Systematic Finite Volume Discretization for the Conservative, Robust and Accurate Simulation of Multiphase Flows

P. Brady*, and O. Desjardins
Sibley School of Mechanical and Aerospace Engineering,
Cornell University, Ithaca, NY 14853

Abstract

The discontinuous nature of the equations governing multiphase flow make their accurate discretization a challenging problem. Various numerical methods have been developed to address this problem, but no clear standard has emerged. In this paper a new, systematic finite volume discretization procedure for multiphase flows is presented. This new method is based on recent developments in conservative immersed boundary (IB) schemes with sharp boundary representations. The IB treatment has been verified using the method of manufactured solutions (MMS) to be second order accurate. This IB treatment is generalized such that the Navier-Stokes equations can be solved on both sides of the boundary (interface) using a systematic finite volume discretization. This allows to solve fluid-structure and gas-liquid flows in a sharp, robust, conservative, accurate, and straightforward way. The order of accuracy of this method will be convincingly demonstrated using novel techniques for applying MMS to finite volume multiphase flows. The conservative properties of this method as well as its robustness will be demonstrated by analyzing several flow scenarios.

*Corresponding Author: peter.brady@cornell.edu
Introduction

A number of physical problems of interest to the scientific and engineering community involve discontinuities, and multiphase flows provide a striking illustration of this fact. Computational modeling for such flows often requires different phenomena to be simultaneously represented within a single cell. For example, fluid-solid flows can be solved on non body fitted grids, in which case one part of a cell obeys the Navier-Stokes equation, while another part is solid and obeys Newton's laws of motion. In the case of liquid-gas flows, where the grids are rarely fitted to the geometry of the phase-interface, a fraction of a cell can contain liquid and obey the Navier-Stokes equations with the density and viscosity of the liquid, while the rest of the cell contains gas and obeys the Navier-Stokes with the density and viscosity of that gas. This leads to discontinuities in equations, variables, or properties that need to be accounted for within a grid cell. As a result, both types of flows share many similarities, however they have typically be considered independently. Schemes that focus on fluid-solid flows on non body fitted meshes are typically called immersed boundary (IB) schemes. A wide variety of such schemes exist; they can be regrouped into three classes [1]: schemes based on velocity forcing (e.g., [2]), schemes based on velocity reconstruction (e.g., [3]), and cut-cell schemes (e.g., [4]). These different strategies lead to different properties for the resulting scheme, including different drawbacks. IB forcing schemes tend to rely on smearing of the forcing term over a few cells, thus do not lead to a sharp treatment of the solid boundary condition. In addition, conservation is difficult to achieve with such an approach. A notable exception was proposed for two-dimensional problems recently [5], however the extension to three-dimensional flows for complex solid geometries leads to major challenges. IB reconstruction schemes tend to lack robustness, generating oscillations when the boundaries are moving, and lack local conservation properties [3]. Cut-cell schemes are challenging to implement, and suffer from stringent time step restrictions due to the small cells they generate [6, 7]. While this can be alleviated, this is often at the price of accuracy [6]. For incompressible liquid-gas flows, two main types of schemes have been proposed: sharp schemes like the ghost fluid method [8], and non sharp schemes like the continuum surface force approach [9]. The ghost fluid method relies on a generalized Taylor series expansion of the discontinuous solution in order to provide a finite difference discretization capable of differentiating a discontinuous quantity, leading to a sharp scheme that is however limited to first order accuracy formally. The continuum surface force algorithm [9] shares similarities with IB forcing schemes, in that it smears out the discontinuous aspects of the two-phase problems such that they can be solved on a mesh using standard discretization schemes. The accuracy and robustness of this strategy tends therefore to be limited.

State-of-the-art discretization schemes for classical conservation laws are generally expected to be discretely conservative, stable, and accurate. Yet, this paradigm is lost when considering discontinuous conservation laws. The goal of the work present herein will be to formulate, implement, test, and deploy a novel finite volume strategy for discretizing discontinuous conservation laws with the following properties: sharp, conservative, robust, and accurate. The present work will be based on the recently developed conservative immersed boundary scheme of [10] which combines all these properties and extend the method to fluid-fluid problems.

Immersed Boundary Treatment

As the fluid-fluid methodology is an extension of a solid-fluid immersed boundary treatment, an overview of that treatment is given here. When considering flows in complex geometries, immersed boundary (IB) methods have have been studied extensively because they provide an alternative to using a full body-fitted mesh, which often requires an unstructured CFD code. However, using a non body-fitted mesh with IB creates new challenges, including insufficient accuracy and the potential lack of conservation properties. Yet, discrete conservation can be obtained by using a cut-cell IB approach, where the cells that intersect with the solid body are cut such that they become body-fitted [1]. This approach requires extensive geometric manipulations and a modified discretization in those cut-cells [6], which can make implementation difficult. In addition, arbitrarily small cells are formed that negatively impact the simulation by requiring smaller time steps [7]. The recently developed IB method [10] contains several modifications to the traditional cut-cell IB formalism in order to alleviate these issues :

- The interface was implicitly represented using a level set function, and all geometric manipulations were performed using a formally second order accurate marching simplex library.
- The cut-cells were formed through a simple modification of the discrete divergence operators only. Using the method of manufactured
solutions, it was shown that this vastly simplified approach achieves second order accuracy.

