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Direct numerical simulation of multiphase flow for arbitrary geometry using level contour reconstruction method †

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Abstract

Direct numerical simulation of multiphase flow on fixed Eulerian grid became increasingly popular due to its simplicity and robustness. Some of the well-known methods include VOF, Level Set, Phase field, and Front Tracking method. Lately, hybridization of above methods gets its attention to overcome the disadvantages pertaining to each method. One hybrid approach developed by the author is the Level Contour Reconstruction Method (LCRM) which combines characteristics of both Front Tracking and Level Set method. Many engineering problems also contain complex geometry as boundary condition and proper representation of grid structure plays very important role for the successful outcomes. In this paper, an algorithm for handling arbitrary geometry inside fixed Eulerian computational domain with multiphase flow has been presented. Interface reconstruction between liquid and vapor phase has been performed outside of arbitrary solid boundary explicitly along with dynamic contact angle model. Sharp interface technique using ghost fluid point extrapolation method has been utilized for correct implementation of no-slip boundary condition at the wall.

Keywords: Numerical simulation; Multiphase flow; Arbitrary geometry; Ghost point method

1. Introduction

The use of a fixed Eulerian grid to simulate multiphase flow with additional advection schemes to preserve the sharpness of interfacial front has become increasingly popular. Variety of numerical techniques such as VOF, Level Set, and Front tracking has been devised and successfully used for many engineering applications. Numerous engineering problems also involve stationary solid surface which has complex geometry as well as moving interface boundary. Thus proper representation of the arbitrarily shaped solid structure poses additional difficulties in numerical simulation of multiphase flows.

An unsuitable grid structure usually makes solution convergence difficult and may even lead to instability of simulation. Hence, accurate grid formation has been one of the key issues in computational fluid dynamics. Two different approaches have been suggested for arbitrarily shape stationary surface and widely used in many engineering fields. The one is to use unstructured body fitted grids and the other approach is to force specific boundary values along the immersed boundary while the governing equations are discretized on a regular Cartesian gird. This so-called "immersed boundary method" has become very attractive due to not only its significantly reduced CPU savings compared to body fitted type, but also its simplicity in implementation along with moving interface formulation.

In this paper, ghost point method for complex geometry has been extended to account for arbitrarily shaped stationary geometry with moving phase boundary.

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2. Numerical formulation

2.1 Governing equation

The governing equations for incompressible multi-fluid motion can be expressed in a single field formulation as:

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

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla p + \rho\mathbf{g} + \nabla\cdot\mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T) + \mathbf{F} \tag{2}$$

here, $\mathbf{u}$ is the velocity, p the pressure, $\mathbf{g}$ the gravitational acceleration, and $\mathbf{F}$ is the local surface tension force at the interface which can be described by the hybrid formulation [1] as:

$$\mathbf{F} = \sigma\kappa_H \nabla I \tag{3}$$

where σ is the surface tension coefficient (assumed constant here), I is the indicator function, a Heavi function which varies from zero to one near the interface, and κ_H is the compact curvature field calculated on the Eulerian grid. The expression for the compact curvature field, κ_H, is given by:

$$\kappa_H = \frac{\mathbf{F}_L \cdot \mathbf{G}}{\sigma \mathbf{G}\cdot\mathbf{G}} \tag{4}$$

where

$$\mathbf{F}_L = \int \sigma\kappa_f \mathbf{n}_f \delta_f(\mathbf{x} - \mathbf{x}_f)ds \tag{5}$$

$$\mathbf{G} = \int \mathbf{n}_f \delta_f(\mathbf{x} - \mathbf{x}_f)ds \tag{6}$$

here, $\mathbf{n}_f$ is the unit normal to the interface, $\mathbf{x}_f = \mathbf{x}(s,t)$ is a parameterization of the interface, and $\delta_f(\mathbf{x}\text{-}\mathbf{x}_f)$ is a two-dimensional dirac delta distribution that is non-zero only when $\mathbf{x} = \mathbf{x}_f$. ds is the length of the element, and κ_f is twice the mean interface curvature computed in a Lagrangian fashion. The detailed procedure for calculating the curvature field can be found in [1, 2]

