DIRECT NUMERICAL SIMULATION
OF FREE-SURFACE AND
INTERFACIAL FLOW

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KEY WORDS: interfaces, free surfaces, surface tension, multiphase flow

1. INTRODUCTION

The numerical simulation of flows with interfaces and free-surface flows is a vast topic, with applications to domains as varied as environment, geophysics, engineering, and fundamental physics.

In engineering, as well as in other disciplines, the study of liquid-gas interfaces is important in combustion problems with liquid and gas reagents. The formation of droplet clouds or sprays that subsequently burn in combustion chambers originates in interfacial instabilities, such as the Kelvin-Helmholtz instability. What can numerical simulations do to improve our understanding of these phenomena? The limitations of numerical techniques make it impossible to consider more than a few droplets or bubbles. They also force us to stay at low Reynolds or Weber numbers, which prevent us from finding a direct solution to the breakup problem. However, these methods are potentially important. First, the continuous improvement of computational power (or, what amounts to the same, the drop in megaflop price) continuously extends the range of affordable problems. Second, and more importantly, the phenomena we consider often happen on scales of space and time where experimental visualization is difficult or impossible. In such cases, numerical simulation may be a useful prod to the intuition of the physicist, the engineer, or the mathematician.

A typical example of interfacial flow is the collision between two liquid droplets. Finding the flow involves the study not only of hydrodynamic fields in the air and water phases but also of the air-water interface. This latter part
is more difficult than the former because the interface is subject to a number of relevant physical phenomena, at scales much smaller than the typical sizes of the droplets. For instance, a major difficulty is caused by the change in interface topology that occurs when the colliding droplets coalesce. This complicates the physics and sharpens the requirements that a numerical method must satisfy in order to resolve the motion in a satisfactory way.

These difficulties are dealt with in a variety of ways, depending on the physical modeling and the numerical methods. First comes a choice of modeling the interface as either a thin or a thick region of space. In engineering problems, such as combustion studies, the interface may be considered a discontinuity of density and pressure as well as of other physical variables. The location of this discontinuity in three-dimensional space will be assumed to be a two-dimensional, twice-differentiable manifold (to simplify, a smooth surface $S$) that evolves according to predetermined rules.

The second choice is to decide which forces and thermal effects to model. The main thrust of this review is as follows. In the bulk of the fluids, we restrict ourselves to viscosity, constant in each phase, and perhaps gravity. On interfaces, we assume a constant surface tension. Our physical assumptions thus lead us to a version of the Navier-Stokes equation, with variable density and viscosity and capillary tension on $S$. This should be contrasted with both a more elementary approach, in which only perfect fluids are considered, and many more complex approaches, where more realistic theories of interfaces or other transport effects (involving temperature, passive scalars, and surface-active substances) are considered.

Once this framework is set, we attack the subject matter of this review: simulation methods for the Navier-Stokes equation with interfaces. On one hand the numerical methods are analogous to otherwise well-known methods in the bulk of the phases, such as finite elements, finite volumes, and finite differences. On the other hand, there are specific problems due to the presence of the interface: location of the discontinuity and computation of surface stresses.

From this point of view the various methods for interface simulation can be divided into two great classes, depending on the nature, fixed or moving, of the grid used in the bulk of the phases. In fixed-grid methods, there is a predefined grid that does not move with the interface. The interface has to somehow cut across this fixed grid. As shown in Figures 1 and 2, this fixed grid may be either structured or unstructured. In moving-grid methods, the interface is a boundary between two subdomains of the grid. The interface then identifies, at some order of approximation, with element boundaries. Again, the grid may be structured and even near-orthogonal or more general. This simplifies the analysis near the interface. However, when the interface undergoes large deformations, the grid has to be remeshed. Other complications may occur, especially when the
Figure 1  An interface cutting across a fixed, structured grid.

topology changes. In addition to the moving-grid and fixed-grid methods, there
are special cases, such as particle methods, in which grids are not needed.

In this article we emphasize fixed-grid methods. These are more interesting
because of their relatively simple description and greater ease of program-
ming. Easier extension to three dimensions of space is one of the principal

Figure 2  An interface cutting across a fixed, unstructured grid.
advantages expected from this simplified formulation. Moreover, much of this paper is concerned with so-called volume-of-fluid (VOF) methods. Many commercially available codes use this method to represent interfaces: SOLA-VOF (Nichols et al. 1980), NASA-VOF2D (Torrey et al. 1985), NASA-VOF3D (Torrey et al. 1987), RIPPLE (Kothe & Mjolsness 1992), and FLOW3D (Hirt & Nichols 1988).

This review remains at an introductory level. The reader may read with profit other reviews and books (i.e. Floryan & Rasmussen 1989, Shyy et al. 1996, Sethian 1996, Rothman & Zaleski 1997). The review by McHyman (1984) is particularly clear, pleasant to read, and refreshing, as well as informative to the novice practitioner.

