

A Level Set Approach for High Performance Computing for Multiphase Fluid Flows

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Abstract-- The study of fluid dynamics has applications in many areas of engineering and science. This includes the understanding environmental, biological and chemical flows. Laboratory experiments and computer simulations are the two main approaches for the study of complex flow problems. Computer simulations can help one to understand and analyse the complexity involved in these flows more clearly without having to perform time consuming, expensive and complicated experiments. Advancements in modern computers have facilitated the solution and analysis of fluid flows with high accuracy (close-to-reality) and reduced computational time. In computational fluid dynamics, one has to employ basic physical principles to develop mathematical models and therefore obtain accurate numerical solutions. Development and improvements of numerical schemes have encouraged researchers to investigate almost too every branch of fluid dynamics and its applications to real life problem. But multiphase flows occur in many industrial and natural phenomena such as petroleum refining, biological flows and interaction with air with sea surface. The simulation of multiphase fluid flows is one of the most challenging problems in CFD as it involves the modelling of sharp interfaces separating multiple fluids.

I. INTRODUCTION

The physical behaviour of two-phase flows can be predicted by computer modelling [1]. Recent advances in computational methods for multiphase flow involving gas, solid and liquid phases [2-3]. The mathematical interpretations of the mass and momentum conservation principles [4]. The governing equations are presented by a set of PDEs [5].

The continuity equation at a point in a compressible fluid such as

$$\frac{\partial}{\partial t}(\rho) + \nabla \cdot (\rho V) = 0 \quad (1)$$

Where t , ρ , V and ∇ denotes time, density, velocity vector and nabla operator. The transportation of fluid is described by the momentum equation as

$$\left(\frac{\partial}{\partial t}(\rho V) + \nabla \cdot (\rho V V) \right) = -\nabla p + \gamma \nabla^2 V + S_v \quad (2)$$

Equations (1)-(2) are Navier Stokes equation [6], which are difficult to solve analytically and numerical solutions are applied for simulation. Furthermore, in the simulation the properties of the fluid change abruptly across the interface whose location must be known at every time-step. This position is determined by interface advection methods and fluid motion is predicted applying N-S solvers [7-8]. The main two approaches to the solution of the multiphase fluid flows- air and water flow which involves large viscosity and density ratios. On the other hand, in the first approach only the liquid phase (to be inviscid) is modelled. But N-S equations can be converted into Laplace's equation [9]. In

the second approach viscous effects have been considered [1]

And the both the liquid and gas are modelled with the full N-S equations.

We mainly focussed on the second approach for multiphase flow the flow of two-immiscible fluids (multifluid flow).

2. Numerical Methods The numerical solution calls for the discretization of the computational domain using a grid arrangement to store variables for the fluid properties. Therefore, the PDEs are discretized according to the chosen grid resulting in a linear system of equations which is then solved to obtain the numerical solution.

2.1 Method for multiphase flows- Modelling the advection of the sharp interface numerically is a challenging task [10] and range of methods [11] have been developed over the last 30 years to achieve this. We studied two phase flows applied to immiscible fluids can be classified into two categories – *interface tracking* and *interface capturing* [7][12-13].

2.1.1 *The interface tracking method*- the interface between two fluids is explicitly tracked during the fluid motion to maintain a sharp discontinuity in the fluid viscosity and density. The motion of the interface is tracked either by marker points located on the surface or by attaching it to a mesh boundary surface. The second is the front tracking method, a separate front, on a fixed grid is used to identify the interface for each phase with the help of additional computational elements introduced explicitly. These elements are marker particles on the surface and form a moving internal boundary. Both phases are treated as one fluid with variable material properties and one set of the N-S equations is solved over the whole computational domain. Furthermore, fluid properties, density and viscosity are calculated with respect to the interface position. On the other hand, this method uses piecewise linear, higher order polynomial to fit the interface which is advected with the flow fields in a Lagrangian manner [14-15]. Henceforth another interface tracking method is the moving mesh method [16-17] wherein a boundary fitted grid is

employed and the grid points are embedded in the fluid and these points are moved in a Lagrangian manner. The same fluid elements are kept in all computational cells which are adjacent to the interface and the fluid always coincides with the specified regions facilitating the piecewise tracking of the fluid surface [18]. The interface is integrated with these points and is tracked by the nodes affixed on both phases. The movement of the interface is determined utilizing the knowledge of velocities known at the current time-step [19].

Moreover, N-S equations are solved for both fluids (liquid and gas). For the liquid phase, these equations are solved on a deforming unstructured mesh [17] and one of the advantages of this method is that it permits the accurate prescription of the boundary conditions of the interface [20].

