A High-Order Projection Method for Tracking Fluid Interfaces in Variable Density Incompressible Flows

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Abstract

We present a numerical method for computing solutions of the incompressible Euler or Navier-Stokes equations when a principal feature of the flow is the presence of an interface between two fluids with different fluid properties. The method is based on a second-order projection method for variable density flows using an "approximate projection" formulation. The boundary between the fluids is tracked with a second-order, volume-of-fluid interface tracking algorithm. We present results for viscous Rayleigh-Taylor problems at early time with equal and unequal viscosities to demonstrate the convergence of the algorithm. We also present computational results for the Rayleigh-Taylor instability in air-helium and for bubbles and drops in an air-water system without interfacial tension to demonstrate the behavior of the algorithm on problems with larger density and viscosity contrasts.

1. Introduction

Fluid flows with free surfaces or material interfaces occur in a large number of natural and technological processes. Casting processes, mold filling, thin film processes, extrusion, spray deposition and fluid jetting devices are just a few of the areas in which material interfaces occur in industrial applications. Often properties that depend on the shape of the interface itself (e.g., surface tension) play an important role in the dynamics of the problem, and the interfacial physics (e.g., capillarity) can drive the flow making it essential to accurately determine the position, curvature, and topology of the interface. Numerical simulations are, in principle, ideally suited to study these flows; not only can the data be much more easily gathered but various physical processes can be turned on and off at will. In practice, however, the numerical computation of flows with material interfaces can be difficult. The interface can separate fluids of dramatically different densities such as air and water, and computational difficulties arise due to the local lack of smoothness at the interface.

There are two basic approaches that one can use to approximate flows with a material interface: "capturing" and "tracking." In interface capturing, the interface is treated as a region of steep gradient in some quantity (e.g., density ρ) that satisfies an advection equation of the form

$$\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{1}$$

where $\mathbf{u}$ denotes the fluid velocity. To obtain high-order accuracy one typically approximates solutions of (1) with an advection algorithm that is high-order in smooth regions and subject to some sort of monotonicity constraint (e.g., see [6, 14, 29]). This approach has been successfully used by Bell and Marcus to study a variety of problems [7, 31]. The primary advantages of this approach are that it is easy to implement and no additional algorithmic details are required to model topological changes of the interface. However, the front diffuses over several computational zones, resulting in a corresponding loss of accuracy (see e.g., [19]).

In an interface tracking method the interface is treated explicitly as a sharp discontinuity moving through the grid. Tracking can offer better accuracy than capturing, but at the cost of greater algorithmic complexity. There are basically three possible representations of an interface in an interface tracking method:

- a piecewise polynomial function ("front tracking" and boundary integral methods)
- the level set of some function (level set methods)
- a collection of volume fractions (volume-of-fluid methods)

Each of these three approaches has its strengths and weaknesses. For example, the advantage of using a piecewise polynomial method is that one can design arbitrarily high-order accurate approximations to a smoothly varying front. This intrinsic accuracy can often allow one to resolve fine scale features of the front on relatively coarse underlying grids. Examples of piecewise polynomial methods include boundary integral methods (e.g., [3, 36, 49]), the front tracking methods of Glimm et. al [17, 18] and the algorithm developed by Tryggvason [59]. The piecewise polynomial approach has several weaknesses: it is relatively difficult to extend a piecewise polynomial method to three-dimensions (e.g., see [20]), one must design special procedures for handling the changes in the front topology and it is not intrinsically conservative. (We note that Tryggvason and his coworkers have developed a three-dimensional piecewise polynomial method [59] and report that the mass loss is negligible for the flows they have studied [58].)

The level set approach was originally introduced by Osher and Sethian [37] and has since been applied to a wide variety of problems including bubbles and drops [52], Rayleigh-Taylor instability [33], flow by mean curvature [47], and dendritic growth and solidification [48]. In a level set method the interface is represented as the level set of some function ϕ. This approach has two inherent strengths. One very useful feature of level set methods is that the representation of the interface as the level set of some function ϕ leads to convenient formulas for the interface normal and curvature. Another advantage of this approach is that no special procedures are required in order to model topological changes of the front. One simply updates the value of the level set function ϕ at each time step, and the location of the front at the new time is simply the zero contour of ϕ.

The volume-of-fluid approach tracks the volume of each individual material in cells that contain a portion of the interface, rather than the interface itself. At each time these volumes are used to reconstruct an approximation to the interface and this approximate interface is then used to update the values of the fluid volumes in each cell at the next time. A volume-of-fluid interface tracking method consists of two parts: an *interface reconstruction algorithm* for determining an approximation to the interface from a given collection of volumes and a volume-of-fluid *advection algorithm* or *transport algorithm* for determining the values of the fluid volumes at the new time from a given velocity field and this reconstructed interface. Volume-of-fluid methods, like level set methods, do not require special procedures to model topological changes of the front. For this reason level set methods and volume-of-fluid methods are somewhat easier to implement in three dimensions than piecewise polynomial methods while retaining the improved accuracy obtained by explicitly modeling the interface motion.

A fundamental property of all volume-of-fluid methods is that they are based on discretizing the *volume*, or equivalently the *volume fraction* f, of one of the fluids. Therefore, since in an incompressible flow conservation of mass is equivalent to conservation of volume, the motion of the interface in an incompressible flow is modeled by solving a conservation law for the volume fraction. As a consequence one can use a conservative finite difference method to update the volume fractions and, except for errors that occur as a result of numerical overshoot and undershoot, the volume (mass) of each fluid in the computation is conserved.

It is interesting to contrast this with the discretization in a level set method. In a level set method the level set function ϕ, which is initially taken to be the (signed) distance from the interface (e.g., see [52]), also satisfies a conservation equation. However, conservation of ϕ does not imply that the volume of each fluid is conserved. It has been found that this can lead to loss of mass, cf. Sussman, Smereka and Osher [52]. Chang et al. [10] and Sussman et al. [51, Sussman-Fatemi-Smereka-Osher:1996] have since developed various "reinitialization" techniques for maintaining ϕ as a distance function that ameliorates this problem.

The approach we present here is based on a volume-of-fluid formulation. Volume-of-fluid methods have been in use for several decades. One of the early algorithms of this type was the SLIC algorithm of Noh and Woodward [35]. Chorin [12] developed an improved version of SLIC in order to model flame propagation and combustion. Ghoniem, Chorin, and Oppenheim [16] and Sethian [46] have used this idea to model turbulent combustion. Another variation of the volume-of-fluid approach was the VOF algorithm of Hirt and Nichols [25]. Several codes based on the VOF idea, namely, SOLA-VOF [25, 34] and its descendants NASA-VOF2D [55], NASA-VOF3D [56], RIPPLE [27, 28] and FLOW3D [24] are used widely for modeling interfaces and free surfaces in industrial applications today. For example, researchers at Xerox have used a modified version of SOLA-VOF to model the flow in thermal ink jet devices [15, 54] and SOLA-VOF and FLOW3D have been used extensively by material scientists to model problems involving melting and solidification (e.g. [9, 30, 57]).