Material property fields can be described using the indicator function, $I(\mathbf{x},\mathrm{t})$ as:

$$b(\mathbf{x},t) = b_1 + (b_2 - b_1)I(\mathbf{x},t) \tag{7}$$

where the subscripts 1 and 2 refer to the respective fluids. The interface is advected in a Lagrangian fashion by integrating

$$\mathrm{d}\mathbf{X}_f / dt = \mathbf{V} \tag{8}$$

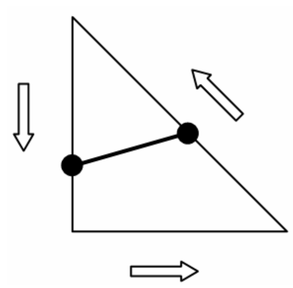
where $\mathbf{V}$ is the interface velocity vector interpolated at $\mathbf{X}_f$. The detailed solution procedure and discretization of the governing equations can be found in Shin and Juric [2].

2.2 Level contour reconstruction method with tetra-marching procedure

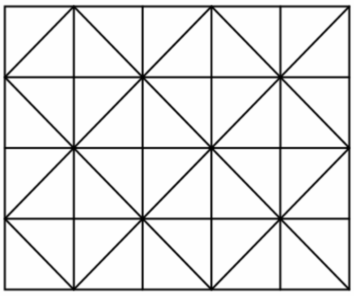
Recently, there have been efforts to construct hybrids from existing well-known methods with the intention of overcoming the inherent drawbacks of each method for the direct simulation of multiphase flow. Level Contour Reconstruction Method [2] is one of the hybrid type method which combines Front Tracking and Level Set method. It is a Front Tracking type method since it uses Lagrangian elements (line segments for 2D and triangles for 3D) to describe the interface. However, it does not have logical connectivity between interfacial elements which was the huge burden with conventional Front Tracking method especially for 3D flow.

During the course of a simulation the interface is periodically regenerated from contour field values (usually the given level of indicator function, $I(\mathbf{x},\mathrm{t})$) to maintain certain regularity of its size. Reconstructed interface elements automatically take on the topological characteristics of the indicator function. Thus it utilizes the Level Set characteristic of indicator function. A primary advantage of the Level Contour Reconstruction Method is the ability to naturally and automatically handle interface merging and breakup while retaining the accuracy of convectional Front tracking technique.

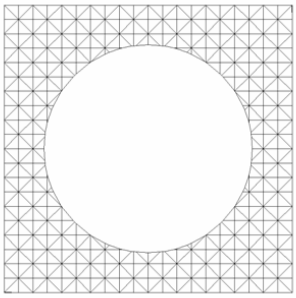
The reconstruction procedure can be undertaken, in generally, with same rectangular shaped Eulerian grid structure as flow computation. With this rectangular shaped grid, there can be more than two lines in single cell during the reconstruction procedure. Thus there can be ambiguity to draw lines between these points. This problem can be avoided by using triangular mesh [3] instead of rectangular one as in Fig. 1(a). There can be only one line from each triangular cell of interest for 2D simulation. To make the reconstructed surface continuous, triangular grid has been oriented in alternative fashion as shown in Fig. 1(b).



(a) Tetra-marching process for each 2D cell



(b) Distribution of triangular shaped cells for interface reconstruction



(c) Grid structure of interface reconstruction for droplet and cylinder interaction

Fig. 1. Tetra-marching procedure for Level Contour Reconstruction Method.

2.3 Sharp interface technique for wall boundary condition with arbitrary geometry

To implement correct non-slip boundary condition at arbitrarily shaped wall, a sharp interface technique near the solid wall based on the ideas of Gilmanov *et al*. [4] has been used.

