

Efficient Computation of Interfacial Flows

Ram Kumar, Balaji Srinivasan

Abstract: Many methods were proposed so far to compute interfacial flows. Most of them explicitly use the value of Surface Tension to calculate the Surface Tension force which induces discretisation errors. Recently Date[5] has suggested a method to alleviate this problem by calculating the surface tension force as the difference of pressures on either sides of the interface. Because this method is first order in nature it required finer mesh near the interface to track the interface exactly which ultimately increased the computation time. This project has been done in two phases. In phase 1 Interfacial flows were computed by coding in C language and tried to replicate Date's[5] method which took too much time to solve. In phase 2 Interfacial flows were computed using a software called Open Foam and some of the results obtained were compared with the standard test results.

Keywords: Open-Foam, FLUENT, SIMPLE algorithm, Single fluid formalism, Staggered grid.

1 INTRODUCTION

Interfacial flows are ubiquitous in industrial and research applications. They are encountered in a variety of important processes like fluid atomization, casting, and oil recovery etc. Numerical simulations are a powerful and cost effective tool to model interfacial flows but accurate solutions are possible only with careful treatment of all phenomena in such flows.

One of the most challenging effects in modeling such flows is the large density jumps across the interface. In many industrial applications the density ratio between the two fluids is about 1000. There are various methods proposed to capture the interface and most of them are for fixed boundaries and when these methods are extended to solve a 2D incompressible flow problem with a moving interface the grid has to be regenerated every time as the boundary change shape or distorts. It is also important to note that all the methods require extremely fine meshes to resolve fine flow structures when fluid splits or tiny bubble entrappings in liquid occur. Adaptive grid generation techniques overcome this need for very fine grids by embedding additional cells in regions where grid fineness is required. But in an unsteady calculation where the interface locations are continuously changing the adaptive procedures must be programmed for both adding as well as for deleting computational cells. Such methods achieve economy. Thus the problem of accurately predicting interfacial flows is computationally very demanding requiring continuous improvements both in physics of modeling as well as in solvers used for discretised equations.

1.1 Sharp Interface Method[9]

One of the subcategory of methods under sharp interface methods is 'Finite Volume Cut cell Method'.

In this method finite volume method based on central differencing scheme is used with a two step fractional step procedure by Takahira et al [4]. In this method he has used a fractional step method to solve unsteady flows. He used the same method to capture the interface as used by Udaykumar [8]. The interface is identified by interfacial markers defined by the coordinate $X(s)$.

The spacing between the markers are kept at some fraction of grid spacing. To minimize the complexity of handling the fluxes and pressure gradient a finite volume discretisation method is used in a trapezoidal cell. The interface is assumed to be a straight line. Depending on the location and orientation of the interface trapezoidal cells of various dimensions can be created. The convective flux, diffusive flux mass and pressure gradient can be calculated at the cell faces of these trapezoidal cells from the neighboring cell centre values with sufficient accuracy so that global second accuracy of the method is preserved. The method is able to predict the critical Reynolds number of vortex shedding with high degree of precision for immersed boundary problems.

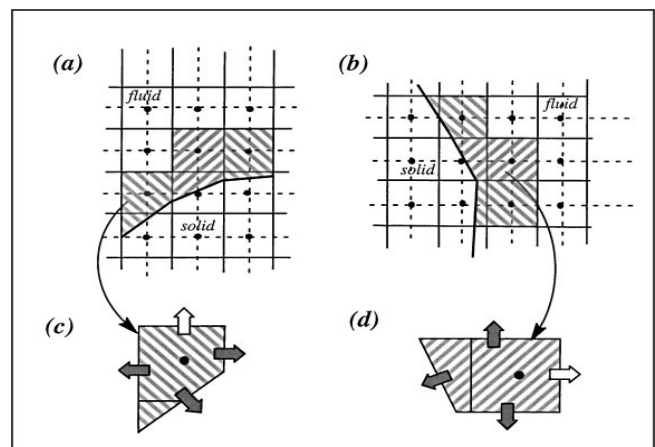


Fig.1.1 (Schematic of Computational domain with immersed boundaries for cut-cell method)

A major difficulty in implementing this method is the number of possible intersections between the fixed grid and the surface of the deforming body which leads to

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irregular interfacial grid size. Applying boundary condition in this method requires a complex coding. It is also difficult to employ this method for 3D non axisymmetric flows. The irregularly shaped cell does adversely affect the conservation and stability properties of the solver. In spite of the extendable nature of this method it can't be used for 3D flows.