However all of these codes are built around a relatively crude volume-of-fluid interface reconstruction algorithm that relies on a piecewise-constant or "staircase" representation of the interface and advection algorithms that are at best first-order accurate. More modern volume-of-fluid interface reconstruction methods use a linear approximation to the interface in each multifluid cell (e.g., see [38, 41, 44, 60]) that results in a piecewise-linear approximation to the interface. For example, Youngs and his colleagues [60, 61] have used several first-order, piecewise-linear algorithms coupled with numerical integration schemes for gas dynamics to model turbulent mixing and the Rayleigh-Taylor and Richtmyer-Meshkov instabilities in compressible flows. Youngs [61] also applied a piecewise linear algorithm for compressible flow in three dimensions (also see [26, 44]).

In recent work Puckett [41] and Pilliod and Puckett [40] introduced two second-order volume-of-fluid interface reconstruction algorithms. One of these algorithms, the Least Squares Volume-of-Fluid Interface Reconstruction Algorithm (LVIRA) [41]) has been coupled to a second-order Godunov algorithm for gas dynamics for modeling compressible flows with two fluids having different equations of state. This algorithm has been used extensively to compute Richtmyer-Meshkov instabilities [32] and shock refraction [22, 23, 21, 43, 42].

The goal of this paper is to develop a second-order algorithm for incompressible flows with two fluids of different densities. The basis for the numerical algorithm is a variable density version of the approximate projection method developed by Almgren, Bell and Szymczak [2] for the incompressible Navier-Stokes equations. This algorithm is based on high-resolution upwind methods that provide a robust discretization of the basic flow equations, making it an suitable framework for modeling variable density flows with a sharp interface. The density interface is constructed from volume fractions using the LVIRA reconstruction algorithm. We present both an operator-split advection algorithm and an unsplit advection algorithm due to Pilliod and Puckett [40] for advecting the volume fractions to update the density field. The unsplit algorithm is based on the ideas of Bell, Dawson and Shubin [6] for approximating solutions of scalar conservation laws. Both of these approaches use the geometric information from the reconstructed interface to compute fluxes in the update of the volume fraction rather than a simple upwind discretization of it. Consequently, the front does not diffuse as it would if one were to use a standard conservative finite difference method to update the values of f. The resulting algorithm is second-order accurate for smooth flows with a discontinuous density interface while degrading to first-order accuracy when the velocity field is not smooth.

The remainder of this paper is organized as follows. In the next two sections we give a detailed description of the interface tracking method, review the basic projection algorithm and discuss how the VOF interface tracking algorithm is coupled to the basic flow algorithm. In Section 4 we present computational examples that demonstrate the convergence properties of the algorithm and demonstrate its performance on several realistic model problems. In Section 5 we state our conclusions.

2. The Interface Tracking Algorithm

In this section we describe a method for tracking the interface between two materials, say a dark fluid and a light fluid, in a two-dimensional, incompressible, non-reacting flow. We consider the problem of advancing a front in a known divergence-free velocity field $\mathbf{u} = (u, v)$. In the following section we describe our method for obtaining this velocity field as a solution of the Navier-Stokes equations. We begin by covering the problem domain with a uniform grid with spacing $h = \Delta x = \Delta y$. With each grid cell we associate a number $f_{i,j}$ that represents the fraction of the i,jth cell that is occupied by dark fluid; i.e.,

$$f_{i,j}\, h^2 \;=\; \text{volume of dark fluid in the } i,j\text{th cell.} \tag{2}$$

The number $f_{i,j}$ is called the *volume fraction* (of dark fluid) in the i,jth cell. It is apparent that

$$0 \le f_{i,j} \le 1\,, \tag{3}$$

that the volume fraction associated with the light fluid is $(1 - f_{i,j})$ and that a portion of the interface lies in the i,jth cell if and only if $0 < f_{i,j} < 1$. The discrete variable $f_{i,j}$ is a discretization of the characteristic function associated with the dark fluid,

$$f(x,y) \equiv \begin{cases} 1 & \text{if there is dark fluid at the point } (x,y), \\ 0 & \text{if there is light fluid at the point } (x,y), \end{cases} \tag{4}$$

in the sense that

$$f_{i,j}\, h^2 \approx \int \int_{i,j\text{th cell}} f(x,y)\, dx\, dy\,. \tag{5}$$

Since the fluid type does not change along particle paths the characteristic function f is passively advected with the flow. Hence f satisfies the advection equation,

$$f_t \,+\, u f_x \,+\, v f_y \;=\; 0\,. \tag{6}$$

Since the flow is incompressible, $\mathbf{u}$ satisfies

$$u_x \,+\, v_y \;=\; 0\,. \tag{7}$$

Multiplying (7) by f and adding it to (6) we obtain a conservation law for the characteristic function f,

$$f_t \,+\, (uf)_x \,+\, (vf)_y \;=\; 0\,. \tag{8}$$

Equation (8) reflects the fact that in an incompressible flow conservation of mass is equivalent to conservation of volume, and hence conservation of f. If one uses a conservative finite difference method to update $f_{i,j}$ then the mass of dark fluid is conserved,

$$h^2 \sum_{i,j} f^0_{i,j} \;=\; \ldots \;=\; h^2 \sum_{i,j} f^n_{i,j} \ldots \;=\; h^2 \sum_{i,j} f^{n+1}_{i,j}\,. \tag{9}$$

Here $f_{i,j}^n$ denotes the volume fraction in the i,jth cell at time $t^n = n\,\Delta t$ and we have assumed that no mass enters or leaves the problem domain during the computation.

During the numerical solution of (8) numerical overshoot and undershoot may cause some volume fractions to violate (3). Although in the computations presented here we found that this effect was negligible, we satisfy (3) explicitly by truncating the values of volume fractions which leave the interval $[0,1]$ during the advection step,

$$f_{i,j}^{n+1} \;:=\; \min(1, \max(f_{i,j}^{n+1}, 0))\,, \tag{10}$$

where := denotes assignment in place. In the computations presented here we have found that the net change in total mass over the entire length of the computation is at most one hundredth of one percent of the total mass of either fluid. We note that one can also remedy overshoot and undershoot with a technique similar to the flux redistribution ideas in [5, 11] (e.g., see [45]).

2.1 The Interface Reconstruction Algorithm In order to advance the solution of (8) in time we first need to construct an approximation to the interface given the values of the volume fractions $f_{i,j}^n$ at time $t = n\,\Delta t$. We refer to an algorithm for doing this as a volume-of-fluid *interface reconstruction algorithm*. In this work we use a volume-of-fluid interface reconstruction algorithm known as the Least Squares Volume-of-Fluid Interface Reconstruction Algorithm (LVIRA) due to Puckett [40, 41]. This algorithm produces a linear approximation to the interface in each multifluid cell, i.e., each cell for which $0 < f_{i,j} < 1$. In general, this piecewise linear approximation is not continuous. The LVIRA algorithm uses the volume fractions $f_{i,j}$ in a 3×3 block of cells to determine the approximate interface in the center cell of the block. An important property of this algorithm, common to all volume-of-fluid algorithms, is that the approximate interface is always chosen so that it reproduces the correct (*i.e.*, given) volume fraction in each multifluid cell. In other words, if we denote the volume fraction due to the linear approximation in the i,jth cell by $\tilde{f}_{i,j}$, then we require that

$$\tilde{f}_{i,j} = f_{i,j} \qquad \text{for all}\, i\,,\, j\,. \tag{11}$$

The LVIRA algorithm also returns a vector $\mathbf{n}$ normal to the interface. In this article we adopt the convention that $\mathbf{n}$ always points away from the dark fluid. The normal vector $\mathbf{n}_{i,j}$ in the i,jth cell together with the given volume fraction $f_{i,j}$ uniquely determines the approximate linear interface in the i,jth cell. Thus, since the volume fraction $f_{i,j}$ is given, the interface reconstruction algorithm is simply a rule for determining a unit normal vector from the 3×3 block of volume fractions centered on the i,jth cell.