- The time step restriction due to arbitrarily small cut-cells was lifted by using implicit time integration, which is readily available for structured solvers.

This novel approach provides exact primary conservation, i.e., local discrete conservation of both fluid mass and momentum. In addition, this method is second order accurate and runs robustly at unity Courant-Friedrichs-Lewy (CFL) numbers. Details on this approach are given in the following section.

**Cut-Cell Geometry**

In order to characterize the geometry of the cut-cells that are the basis of this approach, it is necessary to fully characterize the location of the immersed geometry surface. This is accomplished through the use of an implicit description in the form of an iso-surface of a smooth function, called level set function. The level set function, \( G \), is chosen such that it corresponds to a standard signed distance function, i.e.,

\[
|G(x, t)| = |x - x_\Gamma|,
\]

(1)

where \( x_\Gamma \) corresponds to the closest point on the solid-fluid interface from \( x \), and \( G(x, t) > 0 \) on one side of the interface, and \( G(x, t) < 0 \) on the other side. With this definition, the immersed boundary surface \( \Gamma \) in a domain \( \Omega \) is defined by \( \Gamma(t) = x \in \Omega : G(x, t) = 0 \).

Once such information is made available, simple operations can be used to estimate the location of the surface, such as a linear interpolation between two points of different \( G \)-sign. We then reconstruct the wetted volumes and surfaces by first decomposing each cell (assumed here to be hexahedral without loss of generality) into five simplices (tetrahedra in three dimensions), followed by a marching simplex algorithm to triangulate the interface [11], as illustrated in Fig. 1. Note that in three dimensions, intersecting a tetrahedron with a plane is a straightforward operation. Accounting for all possible symmetries, only three cases need to be considered: (1) no intersection, i.e., the cell is not a cut-cell, (2) an intersection leaving one vertex on one side of the plane and three on the other, and (3) an intersection leaving two vertices on one side and two on the other. The result of this process is a second order discrete representation of the cut-cell in the form of a collection of tetrahedra, from which quantities such as the cut-cell volume and surface areas can be readily extracted.

![Figure 1. Optimal decomposition of hexahedral into five simplices, followed by a marching simplex procedure to intersect the immersed surface with the cell volume.](image)

**Cut-Cell Implementation**

The IB formulation of Meyer et al. [7] forms the basis of our cut-cell implementation. Instead of the full Navier-Stokes equations, consider a generalized conservative transport equation for a quantity \( \phi \) given by

\[
\frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{F}(\phi) = 0,
\]

(2)

where \( t \) is time, and \( \mathbf{F}(\phi) \) represents the flux of \( \phi \), possibly a diffusive, viscous, advective, or convective flux. A typical second-order finite volume discretization of this equation leads to the following form

\[
\phi^n_{c+1} = \phi^n_c - \frac{\Delta t}{V_c} \sum_{faces} (A_f \mathbf{F}^{n+1/2}_f \cdot \mathbf{n}_f)
\]

(3)

where the \( \phi^n_c \) represents the cell-average value of \( \phi \) at time \( t^n \), \( \Delta t \) is the time step size, \( V_c \) is the cell volume, \( A_f \) is the face area, \( \mathbf{n}_f \) is the face outward normal, and \( \mathbf{F}_f \) represents the face-average flux. The presence of the IB leads to many instances where cells are cut by the fluid-solid interface, as illustrated by Fig. 2. In that case, it is appropriate to replace the cell volume \( V_c \) by the wetted volume \( V_w = \alpha^W V_c \), and the face area \( A_f \) by the wetted face area \( A_w = \alpha^S A_f \), which is equivalent to saying that the finite volume formulation should be obtained by integrating over the fluid part of the cell only. This
leads to the following expression,

\[
\phi^{n+1}_c = \phi^n_c - \frac{\Delta t}{\alpha^{s}_c V_c} \left[ \sum_{faces} \left( \alpha^{s}_f A_f \mathbf{F}^{n+1/2}_f \cdot \mathbf{n}_f \right) + A_{IB} \mathbf{F}^{n+1/2}_{IB} \cdot \mathbf{n}_{IB} \right], \tag{4}
\]

where the volume and area fractions \( \alpha_c \) and \( \alpha_f \) are unity except in cut cells. The last term represents the flux of \( \phi \) at the immersed boundary surface, where \( A_{IB} \) is the immersed boundary area in the cell, \( \mathbf{n}_{IB} \) is the outward-oriented immersed boundary normal, and \( \mathbf{F}_{IB} \) is the average flux along the immersed boundary surface in that cell.