1.2 Diffusive interface method

The diffusive interface method circumvents certain problems associated with the classical sharp interface method. Some of the methods that come under the diffusive interface method are discussed here.

Harlow and Welsh [1] used the Marker and Cell method using a staggered arrangement of vector and scalar variables. In order to capture the interface one of the fluids is identified by marker particles.

Hirt and Nicolls [2] introduced the Volume of fluid method (VOF) which by solving an advection equation the volume fraction of heavier fluid at the interface is calculated and this value of volume fraction is used to evaluate the interface properties.

1.3 Phase Field Method [10]

In this method the diffuse interface method is introduced through an energetic variational procedure that results in a thermodynamic consistent coupling system. The basic idea is that though two components are immiscible does mix in reality in a narrow region of very low thickness called interface. A phase field variable σ which indicates volume fraction is used to demarcate the two species and capture the location of the interface. A mixing energy is defined based on σ through convection diffusion equation which defines the interface profile. It can be viewed as a physically motivated level set method which has the advantage of using a physically determined σ profile instead of using an artificial smoothing function for the interface. When the interface thickness approaches zero this method becomes asymptotically identical to the sharp interface model.

1.4 Ghost Fluid Method [11]

This method helps to handle the large density jumps and forces in two phase flows with sufficient accuracy while avoiding artificial spreading of the interface. Since the method is based on partial differential equations it can be applied in all coordinate systems and benefits from parallel efficiency. The robustness and efficiency of the approach is further improved by using implicit schemes for both interface transport and reinitialisation equations as well as for the momentum solver. The accuracy of the method is assessed through classical level set transport tests and simple two phase flow examples using topology changes.

Another class of interface capturing method is the Level set method [4] in which the advection equation is written for the signed interface function Ψ . The form of the Ψ

equation is same as that of the conservative scalar equation. Some of the modifications brought in this method have shown great ability in predicting liquid break ups and fine fluid atomisations.

A third approach relies on the geometric reconstruction of the interface based on the predicted distributions of volume fraction at the interface. Rudman and Gerlach [7] refer to such methods for solving 2D problems. However for 3D problems these methods prove to be cumbersome and difficult to solve.

1.5 Interface Reconstruction with Least square fit and split Eulerian Lagrangian advection [14]

This method uses the combined Lagrangian Eulerian advection scheme to solve the interface advection equation and its reconstruction with least square fit. The scheme is tested for some standard test shapes and found superior to other existing approaches.

1.6 An adaptive coupled Level Set/ Volume of Fluid Interface Capturing Method for Unstructured Triangular Grids [13]

In this method at each time step both the level set and volume fraction is evaluated. Level set function is evolved by solving the level set advection equation using a discontinuous Galerkin Finite element Method. The volume fraction advection is performed using a Lagrangian-Eulerian Method. The interface is reconstructed based on both the level set and volume fraction information. In particular interface normal vector is calculated from the level set function while the line constant is determined by enforcing the mass conservation based on volume fraction. Unlike the other methods here an analytic method is used to determine the line constant. This makes interface reconstruction efficient and conserves volume of fluid exactly. Since the level set function is continuous the normal vector calculation is easy and accurate compared to a classical volume of fluid method. In addition owing to the adaptive grid algorithm it is possible to resolve complex interface changes and interfaces of high curvature efficiently and accurately.

1.7 Parabolic reconstruction of Surface Tension for the Volume of Fluid Method [12]

Volume of fluid method is not accurate when the flow is surface tension dominant or when the density ratio between the two fluids is extremely large. Grid refinement also does not lead to convergence. In addition artificial velocity field (spurious currents) is generated at the interface which can destabilize the interface significantly. In this method an accurate representation of body force due to surface tension is developed which eliminates the problem of spurious currents. There are several steps in this procedure including

- Solving the new body force algorithm
- Improvements in the projection method for Navier stokes solver

- Develop a higher order interface advection scheme.

The curvature to the interface is calculated from an optimal fit for a quadratic approximation to the interface over group of cells.