In the LVIRA algorithm we choose the unit normal $\mathbf{n}$ which minimizes the function

$$G_{i,j}(\mathbf{n}) \;=\; \sum_{k,l=-1}^{1} \left(f_{i+k,j+l} \;-\; \tilde{f}_{i+k,j+l}(\mathbf{n})\right)^2 . \tag{12}$$

where $f_{i+k,j+l}$ are the given volume fractions in the 3×3 block centered on the i,jth cell and $\tilde{f}_{i+k,j+l}(\mathbf{n})$

are the volume fractions due to the line with unit normal $\mathbf{n}$ which divides the (i, j)th cell into fractions $f_{i,j}$ and $1 - f_{i,j}$. Our approximation to the interface is this line.

This algorithm has the property that if the original volume fractions in the 3×3 block centered on the i, jth cell are due to a linear interface, then it will reproduce the interface exactly. We conjecture the approximate interface will be a second-order approximation to the true interface whenever the true interface is C^2. Computational tests presented in [39, 40] support this conjecture and indicate that the algorithm is first-order accurate whenever the interface fails to be this smooth.[1]

We note that the basic principles of LVIRA are applicable to both axisymmetric and three-dimensional interface reconstruction. LVIRA will exactly reconstruct conical interfaces in axisymmetric geometry and planes in three dimensions.

2.2 The Volume-of-Fluid Advection Algorithm The second step in the solution of (8) is an algorithm for evolving the volume fractions in time. Suppose that at time $t^n = n\,\Delta t$ we have values of the velocity field $(u_{i\pm\frac{1}{2},j}, v_{i,j\pm\frac{1}{2}})$ defined at the centers of the cell edges and that these velocities satisfy a discrete form of (7),

$$\frac{(u_{i+1/2,j} - u_{i-1/2,j})}{\Delta x} + \frac{(v_{i,j+1/2} - v_{i,j-1/2})}{\Delta y} = 0\,. \tag{13}$$

Given an approximation to the interface in each cell for which $0 < f^n_{i,j} < 1$ we wish to determine the volume fractions $f^{n+1}_{i,j}$ at the new time $t^{n+1} = (n+1)\,\Delta t$. We refer to algorithms for doing this as volume-of-fluid *advection algorithms.*

In our work we have used two types of advection algorithms. Both are based on the standard conservative finite difference update of (8),

$$f^{n+1}_{i,j} = f^n_{i,j} + \frac{\Delta t}{\Delta x}\,[F_{i-\frac{1}{2},j} - F_{i+\frac{1}{2},j}] + \frac{\Delta t}{\Delta y}\,[G_{i,j-\frac{1}{2}} - G_{i,j+\frac{1}{2}}]\,, \tag{14}$$

where $F_{i-\frac{1}{2},j} = (fu)_{i-\frac{1}{2},j}$ denotes the flux of f across the left edge of the i, jth cell and $G_{i,j-\frac{1}{2}} = (fv)_{i,j-\frac{1}{2}}$ denotes the flux across the bottom edge of the i, jth cell, etc.

2.2.1 The Operator Split Advection Algorithm The simplest of the two advection algorithms is the *fractional step* or *operator split* method,

$$\tilde{f}_{i,j} = f^n_{i,j} + \frac{\Delta t}{\Delta x}\,[F_{i-\frac{1}{2},j} - F_{i+\frac{1}{2},j}]\,, \tag{15}$$

$$f^{n+1}_{i,j} = \tilde{f}_{i,j} + \frac{\Delta t}{\Delta y}\,[\tilde{G}_{i,j-\frac{1}{2}} - \tilde{G}_{i,j+\frac{1}{2}}]\,. \tag{16}$$

[1] In [39, 40] it is demonstrated numerically that these algorithms are first/second-order in the following sense. If the interface between materials 1 and 2 is C^2 with bounded second derivative, then the L^1 norm of the difference between the true characteristic function for material 1 and the approximate characteristic function decays at the appropriate rate. It is also shown (numerically) in [39, 40] that when the interface fails to be C^2 everywhere the algorithm exhibits first-order convergence.

There is a simple geometric interpretation of the fluxes in (15)-(16). Suppose that $u_{i+\frac{1}{2},j}$ is positive. Divide cell (i,j) into two disjoint rectangles, with areas $u_{i+\frac{1}{2},j}\ \Delta t\ \Delta y$ on the right and $(\Delta x - u_{i+\frac{1}{2},j}\ \Delta t)\ \Delta y$ on the left, as shown in Fig. 1. All of the fluid in the first rectangle will cross the right-hand edge during this time step. In particular, the flux of dark fluid across this edge is equal to the amount of dark fluid contained in this rectangle. In a volume-of-fluid method, this is determined by the location of the reconstructed interface. Thus, if $V_{i+1/2,j}$ denotes the volume of dark fluid in this rectangle then the flux is given by

$$F_{i+\frac{1}{2},j} = u_{i+1/2,j}\, V_{i+1/2,j} \,/ (u_{i+1/2,j}\ \Delta t\ \Delta y) = V_{i+1/2,j} \,/ (\Delta t\ \Delta y)\,. \tag{17}$$

After using (17) in (15) to determine the intermediate volume fractions $\tilde{f}_{i,j}$, one then uses these values to reconstruct the interface in all cells which satisfy $0 < \tilde{f}_{i,j} < 1$. The vertical fluxes $\tilde{G}_{i,j+1/2}$ are then determined by a geometric construction analogous to the one described for the horizontal fluxes, and the volume fractions at the new time level $f_{i,j}^{n+1}$ are found by inserting these vertical fluxes into (16). This procedure can be made second-order simply by alternating the sweep direction at each time step; i.e., by employing "Strang splitting" [50].