These modifications can be conveniently implemented by modifying the divergence operators using the volume and surface fluid fractions, and adding a source term to account for any flux at the IB surface. Note that with Neumann boundary conditions, the flux through the IB surface is zero. Similarly, the convective momentum flux at a fixed nonporous surface is zero, but the viscous momentum flux is non-zero. A critical aspect of this fictitious cut-cell methodology lies in the presence of small cells. Indeed, there is technically no limitation to how small cut-cells can get, which can lead to unacceptable restrictions in time step size in order to maintain stability. While Meyer et al. [7] rely on a tedious cell-merging technique, our work simply employs an implicit time integration based on the diagonally-dominant alternate direction implicit (DDADI) strategy [12], allowing for stable time stepping at any cut-cell CFL numbers.

While this procedure accounts explicitly for the change in wetted volumes and area, one would expect that the face-average fluxes \( \mathbf{F}^{n+1/2}_f \) also need to be modified in the presence of IB to account for the shift in the face barycenter position. We conveniently ignore this additional complication, and have shown using the Method of Manufactured Solutions (MMS) that this simplified formalism retains second order accuracy. Consequently, we argue that accounting for the change in face area and cell volume is sufficient to properly capture the presence of an immersed solid, and we use unmodified fluxes in the cut-cells. The resulting scheme is therefore surprisingly simple: it requires modifying the discrete divergence operator and including source terms as necessary, while geometric considerations are readily handled using the combined level set/marching simplex approach described in the previous section.

**Fluid-Fluid Treatment**

Note that for incompressible liquid-gas flows without heat and mass transfer, the velocity field \( \mathbf{u} \) is continuous, meaning that there is only a limited challenge in solving the Navier-Stokes equation. The viscous term is a notable exception to this statement, and will need to be investigated separately. The main difficulty lies in the discretization of the pressure Poisson equation, since the pressure \( p \) is a discontinuous variable. Namely, one has to solve

\[
\nabla \cdot \frac{1}{\rho} \nabla p = \frac{1}{\Delta t} \nabla \cdot \mathbf{u} \tag{5}
\]

where \( \rho \) is the fluid density, and where the pressure is discontinuous due to both the surface tension and the discontinuity in viscosity \( \mu \),

\[
[p]_\Gamma = \sigma \kappa + 2 [\mu]_\Gamma \mathbf{n}^T \cdot \nabla \mathbf{u} \cdot \mathbf{n}. \tag{6}
\]

\( \sigma \) is the surface tension coefficient, while \( \kappa \) is the interfacial curvature. The square brackets represent a jump condition between liquid and gas, i.e., \([p] = p_l - p_g\). We stay true to the finite volume formalism when extending the previous method to the discontinuous Poisson equation that arises in liquid-gas problems. Up until now, we formulated equations for the fluid fraction of the cell, since we did not have any equation to solve in the solid part of the cell. Here, an equation needs to be solved for both phases, which suggests that one should consider both the liquid and the gas within the cell when discretizing the problem. Therefore, we introduce a classical cell average pressure in cell \( i \),

\[
p_i = \frac{1}{V_i} \int_{V_i} p(x,t)dV = \frac{1}{V_c} \left[ \int_{V_l} p_l(x,t)dV + \int_{V_g} p_g(x,t)dV \right]. \tag{7}
\]

Using \( \alpha \) as the liquid volume fraction in the cell, we can write \( p_i = \alpha p_l^i + (1-\alpha)p_g^i \), where \( p_l^i \) and \( p_g^i \) are the average cell liquid pressure and cell gas pressure, respectively. Figure 3 illustrates the i problem statement in one dimension. Using this discretization strategy, it can easily be shown that the pressure gradient in both phases can be obtained from the knowledge of \( p_i \), \( p_{i+1} \), and \([p]_\Gamma \), for example

\[
\frac{dp}{dx}\bigg|_i \approx \frac{p_i - p_{i-1}}{\Delta x} - \frac{1 - \alpha_{i-1}}{\Delta x} [p]_\Gamma \tag{8}
\]

This expression is first order accurate only. If the jump in pressure gradient \([dp/dx]_\Gamma \) is known, one can
write a second order accurate pressure gradient discretization for either phase, for example

\[
\left. \frac{dp}{dx} \right|_i \approx \frac{p_i - p_{i-1}}{\Delta x} - \frac{1 - \alpha_{i-1}}{\Delta x} |p|_\Gamma \\
+ \left[ \frac{dp}{dx} \right]_\Gamma \left( 1 - \alpha_{i-1} \right)^2 \frac{1}{2} 
\]

These results suggest that using the same type of volume fraction correction that was introduced in the conservative immersed boundary method, one can write a second order accurate finite volume discretization of the discontinuous pressure Poisson equation that appears in liquid/gas flows. This is really the finite volume equivalent to the ghost fluid method [8], although a second order accurate version of the ghost fluid method has yet to be found.

The accuracy of this method applied to the pressure Poisson system will be verified using the method of manufactured solutions in a manner similar to [11]. This will be then compared to the accuracy achieved using other common interface treatments such as the CSF [9] and finite difference ghost fluid approaches.

References