1.8 Date's Method [5]

Most of the methods mentioned above explicitly includes surface tension for the formulation for interfacial flows. Recently Date [5] has suggested a method which seems to avoid the use of surface

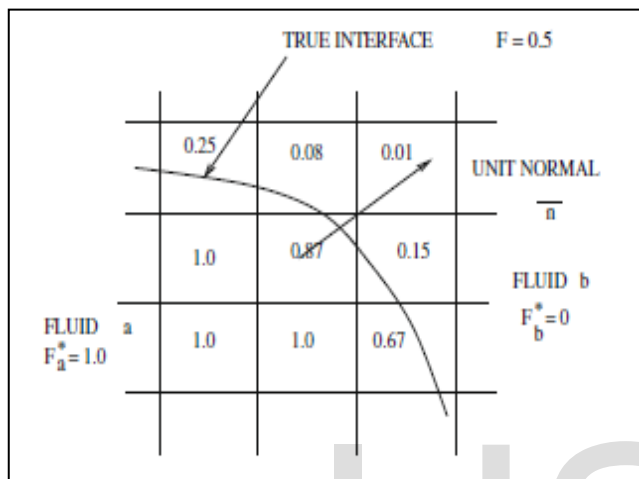


Fig.1.2 (F-distribution and Interface normal)

tension and is fully implicit for simulation of flows with interfaces using primitive variables for two incompressible and immiscible fluids on a fixed grid called single fluid formalism. The convective terms are represented by TVD schemes to predict less smeared interface. Also the method has employed novel means to avoid problems of zigzag pressure predictions on collocated grids and loss or gain of mass/volume encountered in the previous methods. Fluid dynamic evaluation of interface curvature which in turn evaluates the surface tension force without requiring knowledge of surface tension coefficient σ . Eliminating the problem of zig zag pressure distribution as well as the problem of loss of mass /volume during unsteady computations over large times. TVD scheme is used for representation of convective terms to reduce interface smearing.

1.9 Motivation

Various methods have been proposed so far to solve flow of two incompressible and immiscible fluids with moving or deforming boundary. Most of the methods explicitly included the surface tension to formulate these flows which are computationally expensive.

Date [5] has recently suggested a method which alleviates this problem by calculating the surface tension force without the knowledge of the surface tension coefficient σ . But he calculates the volume fraction of heavier fluid (F) and uses first order reconstruction of the interface from F. This requires the need of very small cells near the interface for accurate prediction of interface shape. As a result this

method increases the cost of computation and also consumes more time. But to predict the value of F by knowing the interface shape/location is considerably simple compared to Date's method. So if we can come up with a method which can predict the interface shape more efficiently compared to Date's method it will be a notable advancement in the field of prediction of interfacial flows.

2 PROBLEM FORMULATION

To solve the flow problems we need to solve the 2D Navier stokes equations. These are coupled nonlinear equations (pressure velocity linkage) can be solved by adopting an iterative solution strategy by an algorithm called SIMPLE algorithm proposed by Patankar and Spalding [3]. In this algorithm convective fluxes per unit mass at cell faces are computed using guessed velocity components. Furthermore a guessed pressure field is used to solve the momentum equations and a pressure correction equation deduced from the continuity equation is solved to obtain a pressure correction field which is in turn used to update the velocity and pressure fields. As the algorithm precedes it progressively improve these guessed fields. The process is iterated until converged values of velocity and pressure fields are obtained.

2.1 D-Navier stokes equations for steady incompressible flow

$$\delta' \delta x (\rho u u) + \delta' \delta y (\rho u v) = \mu \delta' \delta x (\delta u / \delta x) + \mu \delta' \delta y (\delta u / \delta y) - \delta p / \delta x$$

(X-momentum equation)

$$\delta' \delta x (\rho u v) + \delta' \delta y (\rho v v) = \mu \delta' \delta x (\delta v / \delta x) + \mu \delta' \delta y (\delta v / \delta y) - \delta p / \delta y$$

(Y-momentum equation)

$$\delta' \delta x (\rho u) + \delta' \delta y (\rho v) = 0$$

(continuity equation)

2.2 Equations Governing SIMPLE Algorithm

$$u_{ij} = \sum a_{nb} u_{nb} + (p_{i-1j} - p_{ij}) A_{ij} + b_{ij}$$

$$v_{ij} = \sum a_{nb} v_{nb} + (p_{ij-1} - p_{ij}) A_{ij} + b_{ij}$$

$$A_{IJ} p_{cIJ} = A_{IJ+1} p_{cIJ+1} + A_{IJ-1} p_{cIJ-1} + A_{I+1J} p_{cI+1J} + A_{I-1J} p_{cI-1J} + b_{IJ}$$

The first two equations are the discretised momentum equations and the last one is the equation for pressure correction. Where u_{ij} , v_{ij} are the guessed velocities and

p_{ij} is the guessed pressure. A_{ij} and b_{ij} are constants.

$$V_{ij} = v_{ij} + v_c$$

$$U_{ij} = u_{ij} + u_c$$

$$P_{ij} = p_{ij} + p_{cIJ}$$

Where v_c and u_c are the velocity corrections. p_{cIJ} is the pressure correction.