To explain the main idea of the sharp interface method, 1D example has been chosen for simplicity. The computational nodes in the fluid (vapor or liquid) can be easily identified using the Level Set field which can be directly obtainable from the given stationary wall boundary. The Cartesian grid node *i* will be inside the solid if the distance function is less than zero or inside the fluid if the distance function is greater than zero. Solid nodes that have direct contact with fluid nodes, *i*-1, will be assigned as ghost nodes. The governing equations are solved only at the fluid nodes with appropriate boundary conditions specified at these ghost nodes.

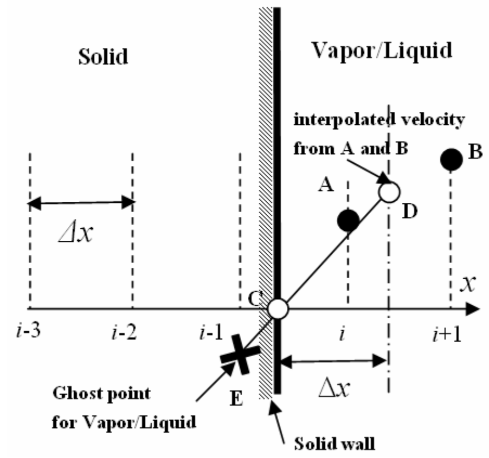


Fig. 2. Sharp interface technique for implementing arbitrarily shaped stationary wall boundary condition.

The values of the ghost nodes will be extrapolated to satisfy non-slip boundary condition (Fig. 2) as:

$$\phi = a_0 + a_1 x \tag{9}$$

where x is the distance from the solid wall. The coefficients a_0 and a_1 can be found using the known information at C (at the wall, usually zero) and D (one cell distance away from the wall). Then Eq. (9) becomes:

$$\phi = \phi_C + (\phi_D - \phi_C)x / \Delta x \tag{10}$$

The value of ϕ_D can be found by linear interpolation using the information of A and B. This method can be readily applicable to multi-dimension. More detailed procedure for sharp interface method can be found in Shin and Abdel-Khalik [5].

2.4 Contact line modeling

We use the Navier-slip model from Liu *et al.* [6], which allows contact line movement proportional to shear stress at the contact point, to account for the contact line behavior at the boundary wall. The contact line velocity can be determined by the following equation:

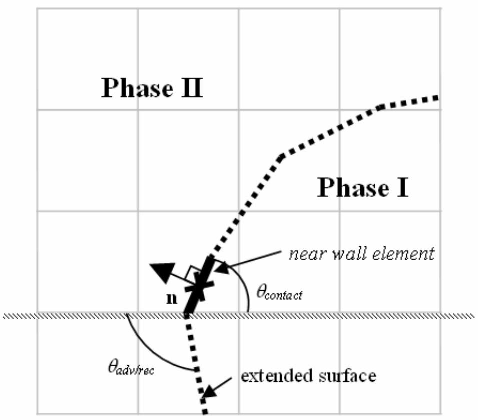


Fig. 3. Schematic diagram of contact line modeling in level contour reconstruction method.

$$U_{cl} = \lambda \frac{\partial u}{\partial n}\bigg|_{wall} \tag{11}$$

here, U_{cl} denotes the contact line speed, $\partial u/\partial n\,|_{wall}$ is the shear stress at the wall, and λ is a proportionality constant. In most cases, we choose λ to be the size of a grid cell as proposed by Liu *et al*. [6].

Since we have explicit information on the interface due to Front Tracking characteristic of LCRM, it is relatively straightforward to implement contact line dynamics in the current formulation. Fig. 3 illustrates the procedure for implementing the contact line model in LCRM. First we identify the "contact points". By calculating the interface normal for the near wall interfaces, we can identify the contact angles associated with those contact points. We then extend the fictitious interface into the wall which has been used to impose the correct interfacial source term, i.e. curvature effect in the governing equations as well as smooth transition of indicator function near the contact region. Due to specific information of the interface location, it is rather easy to modify the geometry near the contact region. We found out that mass conservation is slightly better by forcing the curvature effect implicitly by extending surface rather than changing the actual interface geometry inside the solution domain. The model can also account for contact angle hysteresis. We simply restrict the contact angle if the current contact angle, θ, is less than the prescribed receding angle (θ_{rec}) or greater than the advancing angle (θ_{adv}) then the interface will be extended with the given receding or advancing contact angle, respectively.