A great deal of useful information may be found on a variety of World Wide Web sites. It is difficult to provide a pointer to the rapidly evolving list of these sites. However, useful information and links may be found on our site (http://www.lmm.jussieu.fr/~zaleski/zaleski.html).

This review reflects our personal point of view: Some aspects of the subject have been emphasized; others have been omitted. For instance, interface simulation using boundary integral methods is not described in detail; only relevant references are given below. Similarly, lattice-gas and Boltzmann lattice-gas methods are described in other reviews and books (i.e. Rothman & Zaleski 1994, 1997; Benzi et al. 1992). The same holds for level-set methods (Sussman et al. 1994, Sethian 1996, Sussman & Smereka 1997).

2. PHYSICAL MODELING OF INTERFACES

The study of interfaces starts when equilibrium thermodynamics takes into account spatial inhomogeneities. Consider two pure phases such as water and oil. Oil and water do not mix: The equilibrium state of the mixture in a flask consists of two layers of liquid separated by a thin region called the interface.

2.1 Interface Description

There are many ways in which the geometrical interface $S$ may be defined. The simplest one is to define a height function $h$. We then get the equation $z = h(x, y, t)$. This describes the interface satisfactorily whenever $h$ is single-valued. Alternatively, one may define the phase-characteristic function $\chi$ with $\chi = 1$ in phase 1 and $\chi = 0$ in phase 2. For instance, when $h$ is single-valued, we may take $\chi(x, y, z, t) = H[z - h(x, y, t)]$, where $H$ is the Heaviside step function. Then phase 1 fills the $z > h$ region and phase 2 the $z < h$ region. A short discussion of several equations for interface motion may be found in Whitham (1974). Here we simply remark that evolution of the interface $S$ is defined by its normal velocity $V$ on each point of $S$. We also note $n$, the unit normal to the interface.
The normal velocity is related to the fluid velocity field $\mathbf{u}$ in various ways. In the simplest case, without phase change, one assumes continuity of fluid velocity

$$\mathbf{u}_1 = \mathbf{u}_2. \quad (1)$$

(We note in general $x_i$, the limiting values of a variable $x$ when the interface is approached from phase $i$.) This may be written in jump notation, i.e. the notation $[x] = x_2 - x_1$:

$$[\mathbf{u}]_S = 0. \quad (2)$$

The interface velocity is then the normal velocity, the same on both sides of the interface:

$$V = \mathbf{u}_1 \cdot \mathbf{n} = \mathbf{u}_2 \cdot \mathbf{n}. \quad (3)$$

In the case of evaporation, or more generally phase change, there may be a mass flow $q$ from phase 1 to phase 2. This mass flow is connected to the velocities on both sides of the interface in the following way. Consider the frame of reference where the interface is at rest. The normal velocities in that frame of reference are $u' = \mathbf{u} \cdot \mathbf{n} - V$. The mass flow is the amount of mass that goes from phase 1 to phase 2, and it must be the same on both sides of the interface by conservation of mass (the Rankine-Hugoniot condition):

$$\rho_1 u'_1 = \rho_2 u'_2 = q. \quad (4)$$

Then, in the general frame of reference,

$$\rho_1 (\mathbf{u}_1 \cdot \mathbf{n} - V) = \rho_2 (\mathbf{u}_2 \cdot \mathbf{n} - V) = q. \quad (5)$$

Thus, if there is no phase change, i.e. $q = 0$, one recovers Equation 3, which now appears clearly to be a consequence of mass conservation. The continuity of tangential velocities $[\mathbf{u}_t] = \mathbf{u}_t - (\mathbf{u} \cdot \mathbf{n})\mathbf{n}$, on the other hand, is a physical assumption akin to the assumption that the slip velocity on a solid wall vanishes.

Then interface motion may be described in weak form by

$$\partial_t \chi + V \mathbf{n} \cdot \nabla \chi = 0, \quad (6)$$

which in the no-phase-change case amounts to

$$\partial_t \chi + \mathbf{u} \cdot \nabla \chi = 0. \quad (7)$$

(Notice that $\nabla \chi = \mathbf{n} \delta_S$.) Here we use a weak formulation of the partial differential equation (PDE), since derivatives of the discontinuous function $\chi$ are singular. In this weak formulation, the PDE is interpreted by the space integrals of Equation 7. In other words, the function cannot be differentiated, but integrals of Equation 7 are well-defined: They express volume evolution and correspond to interface motion with velocity $V$. 