3 RESULTS AND DISCUSSIONS

3.1 Replication of Date's Results

Dam break using VOF method in OPEN FOAM

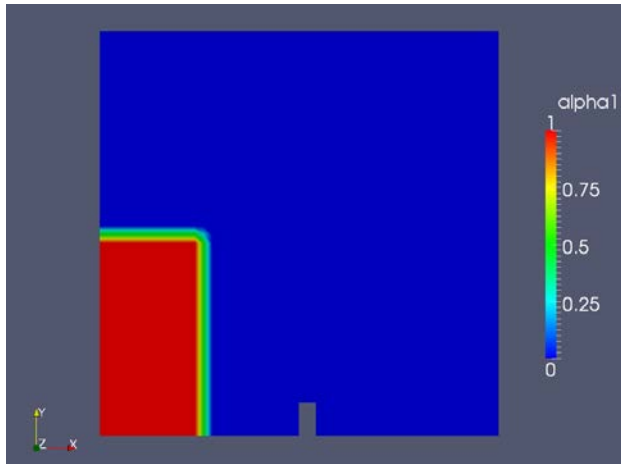


Fig.3.1 (Interface location at time=0)

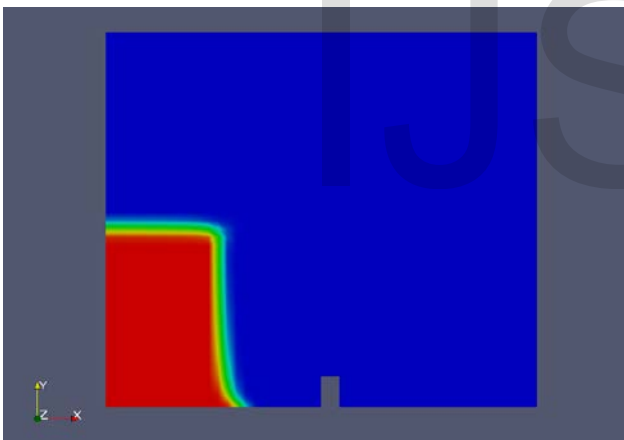


Fig.3.2 (Interface location at time=0.05 seconds)

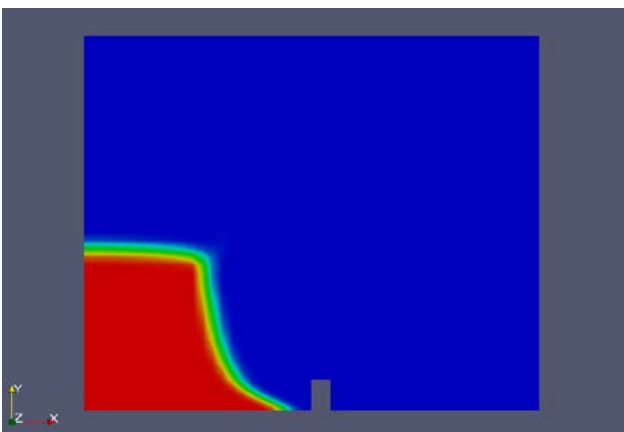


Fig.3.3 (Interface location at t=0.1 seconds)

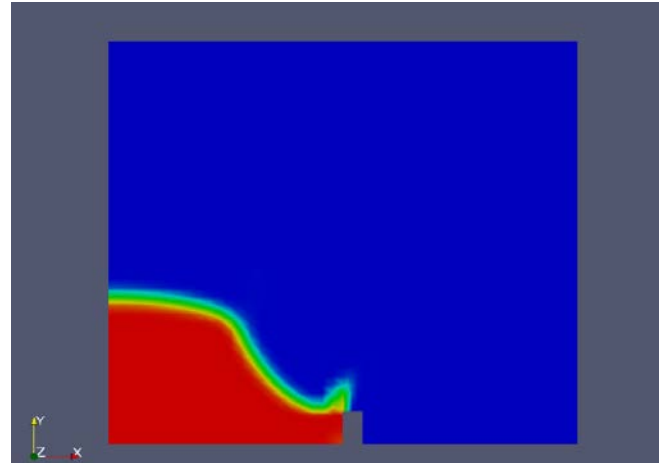


Fig.3.4 (Interface location at time=0.15 seconds)

The above results of the dam break simulation using Open Foam replicates the results of the same problem solved by Date [6] .Hence it can be concluded that Date's [5] method is able to replicate all the features of the flow that have been previously predicted using alternate methods.