3. Result and discussion

To check the performance of current formulation, we have simulated water droplet impacting on cylindrical solid surface similar to Liu *et al*. [6]. Using the length scale as diameter of droplet (D), velocity scale as $\sqrt{gD}$, the governing equation can be nondimensionalized by following dimensionless parameters:

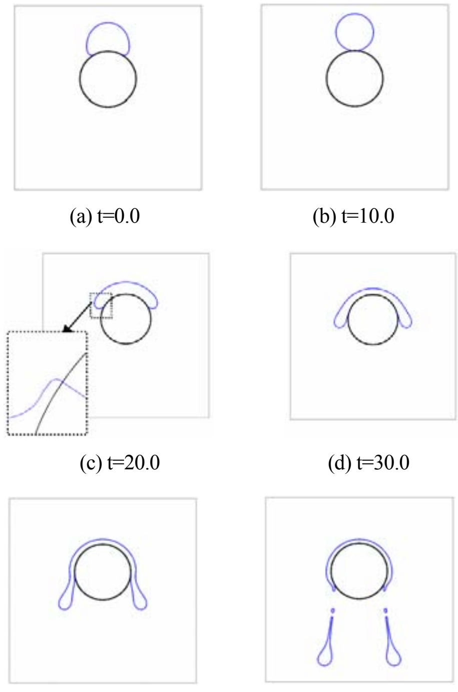
$$\mathrm{Re} = \frac{\rho_L D\sqrt{gD}}{\mu_L}, \mathrm{We} = \frac{\rho_L g D^2}{\sigma}$$
$$\rho^* = \frac{\rho_G}{\rho_L}, \mu^* = \frac{\mu_G}{\mu_L} \tag{12}$$

here subscript L represents liquid phase and G represents gas phase, respectively. For current simulation, Re=10, We=10, ρ*=0.01, and μ*=0.01 has been used. Initially liquid droplet has been placed right above the solid cylinder. Non-dimensional diameter of the cylinder is 1.5. Non-slip boundary condition has been applied at the top and open condition has been used elsewhere. For reconstruction of the moving interface, triangular cell has been subdivided to conform stationary solid wall as in Fig. 1(c) and 100×100 grid resolution was used for the current simulation.

Fig. 4 shows the simulation results with θ_{adv}=θ_{rec}= 90°. The droplet starts to impact on upper surface of the solid cylinder then spread, breaks into smaller droplets, and finally drip down due to gravity. Fig. 5 shows the same experiment except the contact angle which has been prescribed as θ_{adv}=θ_{rec}=45°. As you can see from the figure, the thin film has been maintained for longer period which demonstrate higher wetting characteristic of the liquid.

The interface becomes severely deformed throughout both simulations and current method can capture this subtle feature accurately. The contact angle has been maintained correctly as can be seen in dotted window of Fig. 4(c) and Fig. 5(c). Velocity and pressure distribution at the same time as Fig. 4(c) has been plotted in Fig. 6. The total mass loss during the simulation was less than 3% for both cases.

To see more realistic behavior of contact angle hysteresis, we have tested the droplet impact on flat solid surface inclined at 45° to the horizontal axis (Fig. 7). For this simulation, we have used Re=1000, We=1, ρ*=0.001, and μ*=0.01, respectively. The advancing and receding contact has been prescribed differently as θ_{adv}=110° and θ_{rec}=60°. Initially liquid droplet with non-dimensional diameter of 1.5 has been placed