In our work we have modified the algorithm in (15)-(16) so that we compute a solution of (6) rather than (8) in each sweep direction. In other words, we approximate solutions of

$$f_t + (fu)_x = f\,u_x\,, \tag{18}$$

$$f_t + (fv)_y = f\,v_y\,, \tag{19}$$

rather than

$$f_t + (fu)_x = 0\,, \tag{20}$$

$$f_t + (fv)_y = 0\,. \tag{21}$$

In order to maintain conservation of f it is now necessary to discretize f implicitly on the right-hand side of (18) and explicitly in the right-hand side of (19),

$$\tilde{f}_{i,j} = \{f_{i,j}^n + \frac{\Delta t}{\Delta x}\,[F_{i-\frac{1}{2},j} - F_{i+\frac{1}{2},j}]\}/[1 - \frac{\Delta t}{\Delta x}\,(u_{i+\frac{1}{2},j} - u_{i-\frac{1}{2},j})] \tag{22}$$

$$f_{i,j}^{n+1} = \tilde{f}_{i,j}\,\{1 + \frac{\Delta t}{\Delta y}\,(v_{i,j+\frac{1}{2}} - v_{i,j-\frac{1}{2}})\} + \frac{\Delta t}{\Delta y}\,[\tilde{G}_{i,j-\frac{1}{2}} - \tilde{G}_{i,j+\frac{1}{2}}]\,. \tag{23}$$

To obtain second-order accuracy we simply alternate the sweep directions at each time step, taking care that during the first sweep f is differenced implicitly and that during the second sweep f is differenced explicitly.

2.2.2 A Second-Order Unsplit Advection Algorithm In many cases one will obtain satisfactory results with the second-order fractional step method described above. However, for some problems, such as unstable displacements in porous media, fractional step methods can distort the interface (e.g., see the discussion in [6] and the references therein). A characteristic feature of this problem is the so-called "push-pull" or "staircase" phenomenon. For problems such as these it is preferable to use an unsplit advection algorithm. In this work we have used an unsplit, volume-of-fluid advection algorithm due to Pilliod [39, 40] that is based on an unsplit advection algorithm for scalar hyperbolic conservation laws due to Bell, Dawson, and Shubin [6].

We wish to use the conservative finite difference formula (14) to solve the conservation law (8). To illustrate our approach we assume that $u > 0$ and $v > 0$ and describe how to determine the flux $F_{i+\frac{1}{2},j}$. The other cases are analogous. The flux through the right-hand edge of the i, jth cell in the time interval (t^n, t^{n+1}) is

$$\begin{aligned} F_{i+\frac{1}{2},j} &= \int_{t^n}^{t^{n+1}} \int_{(j-1/2)h}^{(j+1/2)h} u(x,y,t)\, f(x_{i+\frac{1}{2},j}, y, t)\, dy\, dt \\ &= u_{i+\frac{1}{2},j} \int_{t^n}^{t^{n+1}} \int_{(j-1/2)h}^{(j+1/2)h} f(x_{i+\frac{1}{2},j}, y, t)\, dy\, dt\,. \end{aligned} \tag{24}$$

where we have assumed that in our numerical discretization $u_{i+\frac{1}{2},j}$ is constant on the space time interval $(y_{i,j-\frac{1}{2}}, y_{i,j+\frac{1}{2}}) \times (t^n, t^{n+1})$. This integral is the amount of dark fluid in the space-time rectangle $BCEF$ shown in Fig. 2. We can find this volume by tracing back along the characteristics that originate from the rectangle. This gives us the solid region defined by the points $ABCEFGH$ shown in Fig. 2.

This solid is the prism $ABCDEF$, minus the tetrahedron $DEFG$, plus the tetrahedron $ABCH$. We approximate the flux $F_{i+\frac{1}{2},j}$ in (24) by integrating (8) over the prism and integrating by parts. Writing (8) in the form

$$f_t + u_x f + u f_x + (v f)_y = 0\,, \tag{25}$$

and setting $u = u_{i+\frac{1}{2},j}$ and $u_x = (u_x)_{i,j}$ we find that,

$$\int\int\int_{ABCDEF} (f_t + (u_x)_{i,j} f + u_{i+\frac{1}{2},j} f_x + (vf)_y)\, dx\, dy\, dt = 0\,. \tag{26}$$

Integrating the above expression by parts, and noting that $u_{i+\frac{1}{2},j}$ is constant, we find that the flux $F_{i+\frac{1}{2},j}$ is given by

$$\begin{aligned} F_{i+\frac{1}{2},j} = \int\int_{ABDE} f\, dx\, dy &+ \int\int_{ABC} v\, f\, dx\, dt \\ &- \int\int_{DEF} v\, f\, dx\, dt + \int\int\int_{ABCDEF} (u_x)_{i,j}\, f\, dx\, dy\, dt\,. \end{aligned} \tag{27}$$

The integral over $ABDE$ is the volume of dark fluid in this rectangle. In order to evaluate this volume we use the LVIRA algorithm to determine an approximation to the interface in the (i, j)th cell and then compute the area of the intersection of the dark fluid with rectangle $ABDE$. Now let R_1 be the ratio of the volume of dark fluid in $ABDE$ to the area of $ABDE$, and let V_1 be the volume of the prism $ABCDEF$. The volume integral in (27) is approximately

$$\int\int\int_{ABCDEF} (u_x)_{i,j}\, f\, dx\, dy\, dt \approx R_1\, V_1\, (u_x)_{i,j}.$$

Next we explain how to evaluate the integral over DEF. The domain of dependence of DEF is the triangle DEG. The tetrahedron $DEFG$ is related to the triangle DEF through

$$\int\int_{DEF} f\,dx\,dt \;=\; \int\int_{DEG} f\,dx\,dy \;+\; \int\int\int_{DEFG} ((u_x)_{i,j} \;+\; (v_y)_{i,j})\, f\,dx\,dy\,dt\,. \tag{28}$$

The integral over DEG is the volume of dark fluid in the triangle DEG. In order to evaluate the volume of dark fluid in DEG we use the LVIRA algorithm to determine an approximation to the interface in the (i,j)th cell and then compute the area of the intersection of the dark fluid with triangle DEG.

Let R_2 be the ratio of the volume of dark fluid in DEG to the area of DEG, and let V_2 be the volume of the tetrahedron $DEFG$. Then the volume integral in (28) is approximately

$$\int\int\int_{DEFG} \big((u_x)_{i,j} \;+\; (v_y)_{i,j}\big)\, f\,dx\,dy\,dt \;=\; R_2\, V_2\big((u_x)_{i,j} \;+\; (v_y)_{i,j}\big)\,,$$

which, by (13),is approximately zero. The integral over ABC is performed similarly. Thus we are able to evaluate each term of (27), and hence determine the flux of dark fluid through the right edge of the cell.

Note that if $v_{i,j+\frac{1}{2}} < 0$, then the point G will lie in the $(i, j+1)$th cell. Thus the tetrahedron $DEFG$ will lie in the $(i, j+1)$th cell instead of the (i,j)th cell. In this case we add the tetrahedron $DEFG$ to the prism $ABCDEF$, instead of subtracting it as we did above. Thus in (27) we add the integral over DEF instead of subtracting it. In order to avoid the distorted region that arises when $u_{i+\frac{1}{2},j}$ and $u_{i+\frac{1}{2},j+1}$ are of opposite sign we determine the x-coordinate of the vertex G by

$$x \;=\; \min(i\,\Delta x \;+\; \frac{\Delta x}{2}, i\,\Delta x \;+\; \frac{\Delta x}{2} \;-\; \Delta t\, u_{i+\frac{1}{2},j+1})\,.$$

Thus we are assured that if $v_{i,j+\frac{1}{2}} < 0$ then G lies in the $(i, j+1)$th cell. In addition to simplifying the procedure, the presence of shear indicated by the sign change in the velocity makes the implicit assumption of a zero velocity at the cell corner reasonable.