3.2 Sloshing Tank 2D

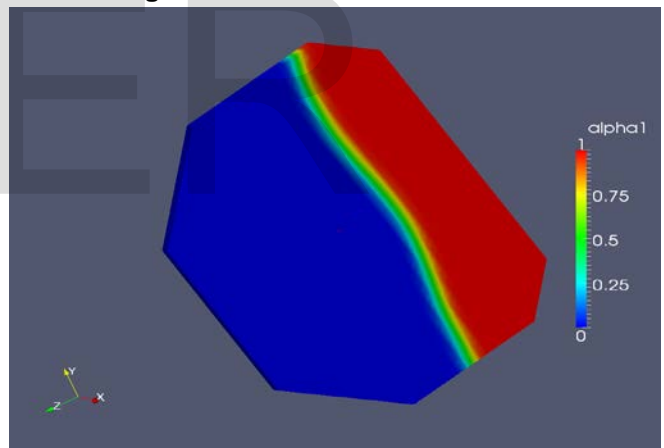


Fig.3.5 (Interface at time=3 seconds)

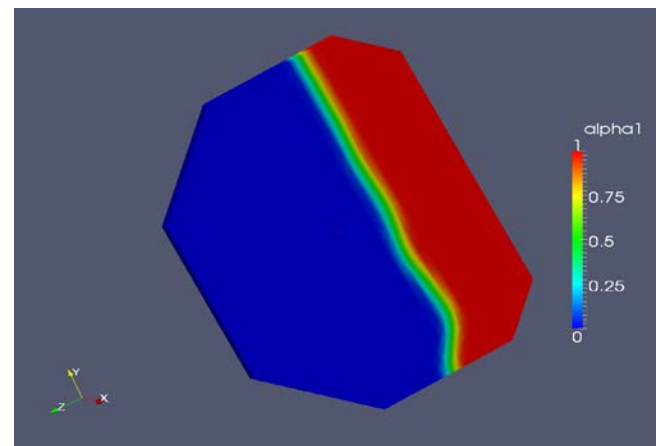


Fig.3.6 (Interface at time=4 seconds)

3.3 Bubble Column Problem

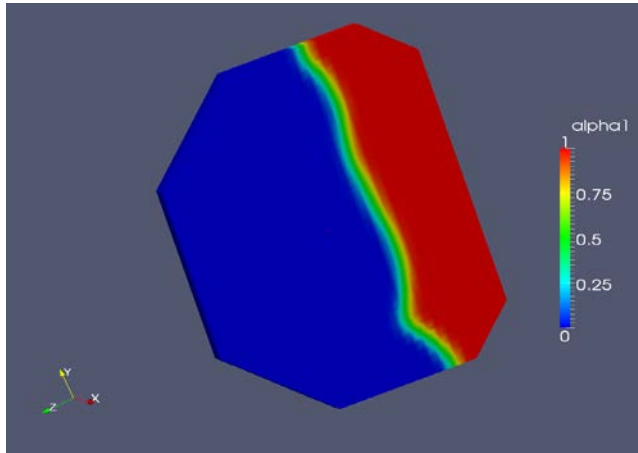


Fig.3.7 (Interface at time =5 seconds)

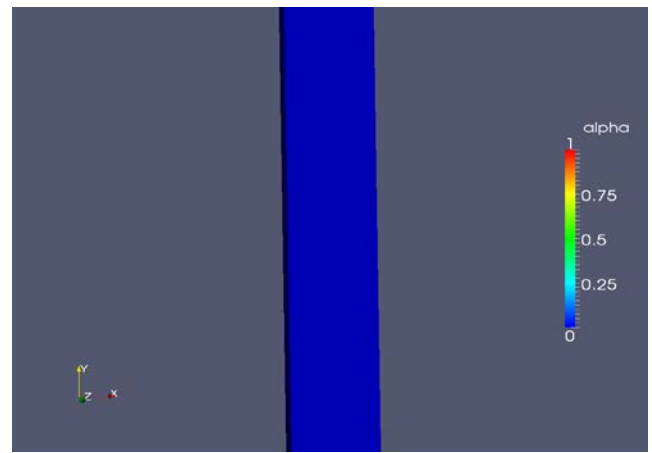


Fig.3.10 (Interface at time =0 seconds)