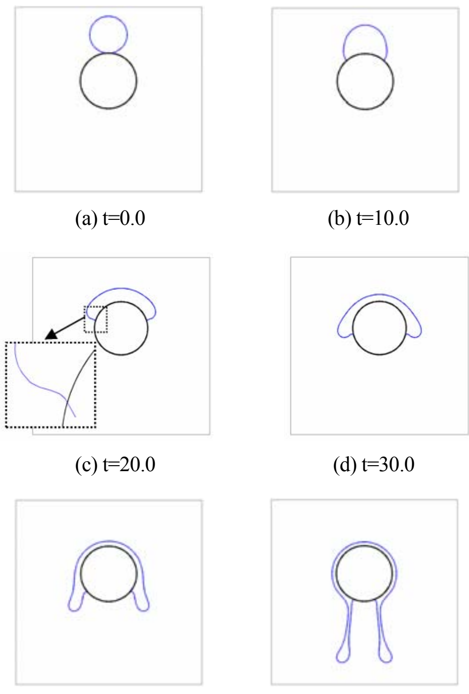


(a) t=0.0 (b) t=10.0

(c) t=20.0 (d) t=30.0

(e) t=40.0 (f) t=55.0

Fig. 4. Interface evolution of droplet during impacting stationary solid cylinder with $\theta_{adv}=\theta_{rec}=90^o$.



(a) t=0.0 (b) t=10.0

(c) t=20.0 (d) t=30.0

(e) t=40.0 (f) t=55.0

Fig. 5. Interface evolution of droplet during impacting stationary solid cylinder with $\theta_{adv}=\theta_{rec}=45^o$.

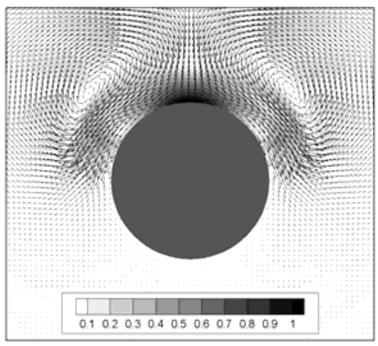
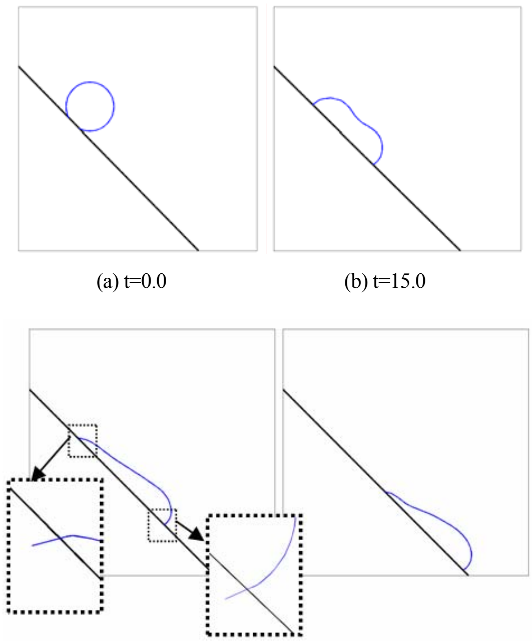


Fig. 6. Velocity and pressure distribution during droplet and cylinder interaction.



(a) t=0.0 (b) t=15.0

(c) t=30.0 (d) t=50.0

Fig. 7. Interface evolution of droplet during impacting stationary flat solid surface inclined at 45^o to horizontal axis ($\theta_{adv}=110^o$, $\theta_{rec}=60^o$).

right above the flat solid surface. As you can see from the Fig. 7, the liquid interface is sliding down the inclined wall with two different contact angles and moving velocities. The advancing contact angle (110^o) and receding contact angle (60^o) has been correctly modelled as in magnified windows of Fig. 7(c). Even thought we prescribed the contact angle implicitly inside the solid domain, the interface evolves to satisfy imposed advancing/receding contact angle eventually.

4. Conclusions

An algorithm for handling arbitrary geometry inside fixed Eulerian computational domain with multiphase flow has been presented. Interface reconstruction between liquid and vapor phase has been performed outside of arbitrary solid boundary explicitly. Sharp interface technique for complex geometry has been applied to implement no-slip boundary condition at the wall which uses extrapolated ghost point values at the near-boundary nodes via linear extrapolation along the local normal to the body. The proposed methodology maintains a sharp fluid/body interface accurately during the course of droplet impacting simulation upon stationary cylindrical surface.

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