3. The Variable Density Projection Method

3.1 The Equations of Motion We solve the variable density Navier-Stokes equations subject to the incompressibility constraint, together with advection equations for density and viscosity.

$$U_t + (U\cdot\nabla)U \;=\; \frac{1}{\rho}\left(\nabla\cdot(2\mu\mathcal{D}) - \nabla p + \mathbf{F}\right)\,, \tag{29}$$

$$\nabla\cdot U \;=\; 0\,, \tag{30}$$

$$\rho_t + (U\cdot\nabla)\rho \;=\; 0\,, \tag{31}$$

$$\mu_t + (U\cdot\nabla)\mu \;=\; 0\,. \tag{32}$$

Here $U = (u(x,y,t), v(x,y,t))$ is the velocity, $p = p(x,y,t)$ is the hydrodynamic pressure, $\rho = \rho(x,y,t)$ is the density, $\mu = \mu(x,y,t)$ is the dynamic viscosity, $\mathbf{F}$ represents body forces such as gravity, and $\mathcal{D}$ is the viscous stress tensor, $\mathcal{D} = 1/2(\nabla U + \nabla U^T)$.

We describe the algorithm for approximating solutions of (29)-(32) with Dirichlet boundary conditions on velocity and uniform grid spacing, $\Delta x = \Delta y = h$. Our strategy for solving the above system of equations is a fractional step scheme having four parts: solving the momentum equation (29) for velocity using a lagged pressure gradient, advancing the volume fractions via the procedure described in §2, using this information to reconstruct the density and dynamic viscosity by volume weighting

$$\rho_{i,j} = f_{i,j}\,\rho_1 + (1 - f_{i,j})\,\rho_2\,, \tag{33}$$

$$\mu_{i,j} = f_{i,j}\,\mu_1 + (1 - f_{i,j})\,\mu_2\,, \tag{34}$$

and projecting the intermediate velocity field onto the space of approximately discretely divergence-free vector fields. Here ρ_1 and ρ_2 are the densities of the "dark" and "light" fluids, respectively.

In the "advection-diffusion step", we solve

$$\frac{U^* - U^n}{\Delta t} = -\left[(U\cdot\nabla)U\right]^{n+\frac{1}{2}} + \frac{1}{\rho^{n+\frac{1}{2}}}\left((\mathcal{L}_h^* + \mathcal{L}_h^n) - \nabla p^{n-\frac{1}{2}} + \mathbf{F}^{n+\frac{1}{2}}\right) \tag{35}$$

for the intermediate velocity U^*, where $\mathcal{L}_h$ is a second-order finite difference approximation to $\nabla\cdot(\mu\mathcal{D})$. The nonlinear advection terms $[(U\cdot\nabla)U]^{n+\frac{1}{2}}$, are evaluated using an explicit predictor-corrector scheme and require only the available data at t^n. The density, ρ, and viscosity, μ, are constructed from the volume fractions calculated at time $t^{n+\frac{1}{2}}$ in the interface tracking step using the predicted velocities at cell edges obtained in the process of differencing $[(U\cdot\nabla)U]^{n+\frac{1}{2}}$. The lagged pressure gradient $\nabla p^{n-\frac{1}{2}}$, and force, $\mathbf{F}^{n+\frac{1}{2}}$, are treated as source terms. Because the viscosity coefficient, μ, is a function of volume fraction and therefore varies in space, the implicit part of (35) corresponds to a coupled parabolic solve for both velocity components.

The velocity field U^* is not, in general, divergence-free. The projection step of the algorithm decomposes the result of the first step into a scalar multiple of a discrete gradient of a scalar potential (the scalar multiple being the inverse density) and a approximately discretely divergence-free vector field, which correspond, respectively, to an updated pressure gradient term and a new velocity. In particular, if $\mathbf{P}$ represents the approximate projection operator, then

$$\frac{U^{n+1} - U^n}{\Delta t} = \mathbf{P}\left(\frac{U^* - U^n}{\Delta t}\right), \tag{36}$$

$$\frac{1}{\rho^{n+\frac{1}{2}}}\nabla p^{n+\frac{1}{2}} = \frac{1}{\rho^{n+\frac{1}{2}}}\nabla p^{n-\frac{1}{2}} + (\mathbf{I} - \mathbf{P})\left(\frac{U^* - U^n}{\Delta t}\right), \tag{37}$$

Discretization of the advection terms. The discretization of the advection terms in this algorithm is a variable density version of the method discussed by Bell, Colella and Howell [4]. It is a predictor-corrector method based on the unsplit Godunov method introduced by Colella [14]. In the predictor, velocities are extrapolated along characteristics to the cell edges at the new half-time-step level, $t^{n+\frac{1}{2}}$. A MAC projection (e.g., see [4]) is applied to make these edge velocities divergence-free. The volume fractions and velocities are advanced using these edge velocities.

In the predictor we extrapolate the velocity to the cell edges at $t^{n+\frac{1}{2}}$ using a second-order Taylor series expansion in space and time. The time derivative is replaced using (29). For edge $(i+\frac{1}{2},j)$ this gives

$$\begin{aligned} U^{n+\frac{1}{2},L}_{i+\frac{1}{2},j} &= U^n_{ij} + \left(\frac{\Delta x}{2} - \frac{u_{ij}\,\Delta t}{2}\right) U^n_{x,ij} - \frac{\Delta t}{2}\left(\widehat{vU_y}\right)_{ij} \\ &+ \frac{1}{\rho^n_{ij}}\frac{\Delta t}{2}\left(\mathcal{L}^n_{ij} - Gp^{n-\frac{1}{2}}_{ij} + \mathbf{F}^n_{ij}\right) \end{aligned} \tag{38}$$

extrapolated from cell (i,j), and

$$\begin{aligned} U^{n+\frac{1}{2},R}_{i+\frac{1}{2},j} &= U^n_{i+1,j} - \left(\frac{\Delta x}{2} + \frac{u_{i+1,j}\,\Delta t}{2}\right) U^n_{x,i+1,j} - \frac{\Delta t}{2}\left(\widehat{vU_y}\right)_{i+1,j} \\ &+ \frac{1}{\rho^n_{i+1,j}}\frac{\Delta t}{2}\left(\mathcal{L}^n_{i+1,j} - Gp^{n-\frac{1}{2}}_{i+1,j} + \mathbf{F}^n_{i+1,j}\right) \end{aligned} \tag{39}$$

extrapolated from cell $(i+1,j)$. Here and in what follows, D and G represent discrete approximations to the divergence and gradient operators, respectively.

Analogous formulae are used to predict values at each of the other edges of the cell. In evaluating these terms the first-order derivatives normal to the edge (in this case U_x) are evaluated using a monotonicity-limited fourth-order slope approximation [13]. The limiting is done on the components of the velocity individually.