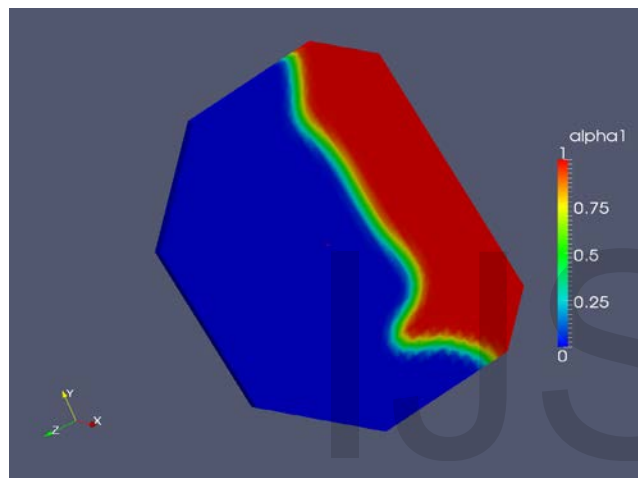


Fig.3.8 (Interface at time =6 seconds)

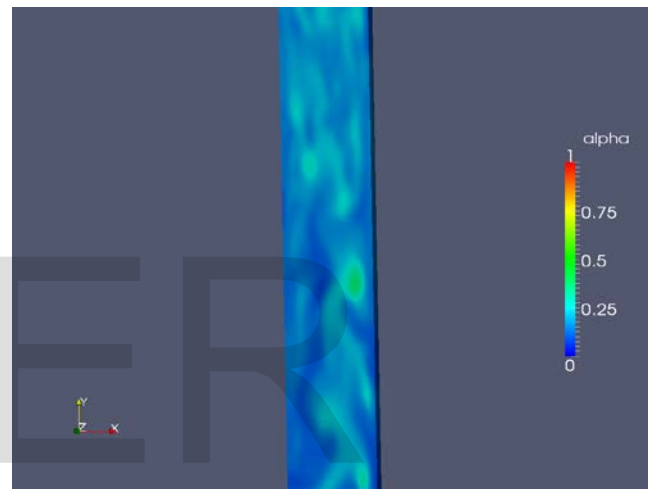


Fig.3.11 (Interface at time =1 second)

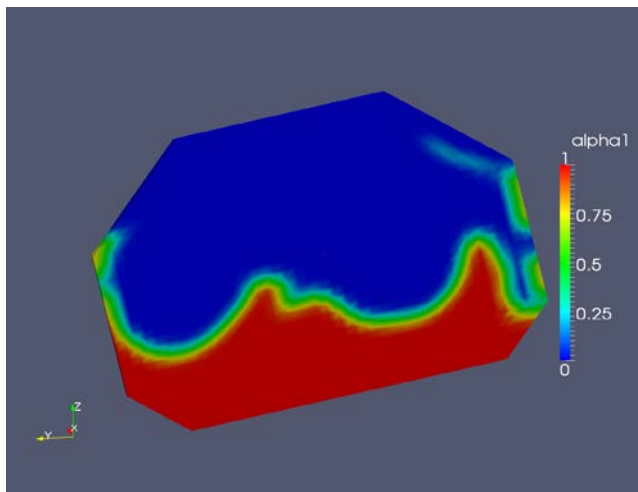


Fig.3.9 (Interface at time=9 seconds)

