculate their properties. When the interface "cuts through" an element, the properties are averaged for that element. Fluid properties inside an element are constant.

3. NUMERICAL RESULTS

In this section, the test cases executed to verify the developed methodology are presented. Three test cases are shown, the static droplet, the oscillating droplet and the rising bubble. The static droplet consists of simulating an spherical droplet of fluid in less dense fluid in absence of gravity forces. The goal of this test is to observe the intensity of the spurious currents that rise due to numerical discretization and curvature error, and to verify the surface tension and pressure balance. The oscillating droplet test has a similar setup to the static droplet, but the droplet radius is disturbed slightly, turning it into an ellipsoidal. The droplet radius should oscillate around its equilibrium diameter, and the frequency and amplitude can be verified against the exact values. Finally, the rising bubble test case consists in releasing a bubble of fluid in denser fluid, subject to gravity force. The bubble should rise against the direction of the gravity force and match the terminal velocity and shape observed in experiments.

3.1 Static Droplet

This test was executed using the following setup, a three dimensional cubic domain with non dimensional edge length $l = 2$ with no slip boundary conditions at its walls, and homogeneous Dirichlet pressure boundary condition at its corners. An spherical interface mesh of non dimensional radius $r = 1$ is positioned at the center of the domain. The simulation parameters are $Re = 1$, $We = 1$ and 1200 time steps of $dt = 0.005$. The fluid parameters are $\rho_{in} = 1$, $\mu_{in} = 1$, $\rho_{out} = 0.001$ and $\mu_{out} = 0.001$. The interface thickness used for this simulation was $e = 2h$, where $h = 0.071$ is the average fluid mesh element edge length, and the 1200 time steps were executed with a time step size of $dt = 0.05$.

The spurious velocities and pressure error obtained for a fluid mesh with $h = 0.071$ (131188 nodes) and several interface meshes are presented in Table 1. In Figure 1, the pressure gradient for the test with the smallest pressure error is displayed. For a droplet of radius $r = 1$, the pressure gradient analytical value is equal to $\Delta p = 4$. It could be observed that the best results were obtained when the refinement of the interface matched the refinement of the fluid mesh. The interface meshes with 4308 and 9500 nodes were much more refined than the fluid mesh, resulting in inaccurate results for the former and an unstable simulation in the latter.

Table 1. Spurious velocity intensity and pressure error for the static droplet test case. The test case was executed with the fluid mesh edge length $h = 0.071$ (131188 nodes, 110464 elements), on a domain of $length = width = height = 2$. The simulation appears to degrade when the interface mesh average edge length is smaller than the fluid mesh average edge length, optimal values are obtained with close average edge lengths.

Number of nodes	v_{max}	Δp_{error}
159	6×10^{-1}	0.408%
317	1.9×10^{-2}	0.118%
625	1.2×10^{-2}	0.102%
1141	4×10^{-3}	0.061%
4308	4.2×10^{-1}	18.4%
9500	366	1223.1%

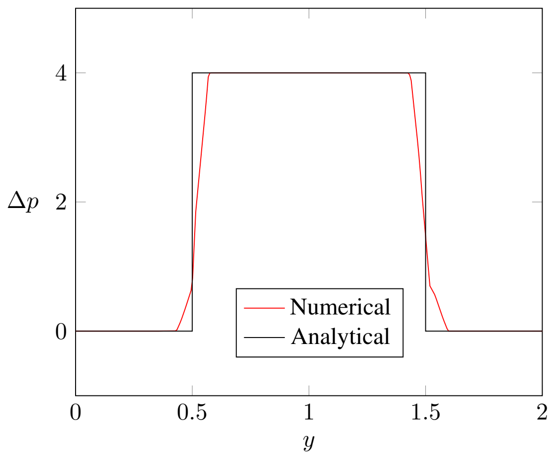

Figure 1. Pressure values from point (1, 0, 1) to point (1, 2, 1) of the fluid domain. These values were obtained using a Droplet of average edge length $h = 0.06$ (1141 nodes). The slight inclination of the red line close to the interface is due to the artificial interface thickness of $e = 2h$ utilized.

3.2 Oscillating Droplet

For this test, the same fluid domain as the static droplet is used. The interface mesh represents an ellipsoidal droplet with diameters $d_a = 1.02$, $d_b = d_c = 0.985246$. This droplet has the same volume as an spherical droplet of diameter $d = 1$. The Reynolds and Weber numbers are given by $Re = 500$ and $We = 125$, and the fluid properties are $\rho_i n = 1$, $\rho_o ut = 0.001$, $\mu_i n = 1$ and $\mu_o ut = 0.01$.

The exact droplet's diameter and oscillation frequency were exhibited by Prosperetti (1980), and are given by:

$$d = d_o + cos(\omega t)a_o e^{\frac{-5t}{Rer^2}} \tag{6}$$

$$\omega = \sqrt{\frac{24}{(3\rho_{in} + 2\rho_{out})r^3 We}} \tag{7}$$

d is the diameter, d_o is the equilibrium diameter, a_o is the initial perturbation, t is time, r is the equilibrium radius and ω is the oscillation frequency.

The obtained results for a fluid mesh with $h = 0.06$ (210724 nodes) and interface mesh of $h = 0.07$ (898 nodes) are presented in Figure 2, along with the exact values for reference. The simulation was executed over 4286 time steps, with a time step of $dt = 0.007$.