The transverse derivative terms ($\widehat{vU_y}$ above) are evaluated as in [4], by first extrapolating from above and below to construct edge states, using normal derivatives only, and then choosing between these states using the upwinding procedure defined below. In particular, we define

$$\begin{aligned} \widehat{U}^B_{i,j+\frac{1}{2}} &= U^n_{ij} + \left(\frac{\Delta y}{2} - \frac{v_{ij}\,\Delta t}{2}\right) U^n_{y,ij}, \\ \widehat{U}^T_{i,j+\frac{1}{2}} &= U^n_{i,j+1} - \left(\frac{\Delta y}{2} + \frac{v_{i,j+1}\,\Delta t}{2}\right) U^n_{y,i,j+1}, \end{aligned}$$

where U_y are limited slopes in the y direction, with similar formulae for the lower edge of cell $B_{i,j}$. In this upwinding procedure we first define the normal velocity on the edge:

$$\widehat{v}^{adv}_{i,j+\frac{1}{2}} = \begin{cases} \widehat{v}^B & \text{if } \widehat{v}^B > 0,\ \ \widehat{v}^B + \widehat{v}^T > 0, \\ 0 & \text{if } \widehat{v}^B \le 0, \widehat{v}^T \ge 0 \text{ or } \widehat{v}^B + \widehat{v}^T = 0, \\ \widehat{v}^T & \text{if } \widehat{v}^T < 0,\ \ \widehat{v}^B + \widehat{v}^T < 0. \end{cases}$$

(Here and in the next equation we suppress the $i, j+\frac{1}{2}$ spatial indices on bottom and top states.) We now upwind $\widehat{U}$ based on $\widehat{v}^{adv}_{i,j+\frac{1}{2}}$:

$$\widehat{U}_{i,j+\frac{1}{2}} = \begin{cases} \widehat{U}^B & \text{if } \widehat{v}^{adv}_{i,j+\frac{1}{2}} > 0, \\ 1/2(\widehat{U}^B + \widehat{U}^T) & \text{if } \widehat{v}^{adv}_{i,j+\frac{1}{2}} = 0, \\ \widehat{U}^T & \text{if } \widehat{v}^{adv}_{i,j+\frac{1}{2}} < 0. \end{cases}$$

After constructing $\widehat{U}_{i,j-\frac{1}{2}}$ in a similar manner, we use these upwind values to form the transverse derivative in (38),

$$(\widehat{vU_y})_{ij} = \frac{1}{2\,\Delta y}(\widehat{v}^{adv}_{i,j+\frac{1}{2}} + \widehat{v}^{adv}_{i,j-\frac{1}{2}})(\widehat{U}_{i,j+\frac{1}{2}} - \widehat{U}_{i,j-\frac{1}{2}}).$$

We use a similar upwinding procedure to choose the appropriate states $U_{i+\frac{1}{2},j}$ given the left and right states, $U^{n+\frac{1}{2},L}_{i+\frac{1}{2},j}$ and $U^{n+\frac{1}{2},R}_{i+\frac{1}{2},j}$:

$$U_{i+\frac{1}{2},j} = \begin{cases} U^L & \text{if } u^L > 0 \text{ and } u^L + u^R > 0, \\ 1/2(U^L + U^R) & \text{if } u^L \le 0, u^R \ge 0 \text{ or } u^L + u^R = 0, \\ U^R & \text{if } u^R < 0 \text{ and } u^L + u^R < 0, \end{cases}$$

where we have again suppressed the spatial indices $i + \frac{1}{2}, j$. We follow a similar procedure to construct $U_{i-\frac{1}{2},j}$, $U_{i,j+\frac{1}{2}}$, and $U_{i,j-\frac{1}{2}}$.

In general the normal velocities at the edges are not divergence-free; in order to make these velocities divergence-free we apply the MAC projection [4] before construction of the convective derivatives. The equation

$$D^{MAC}(\frac{1}{\rho^n}G^{MAC}\phi) = D^{MAC}U^{n+\frac{1}{2}}$$

is solved for ϕ, where

$$D^{MAC}U^{n+\frac{1}{2}} = (\frac{u^{n+\frac{1}{2}}_{i+\frac{1}{2},j} - u^{n+\frac{1}{2}}_{i-\frac{1}{2},j}}{\Delta x} + \frac{v^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} - v^{n+\frac{1}{2}}_{i,j-\frac{1}{2}}}{\Delta y}),$$

and

$$(G^{MAC}\phi)^x_{i+\frac{1}{2},j} = \frac{\phi_{i+1,j} - \phi_{i,j}}{\Delta x},$$
$$(G^{MAC}\phi)^y_{i,j+\frac{1}{2}} = \frac{\phi_{i,j+1} - \phi_{i,j}}{\Delta y}.$$

We then define advection velocities by

$$u^{ADV}_{i+\frac{1}{2},j} := u^{n+\frac{1}{2}}_{i+\frac{1}{2},j} - \frac{1}{\rho^n_{i+\frac{1}{2},j}}(G^{MAC}\phi)^x_{i+\frac{1}{2},j},$$
$$v^{ADV}_{i,j+\frac{1}{2}} := v^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} - \frac{1}{\rho^n_{i,j+\frac{1}{2}}}(G^{MAC}\phi)^y_{i,j+\frac{1}{2}},$$

where $\rho_{i+\frac{1}{2},j}$ and $\rho_{i,j+\frac{1}{2}}$ are defined by

$$\frac{1}{\rho_{i+\frac{1}{2},j}} \equiv \frac{1}{2}(\frac{1}{\rho_{i,j}} + \frac{1}{\rho_{i+1,j}}),$$
$$\frac{1}{\rho_{i,j+\frac{1}{2}}} \equiv \frac{1}{2}(\frac{1}{\rho_{i,j}} + \frac{1}{\rho_{i,j+1}}).$$

In the corrector step, we form an approximation to the convective derivatives in (29)

$$[(U\cdot\nabla)U]^{n+\frac{1}{2}} = \frac{1}{2\Delta x}(u^{ADV}_{i+\frac{1}{2},j} + u^{ADV}_{i-\frac{1}{2},j})(U^{n+\frac{1}{2}}_{i+\frac{1}{2},j} - U^{n+\frac{1}{2}}_{i-\frac{1}{2},j}) + \frac{1}{2\Delta y}(v^{ADV}_{i,j+\frac{1}{2}} + v^{ADV}_{i,j-\frac{1}{2}})(U^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} - U^{n+\frac{1}{2}}_{i,j-\frac{1}{2}}).$$

The CFL Constraint In this method there are two sources of a CFL-like constraint: the volume-of-fluid advection algorithm and the differencing of the nonlinear advection terms in (29). It is apparent from geometric considerations that one must choose the CFL number σ in the volume-of-fluid advection step so that the amount of fluid which leaves a cell in one time step is no more than the amount of fluid that was originally in the cell. In other words, one must choose σ so that

$$V_{i+1/2,j} - V_{i-1/2,j} \leq f_{i,j} \; \Delta x \; \Delta y \tag{40}$$

for all i, j where $V_{i+1/2,j}$ is the volume of dark fluid which crosses the right hand edge of the i,jth cell in one time step. One way to ensure that (40) is always satisfied is to choose $\sigma \in (0,1]$ so that,

$$|u^n_{i+\frac{1}{2},j}| \; \Delta t \; \leq \; \Delta x \, /2 \qquad \text{and} \qquad |v^n_{i,j+\frac{1}{2}}| \; \Delta t \; \leq \; \Delta y \, /2 \qquad \text{for all} \, i \, , \, j \, . \tag{41}$$

Our method of differencing the nonlinear advection terms in (29) is an explicit difference scheme and therefore also requires a time-step restriction; however, this condition is less restrictive than (41) so we use that condition to set the time step.