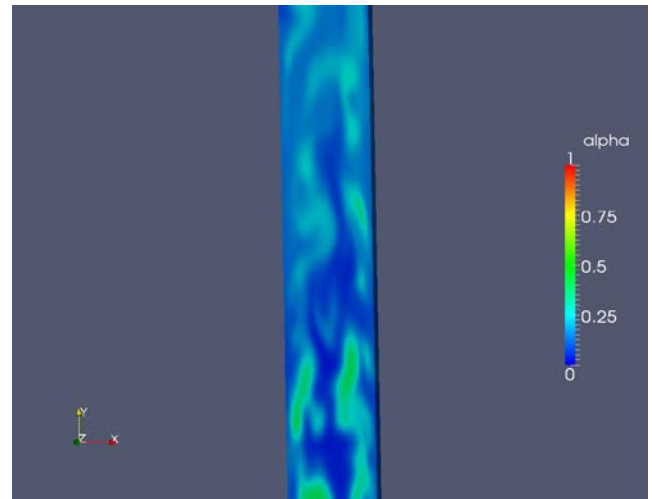


Fig.3.12 (Interface at time =1.85 seconds)

3.4. Rayleigh Taylor Instability

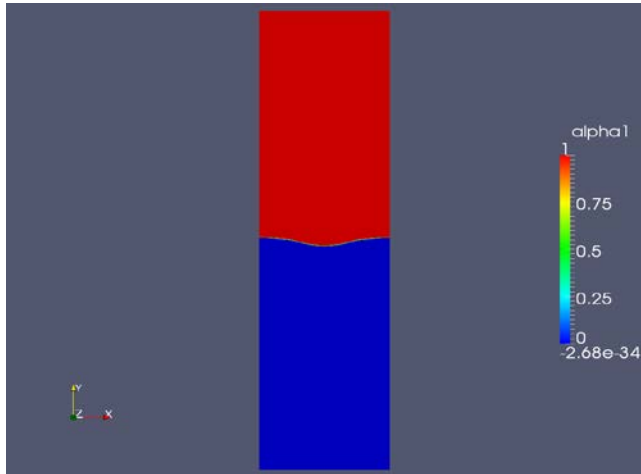


Fig.3.13 (Interface at time =0 second)

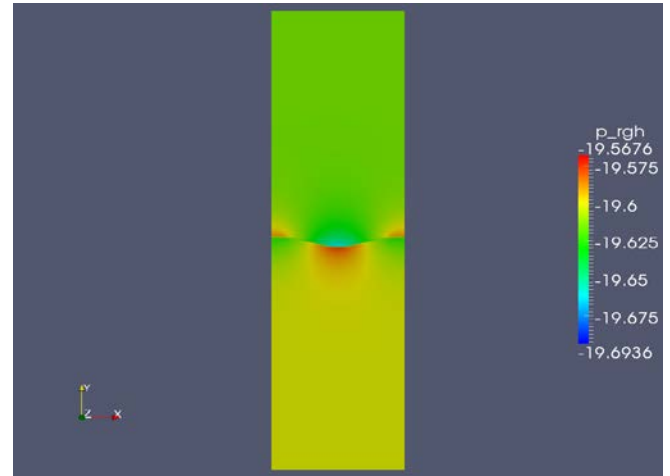


Fig.3.16 (Pressure at time =0.5 seconds)

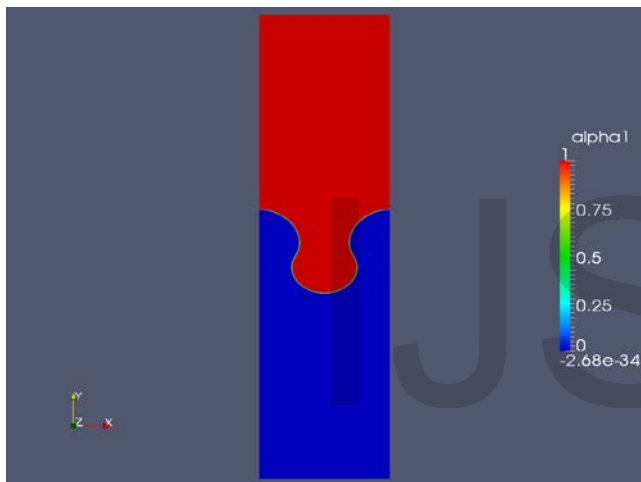


Fig.3.14 (Interface at time =2.55 seconds)