2.1.2 *The interface capturing method* - The volume fraction function which as the colour function is a step function and represents the fraction of volume occupied by one fluid. The interface is reconstructed from the value of the colour function [21-22]. The volume fraction method solves a scalar transport equation Eq.(3) in an Eulerian manner

$$\frac{\partial}{\partial t}(C) + V \cdot \nabla C = 0 \quad (3)$$

where C being the colour function is a step function and represents the fraction volume occupied by one fluid shown in

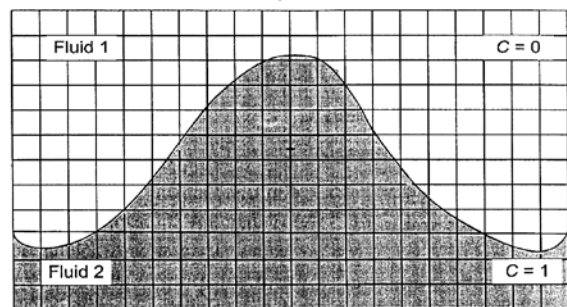


Fig. 1 Interface capturing methods

which shows that the value of the colour function C is only in the fluid 2 and zero in the fluid 1 unity while it lies between zero and unity at the interface. The mesh is kept fixed and a suitable technique is chosen to locate the interface in the interface capturing methods [14][23]. Since the interface is

reconstructed at each time-step from the known value of the indicator function and also this method is able to cope with large stretching and deformation of the interface. On the other hand, this methods can be used for modelling large scale deformations of the interface including breakup and merging [7]. The volume fraction method which uses the colour functions to identify the interface. The volume of fluid methods has been widely used for the numerical simulation of viscous flows having non-zero viscosity with moving interface.

II. KRYLOV-SUBSPACE METHOD (K-S)

Krylov-Subspace method [24-25] are some of the most efficient iterative methods applied to a large sparse linear system of equations obtained from PDEs representing multiphase flow problems [15]. A residual vector $\gamma = B - Ax$ is calculated initially and is minimized or is set to satisfy some other constraints in each iteration. The residual vector on the multiplication by powers of the matrix A in successive iteration, generates a subspace which is Krylov Subspace (K-S) [26-27], as m denotes dimension of the subspace. This method belong to non stationary category [28] as shown in Fig.2

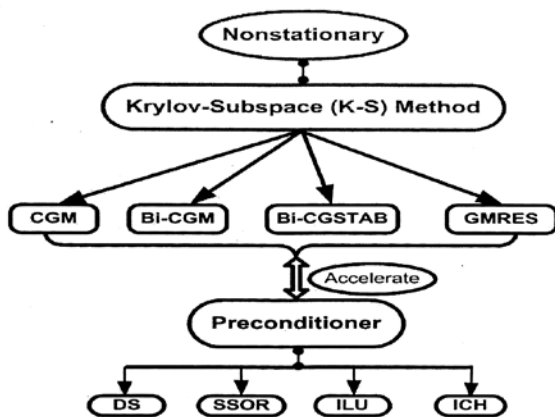


Fig. 2 Nonstationary iterative methods

have been widely adopted as a good choice for solving large sparse linear systems of equations [29-30]

III. MODEL VALIDATIONS AND OTHER NUMERICAL SCHEME

The whole model for multiphase flow problems consists of two parts are shown in Fig.3

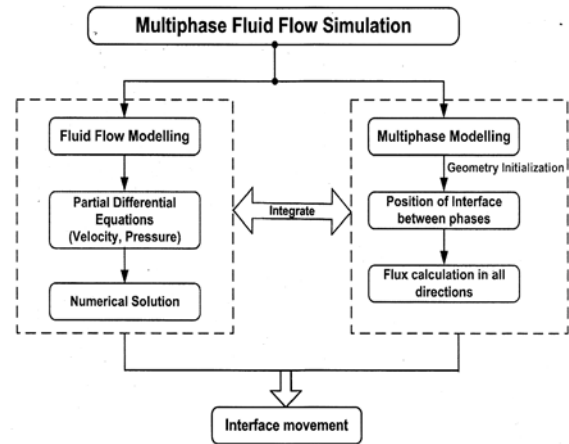


Fig.3 Different steps of the multiphase fluid flow simulation and these parts are PDEs solvers which includes linear system solvers and multifluid methods [31-32]. Furthermore, in case of computer simulation both two parts are integrated together and executed within a time iteration [33].

In order to validate this integrated model many benchmark problems [34-35].

4.1 *Parallel Numerical Algorithm* – Computer simulation of multiphase flow problems involve the implementation of complex algorithms which are as intensive in both time and memory requirements [36-37]. Executing the Algorithm may take days when run on a single processor. Moreover, in the this studies simulation of some problems – dam breaking , the rising of a air bubble, and the fine grid resolution 512×512 takes 6-7 days when executed in a single processor with clock speed 2.8GHz and 8 GB RAM. Henceforth, for higher resolution simulation of CFD problems the matrix size may become too big to fit in the memory and thus, it is difficult to solve the linear system on the available computer [38-39].