3.2 The Approximate projection Since the velocity is defined at cell centers, the projection used to enforce incompressibility at time t^{n+1} must include a divergence operator which acts on cell-centered quantities, unlike the MAC projection. The projection we use here is approximate in the sense that $\mathbf{P^2} \neq \mathbf{P}$. This approximate projection uses a standard finite element basis for representing the pressure so that the linear system that is solved during the projection step corresponds to the system that is solved using bilinear finite element methods for Poisson problems. The introduction of this approach to the projection, as well as the motivation for using an approximate rather than exact projection, is described in detail in [2] for the constant density case; here we extend the discussion to include variable density.

We consider the scalar pressure field to be a C^0 function that is bilinear over each cell; i.e., the pressure is in $S^h = M^1_0(x) \otimes M^1_0(y)$ where $M^t_s(x)$ is the space of polynomials of degree t in the x direction on each cell with C^s continuity at x-edges. For the velocity space we define

$$\mathbf{V}^h = \mathbf{V}^{h,x} \;\times\; \mathbf{V}^{h,y}$$

where $\mathbf{V}^{h,x} = M^0_{-1}(x) \otimes M^1_{-1}(y)$ and $\mathbf{V}^{h,y} = M^1_{-1}(x) \otimes M^0_{-1}(y)$, i.e., u is piecewise constant in x and a discontinuous linear function of y in each cell, with a similar form for v.

For use in the predictor and corrector, the velocity and pressure gradient are considered to be average values over each cell. The vector space, $\mathbf{V}^h$, contains additional functions that represent the linear variation within each cell. These additional degrees of freedom make $\mathbf{V}^h$ large enough to contain $\nabla \phi$ for $\phi \in S^h$. We establish a correspondence between these two representations by introducing an orthogonal decomposition of $\mathbf{V}^h$. In particular, for each vector field $V \in \mathbf{V}^h$ we define a piecewise constant component $\overline{V}_{ij}$ and the variation $V^\perp = V - \overline{V}$ so that for each cell $B_{i,j}$, $\int_{B_{i,j}} V^\perp d\mathbf{x} = 0$. By construction these two components are orthogonal in L^2 so they can be used to define a decomposition of $\mathbf{V}^h$ into two components,

$$\mathbf{V}^h = \overline{\mathbf{V}}^h \oplus \mathbf{V}^{h^\perp}$$

where $\overline{\mathbf{V}}^h$ and $\mathbf{V}^{h^\perp}$ represent the cell averages and the orthogonal linear variations, respectively. The decomposition of $\mathbf{V}^h$ induces a decomposition of $\nabla\phi$ for all $\phi \in S^h$; namely,

$$(\nabla\phi)_{ij} = (\overline{\nabla\phi})_{ij} + (\nabla\phi)^\perp_{ij}.$$

We now define a weak form of the projection on $\mathbf{V}^h$, based on a weak divergence on $\mathbf{V}^h$. In particular, we define a vector field V^d in $\mathbf{V}^h$ to be divergence-free in the domain Ω if

$$\int_\Omega V^d \cdot \nabla\psi \, d\mathbf{x} = 0 \qquad \forall \psi \in S^h.$$

With this definition we can then project any vector field V into an inverse-density-weighted gradient $\frac{1}{\rho}\nabla\phi$ and weakly divergence-free field V^d (with vanishing normal velocities on boundaries) by solving

$$\int_\Omega \frac{1}{\rho}\nabla\phi(\mathbf{x}) \cdot \nabla\psi_{i+1/2,j+1/2}(\mathbf{x})\, d\mathbf{x} = \int_\Omega V \cdot \nabla\psi_{i+1/2,j+1/2}(\mathbf{x})\, d\mathbf{x} \qquad \forall \psi_{i+1/2,j+1/2}(\mathbf{x}) \tag{42}$$

for $\phi(\mathbf{x}) = \sum \phi_{i+1/2,j+1/2}\psi_{i+1/2,j+1/2}(\mathbf{x})$, and setting $V^d = V - \frac{1}{\rho}\nabla\phi$. Here the ψ's are the standard basis functions for S^h, namely $\psi_{i+1/2,j+1/2}(\mathbf{x})$ is the piecewise bilinear function having node values

$$\psi_{i+1/2,j+1/2}(\mathbf{x}_{k+1/2,\ell+1/2}) = \delta_{ik}\delta_{j\ell}\,.$$

The density ρ is considered to be constant over each cell $B_{i,j}$.

For the purposes of the fractional step scheme we define $\overline{V}_{i,j}$ as the approximation to $(U^* - U^n)/\Delta t$ in (35) and

$$\overline{V}^d_{i,j} = \overline{V}_{i,j} - \frac{1}{\Lambda_{i,j}}\int_{B_{i,j}} \frac{1}{\rho_{i,j}}(\nabla\phi)_{i,j}\, dx\, dy = \overline{V}_{i,j} - \frac{1}{\rho_{i,j}}(\overline{\nabla\phi})_{i,j}$$

as the approximation to $(U^{n+1} - U^n)/\Delta t$ in (36). Here $\Lambda_{i,j}$ denotes the volume of $B_{i,j}$ and $\phi_{i,j}$ is the approximation to the update for p; i.e., $\phi(\mathbf{x}) = \delta p^n \equiv p^{n+\frac{1}{2}} - p^{n-\frac{1}{2}}$.

The left-hand-side of equation (42) is, in discrete form, a nine-point stencil approximating the Laplacian of ϕ,

$$\begin{aligned}
(D\frac{1}{\rho}G\phi)_{i+1/2,j+1/2} \;=\; \frac{1}{6h^2}\Big(&\frac{1}{\rho_{i,j}}(2\phi_{i-1/2,j-1/2} + \phi_{i+1/2,j-1/2} + \phi_{i-1/2,j+1/2} - 4\phi_{i+1/2,j+1/2}) + \\
&\frac{1}{\rho_{i,j+1}}(2\phi_{i-1/2,j+3/2} + \phi_{i+1/2,j+3/2} + \phi_{i-1/2,j+1/2} - 4\phi_{i+1/2,j+1/2}) + \\
&\frac{1}{\rho_{i+1,j}}(2\phi_{i+3/2,j-1/2} + \phi_{i+1/2,j-1/2} + \phi_{i+3/2,j+1/2} - 4\phi_{i+1/2,j+1/2}) + \\
&\frac{1}{\rho_{i+1,j+1}}(2\phi_{i+3/2,j+3/2} + \phi_{i+1/2,j+3/2} + \phi_{i+3/2,j+1/2} - 4\phi_{i+1/2,j+1/2})\Big)
\end{aligned}$$

and the right-hand-side, for $V = \overline{V}$, is a standard four-point divergence stencil:

$$(D\overline{V})_{i+1/2,j+1/2} = \frac{V^x{}_{i+1,j} + V^x{}_{i+1,j+1} - V^x{}_{i,j} - V^x{}_{i,j+1}}{2\,\Delta x} + \frac{V^y{}_{i,j+1} + V^y{}_{i+1,j+1} - V^y{}_{i,j} - V^y{}_{i+1,j}}{2\,\Delta y}$$

where V^x and V^y are the x- and y-components of V, respectively.