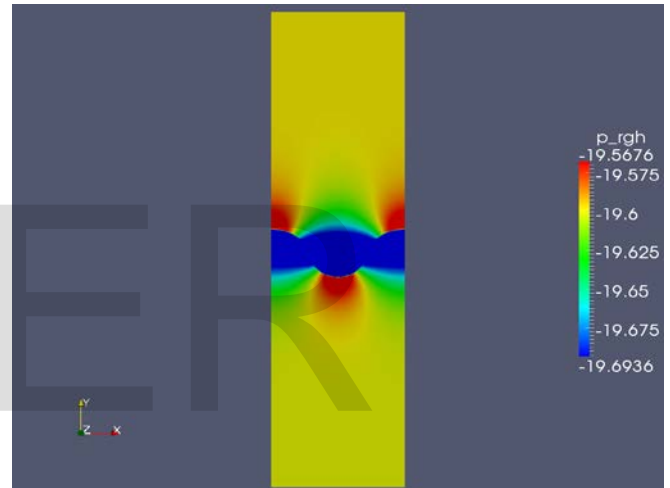


Fig.3.17 (Pressure at time =2 seconds)

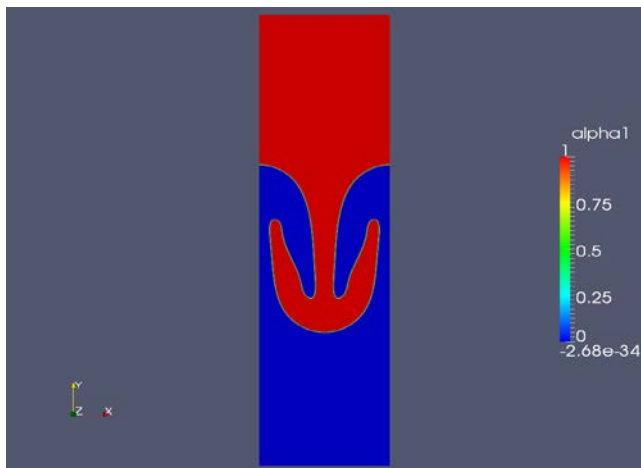


Fig.3.15 (Interface at time =3.8 seconds)

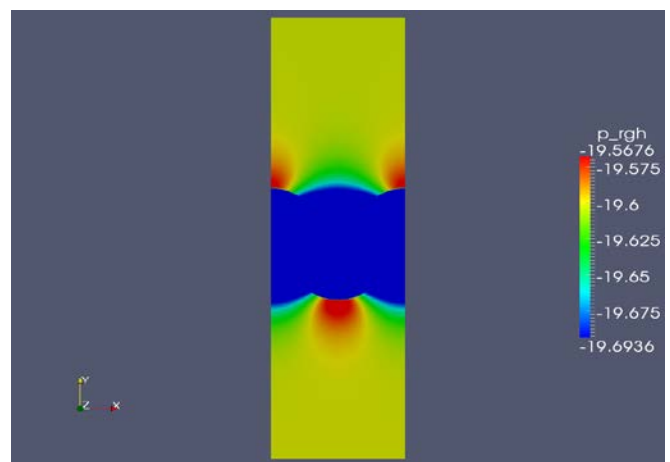


Fig.3.18 (Pressure at time =3 seconds)

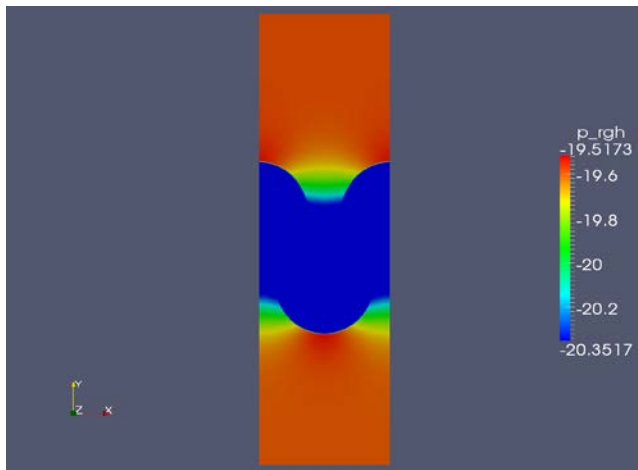


Fig.3.19 (Pressure at time =3.85 seconds)

All the above problems are simulated in Open Foam using Volume of Fluid Method.

4 CONCLUSION

Many methods have been proposed to solve computational methods. Most of them have been explicitly using the value of surface tension which induced discretisation errors. Date proposed a method using which certain problems were solved which was able to replicate the same result as obtained by other methods. But still the method of Date was found time consuming as more number of cells were required near the interface to capture its exact shape. Hence it is necessary to develop a method which can overcome this problem with more efficiency and less computational effort.

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