To deal with memory constraint and to reduce computational time, these complex algorithm need to be implemented on parallel computers consisting the clusters of processors [40-41]. An idea of the importance of the parallel computers can be found from the top 500 site (www.top500.org) the five hundred fastest machines in the world on their performance on the various benchmarks problems. In this

approach one can avail of the huge memory and computational power of many processors. On the other hand, the parallel implementation of CFD code has been carried out for the simulation [42]. The development of parallel algorithms has been focus of intense research in the area of parallel matrix computation [40][43-44]. The quality of parallel algorithms can be measured by using common performance evaluators, speed up S_n and Efficiency E_n [45-46]

$$\frac{T_s}{T_p} = S_n ; \quad \frac{S_n}{n} = E_n \quad (4)$$

Where T_p and T_s denotes time taken by parallel algorithm on n processors and T_s denotes the time taken by its serial version. In the present work, the simulation has been carried out on a Linux cluster which has 56 nodes, each having 2 quad core processors with clock speed 2.8GHz and 8 GBRAM. In the programs related to parallel matrix computation, processor is required to send the executed data to each other within a network [48]. Now, these data are sent in the form of message by using certain parallel communication libraries Message Passing Interface [31] [49-51]. Now for parallel computation of the linear solvers one processor is required to manage the processor communication such as gathering the parts of matrix-vector products calculated by other processor and therefore [43] and these processor act the master processor and therefore the master slave paradigm [42][51] has been adopted in the research studies to design the parallel algorithms for the different steps of the linear solvers

DISCUSSION AND FURTHER RESEARCH

The following conclusions can be drawn from the above studies:

- [i] computer simulation of multiphase flow requires the numerical solution of PDEs. The numerical solution is used to move the interface between two-phases of fluids in the multifluid model.

- [ii] the interface capturing method is more suitable for large deformation and stretching on the interface.
- [iii] the VOF (PLIC) method maintains the sharpness of the interface.
- [iv] an analytic relation between the *interface position* and the volume fraction facilitates extension to 3D problems.
- [v] PDEs are solved numerically in a computational domain which is divided into parts using suitable grid schemes. Now, the under mentioned points and observations are noted for steps from domain discretization to linear system of equations:
 - [a] the FVM enforces conservation the momentum and mass in each CV as well as in the whole domain.
 - [b] the staggered grid is more suitable to deal with the problem involving velocity–pressure coupling.
 - [c] the non-linearity of velocity terms can be dealt with by the SIMPLE method.
 - [d] a special data structure is required to store sparse matrices.
 - [e] the non-stationary K-S solver Bi-CGSTAB provides smooth convergence.
 - [f] effective preconditioners for K-S solvers are DS, ILUT and SSOR.
 - [g] large scale problems are solved on the parallel computer.
 - [h] parallel algorithms are needed to develop to carry out the simulation on these computers.

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Discontinuous Galerkin upwinding for the Level Set approach. Treatment of surface tension effects. Reinitialization procedure for LS-dG(1). NUMERICAL SIMULATIONS. Single phase flow around a cylinder. Two-phase flow of a rising bubble. International journal for numerical methods in fluids. Int. J. Numer. Meth. Fluids 2010; 00:1-10. Prepared using dauth.cls [Version: 2002/09/18 v1.01]. Summarizing the properties of FEM-Level Set techniques for multiphase flow problems, we can conclude the following (potentially) advantageous behaviour in comparison to interface tracking methods as well as VOF and Phase-Field approaches which motivates our recent and future work for the combination of FEM and Level Set methods Shin S and Juric D 2002 Modeling three-dimensional multiphase flow using a level contour reconstruction method for front tracking without connectivity. J. Comput. Phys. 180 (2): 427-470 Google Scholar. Shin S and Juric D 2009 A hybrid interface method for three-dimensional multiphase flows based on front tracking and level set techniques. Int. J. Numer. Sussman M, Samerka P and Osher S 1994 A level set approach for computing solutions to incompressible two-phase flows. J. Comput. Phys. 114: 146-159 Google Scholar. Sussman M, Fatemi E, Semerka P and Osher S 1998 An improved level set method for incompressible two-phase flows. Comput. Fluids 27: 663-680 Google Scholar. The multiphase flow group has developed a suite of in-house numerical codes using different modelling approaches for various applications, including Front Tracking method, Level-set method, Immersed Boundary method, Lattice Boltzmann method, and Boundary Integral method. These modeling tools can be applied to various flow regimes for wide applications from microfluidics, bubble column, boiling, to oil and gas transportation. Figure 1: Particle suspension flow modeling. Figure 2: Droplet splash dynamics.