The resulting linear system can be solved using standard multigrid methods (see [8]). In particular, we have used the standard V-cycle with Gauss-Seidel relaxation. In the presence of large density jumps, however, the standard multigrid solver can require an unreasonably large number of iterations to reach convergence (see [1], e.g., for an explanation). For these cases we use a multigrid preconditioned conjugate gradient solver with two Jacobi relaxations per level in the V-cycle preconditioner [53]. In the Rayleigh-Taylor computations shown below we observed typical improvements of 100 cycles reduced to 15. Although there is more work per iteration in the multigrid preconditioned conjugate gradient method than in the standard multigrid method, the improvement in CPU time was still significant.

4. Computational Results

In this section we demonstrate the convergence properties of both the operator-split and unsplit versions of the method and apply the unsplit version to several realistic problems. We do note that for these type of unstable interface problems the numerics are sensitive to the time step control, particularly on coarse grids where the viscous length scales are not fully resolved. In particular, for the more complex examples we have had to reduce the CFL parameter σ to 0.1 to obtain satisfactory results. For the types of unstable interface problems being considered this more restrictive time step appears to be necessary to prevent growth of parasitic numerical modes.

4.1 Rayleigh-Taylor Computations – Short Time The first numerical examples we compute are Rayleigh-Taylor instabilities with viscosity in order to demonstrate numerical convergence of the method. For the first case we consider the example treated by Bell and Marcus [7]. In this problem a heavy fluid lies above a light fluid in a rectangle 1 m wide by 4 m tall. The densities of the two fluids are $1.225\,kg\,/\,m^3$ and $0.1694\,kg\,/\,m^3$ while the dynamic viscosity of each fluid is $3.1304952 \times 10^{-3}\,kg\,/\,m\,s$. The interface is initially a sine wave with amplitude 5 cm. For this case since the viscosities are equal the velocities are expected to be continuously differentiable but not C^2. We compute to time 0.25 using a fixed time step that satisfies the stability requirement on three different grids, 32×128, 64×256 and 128×512. By comparing the difference in the solutions on grids of adjacent resolution we can approximate the L^1 error in the coarser grid. We then use these estimates of the error to compute numerical convergence rates. For this problem, for volume fraction we obtain a convergence rate of 1.81 for the split volume advection algorithm and 1.77 for the unsplit algorithm. For the velocity field we obtain a convergence rate of 1.72 for the split algorithm and 1.76 for the unsplit algorithm. These rates indicate that the method is performing at near its formal second-order accuracy.

Of course, in most problems of real interest the viscosities of the two fluids are different. In this case there is an additional loss of regularity in the solution. In particular, the velocity at the interface is not continuously differentiable; there is a jump in the velocity gradient. To test the convergence in this more realistic regime we consider an air / helium Rayleigh-Taylor instability in a $0.01m \times 0.04m$ domain computing to time 0.025. For this case the viscosities of air and helium are $1.77625 \times 10^{-5} kg/m\ s$ and $1.941 \times 10^{-5} kg/m\ s$, respectively. Performing the same technique for computing convergence rates as in the previous example we obtain rates of 1.22 and 1.19 for the volume fractions for the split and unsplit algorithms, respectively. For velocity we obtain a rate of 0.91 for the split algorithm and 0.87 for the unsplit algorithm. As expected the convergence rates are reduced because of the loss of regularity of the solution; however, the method still performs at near first-order accuracy. In order to achieve second-order accuracy it would be necessary to develop a substantially more sophisticated treatment of the velocity discretization in the neighborhood of the interface; however, that is beyond the scope of this paper.

4.2 A Rayleigh-Taylor Computation – Long Time For the next example we look at a longer time integration of the air / helium Rayleigh Taylor instability problem in the second convergence example. For this example we have selected a relatively coarse grid of 64×256 to illustrate the behavior of the methodology. In Figure 3 we show a time history of the evolution of the interface. We note that what is being plotted here and in Figures 4 and 5 is the actual reconstructed interface, not a contour of volume fraction. The interface is reconstructed for the plotter using exactly the same interface reconstruction algorithm as is used in the time-stepping. The reconstructed interface retains all small features of the flow, and has not been smoothed as is inherent in plotting contours. The result shows the development of the expected mushroom cap even on a relatively coarse grid.

4.3 Bubble For this example we consider the dynamics of a two-dimensional bubble of air in water. The viscosity of air is $1.77625 \times 10^{-5} kg/m\ s$ and the density is $1.225 kg/m^3$. For water the viscosity is $1.1377 \times 10^{-3} kg/m\ s$ and the density if $999.2 kg/m^3$. The computational domain is $0.007m \times 0.014m$ and we have again, for purposes of illustration, used a relatively coarse grid of 64×128. In Fig. 4, we show a time sequence of the reconstructed interface. (We note the that reconstructed interface retains small features of the flow. Contours of volume fraction, which are not shown, provide a considerable smoother representation of the interface.) The lower edge of the bubble accelerates more quickly than the upper edge and the bubble begins to form a torus. As the bubble continues to rise the center of the bubble is stretched until the bubble breaks into two pieces. The sides of the bubble are also highly stretched and are beginning to fragment. (We emphasize that these are two-dimensional bubbles in a confined box so the dynamics are different than radially symmetric bubbles in free space.) This problem illustrates the ability of the method to handle large density and viscosity ratios and changes in topology of the interface. In this case the changes in topology occur from regions of fluid being highly stretched. Although the interface reconstruction loses accuracy for subgrid filaments of fluid the conservative treatment of volume fractions makes the method robust.

4.4 Droplet Splash The final example is another air / water example using the same computational domain and resolution as the previous example. In this case, the initial conditions are a two-dimensional water droplet above an air / water interface. This example illustrates a different type of change in topology, namely, the merging of two independent regions. Note that because droplet is fairly close to the water surface some air bubbles are trapped in the water after the splash. Another feature of the flow is the formation of water waves resulting from the splash moving toward the walls. As before, in spite of the coarse grid the method predicts a smooth interface and handle the change in topology without any difficulty.

5. Conclusions

We have presented a numerical method for approximating solutions of the incompressible Euler and Navier-Stokes equations for two fluids with different densities and viscosities. This method is based on a variable density version of the "approximate" projection method of Almgren et. al [2]. It incorporates the second-order volume-of-fluid interface tracking algorithms of Pilliod and Puckett [40] including an unsplit volume-of-fluid advection algorithm based on the work of Bell, Dawson and Shubin [6]. We have demonstrated that the interface tracking algorithm is non-diffusive and that the interface is maintained as a sharp discontinuity at all times. We have demonstrated numerical convergence of the method for early time computations of viscous Rayleigh-Taylor instabilities. We have also used the method to compute long time evolution of Rayleigh-Taylor instability. Further tests show the behavior of the model for air bubbles in water and water droplets in air and demonstrate the ability of the method to treat difficult problems with large ratios of density and viscosity.

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