3.3 Rising Bubble

This test consists in placing an spherical bubble in quiescent fluid, subject to gravity force. The bubble phase has an smaller specific mass, causing it to rise in the direction contrary to the gravity force. As it rises, it accelerates and changes shape, until it reaches terminal velocity. The terminal velocity can be compared to experimental data found by Bhaga and Weber (1981).

The fluid domain used for this test is square based prism, with height and width measuring $h = w = 7$, and the length of $l = 11$, with no slip boundary conditions on all faces, except for the face contrary to the gravity force, towards which the bubble rises, which has an homogeneous Dirichlet pressure boundary condition. The bubble's diameter is $d = 1$, and its starting position is given by $P = (2.5, 3.5, 3.5)$.

The fluids simulated are air and a mixture of sugar and water. The non dimensional numbers were obtained based on these fluids properties. The Reynolds number is $Re = 13.96$, Weber number is $We = 115.662$, the fluids properties are $\rho_{out} = \mu_{out} = 1$, $\rho_{in} = 0.000892$ and $\mu_{in} = 0.0000142$.

The bubble's velocity plotted against the terminal velocity obtained by Bhaga and Weber (1981) can be seen in Figure 3. The results were obtained using a fluid mesh with $h = 0.8$ (435385 nodes), and an interface mesh initially constructed with $h = 0.08$ (844 nodes). The simulation was executed over 500 time steps of $dt = 0.012$ and a remeshing procedure was invoked at every iteration, to ensure the bubble interface mesh maintained appropriate resolution.

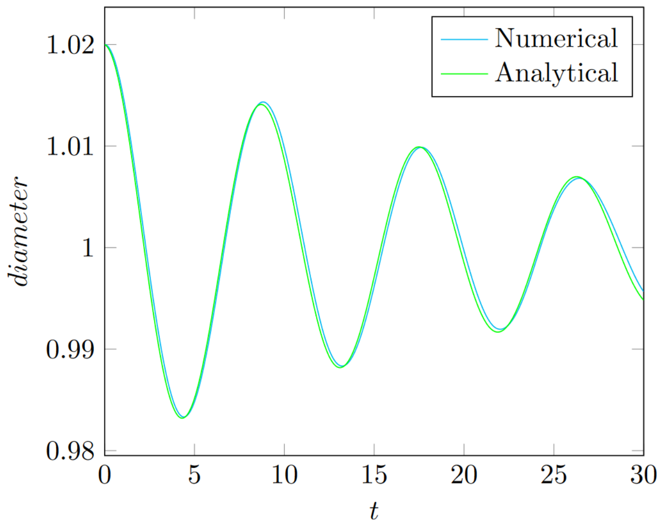

Figure 2. Oscillating Droplet test case for a fluid mesh with 210724 nodes and interface mesh with 898 nodes. $Re = 500$ and $We = 125$. The simulation was executed over 4286 time steps with a time step of $dt = 0.007$

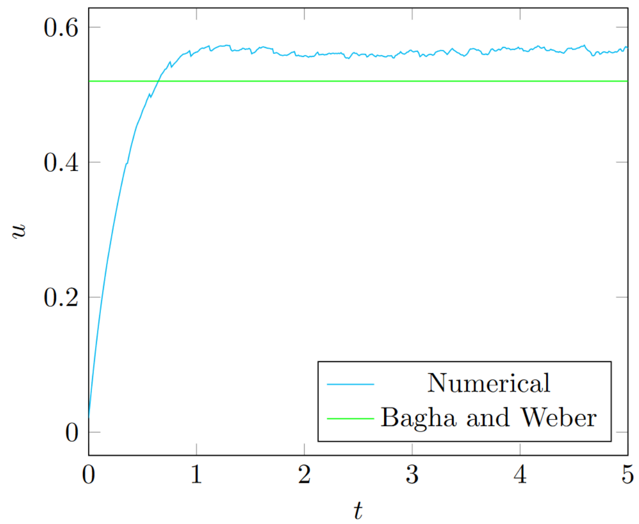

Figure 3. Rising Bubble test case, replicating numerically the air/sugar-water experiment conducted by Bhaga and Weber (1981). $Re = 13.96$, $We = 115.662$, obtained over 500 time steps with a time step of $dt = 0.012$

4. CONCLUSION

The development of a numerical method for the three dimensional simulation of two phase flow, using a front-tracking decoupled mesh method for simulating the interface and calculating the curvature using the Laplace-Beltrami operator was achieved, and the method presented itself stable and accurate for a number of tests. The static droplet test showed results in order with what is available in the literature, with a very small pressure error. It is expected that the intensity of the spurious velocities found in this test can be further reduced. The oscillating droplet test presented very good agreement, and the small discrepancy observed at the end of the graph can be attributed to numerical diffusion, which can be improved by mesh refinement. Finally, the rising bubble test case offers results in reasonable agreement with the experimental reference, and can be further improved by a combination of mesh refinement and interface thickness adjustment. The developed numerical tool exhibits versatile capabilities for simulating a wide range of real-world three-dimensional scenarios. Moreover, ongoing efforts are focused on further enhancing its accuracy through continuous development.

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