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2.2 *Navier-Stokes Equation: Whole-Domain Formulation*

We now consider the incompressible flow of two immiscible liquids. The whole flow fills a domain $\Omega$. This domain may be decomposed into any number of subdomains filled with the individual phases. However, in this paragraph we express the Navier-Stokes equation over the whole domain $\Omega$. Incompressibility implies the divergence free condition

$$\nabla \cdot \mathbf{u} = 0. \tag{8}$$

The momentum balance is modeled by the Navier-Stokes equation,

$$\rho (\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla p + 2\nabla \cdot \mathbf{D} + 2\sigma \kappa \delta_S \mathbf{n}, \tag{9}$$

where $\rho$ is the density and $\mu$ the dynamical viscosity. These are two physical properties of the bulk phases that may have discontinuities across phase boundaries. The rate-of-strain tensor is $\mathbf{D}$:

$$D_{ij} = \frac{1}{2} \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right). \tag{10}$$

In these equations, the term $2\sigma \kappa \delta_S \mathbf{n}$ represents capillary forces, with a surface tension $\sigma$ and $\mathbf{n}$ is again the unit normal to the interface. The mean curvature is $\kappa = (1/r_1 + 1/r_2)/2$. It may also be expressed as

$$\kappa = -\frac{1}{2} \nabla_S \cdot \mathbf{n}, \tag{11}$$

where $\nabla_S$ is the gradient operator restricted to the surface $S$.

2.3 *Whole-Domain Conservation Law Form*

We may also rewrite the Navier-Stokes equation as a set of conservation laws. Conservation of momentum is then obvious. In particular, capillary effects may be represented by a tensor $\mathbf{T}$. This tensor is tangent to the interface and is given by

$$\mathbf{T} = -\sigma (1 - \mathbf{n} \otimes \mathbf{n}) \delta_S, \tag{12}$$

where $1$ is the kronecker symbol tensor $\delta_{ij}$.

One may show that the capillary force may be written (Lafaurie et al 1994)

$$2\sigma \kappa \mathbf{n} \delta_S = -\nabla \cdot \mathbf{T}, \tag{13}$$

with the equivalence of Equation 9 in conservative form

$$\partial_t (\rho \mathbf{u}) = -\nabla \cdot (\rho \mathbf{1} + \rho \mathbf{u} \otimes \mathbf{u} + \mathbf{T} - 2\mu \mathbf{D}). \tag{14}$$
2.4 *Navier-Stokes Equation: Jump-Condition Form*

Another useful formulation of the momentum-balance equation decomposes the problem into any number of bulk-phase domains within which the usual, nonsingular Navier-Stokes equation holds; for the interface between domains, some quantities are required to be continuous, whereas others are required to have specific jumps.

The jumps result from a balance between the singular terms in the whole-domain formulation. Balancing the most singular terms in Equations 9 or 14 leads to

\[
[-p I + 2\mu D]_S \cdot n = 2\sigma \kappa n.
\]

This condition may be split into a normal and tangential stress condition

\[
[-p + 2\mu n \cdot D \cdot n]_S = 2\sigma \kappa,
\]

\[
[\mu t^{(k)} \cdot D \cdot n]_S = 0
\]

where the vectors \(t^k\) may be any set of \(d-1\) independent tangent (to \(S\)) vectors, and \(d\) is the dimension of space.

Away from the interface, Equation 9 takes the usual form

\[
\partial_t u + u \cdot \nabla u = -\nabla (p/\rho) + \nu \nabla^2 u,
\]

with \(\nu = \mu/\rho\). All the above formulations are equivalent.

2.5 *Problems with Reconnecting Interfaces*

When two interfaces reconnect and change topology, as in Figures 3 and 4, the above macroscopic model becomes even more singular. Indeed, immediately after reconnection the surface is no longer a smooth surface but has cusp-like singularities.

The curvature \(\kappa\) is then ill-defined and arbitrarily large in the instants immediately following reconnection. Another difficulty arises in the case represented in Figure 4. In that case it is reasonable to assume that the velocity field is hyperbolic near the reconnection point. The interfaces then approach each other exponentially, and their separation \(d(t)\) varies as \(d_0 \exp(-\lambda t)\), where \(\lambda\) is the largest eigenvalue of the rate-of-strain tensor \(D\) of the local velocity field. It is obvious that the separation \(d(t)\) rapidly reaches scales much smaller than the scales on which microscopic molecular forces act to attract or repel interfaces (de Gennes 1985). The exact nature of these forces depends on the fluids and on the presence of surfactants. As a rule of thumb, they must be considered prevalent on scales of 10–40 nm.

This difficulty is less important, from the numerical point of view at least, in the case of the filamentary reconnection (Figure 3). Indeed, in that case the
macroscopic impact of microscopic physics may be limited. In other words, the macroscopic interface motion may be relatively less dependent on interface physics. This is because universal macroscopic solutions that lead to a singularity in finite time may be found (Eggers 1997). The nature of this universal singularity does not depend on the large-scale flow around the singularity or on microscopic properties (Eggers 1993, Stone 1994). One may then hope to solve the problem on a sufficiently fine scale to capture the singularity, just as one captures a shock in computational aerodynamics.

2.6 Free-Surface Flow

Free-surface flow is a limiting case of flow with interfaces, in which the treatment of one of the phases is simplified. For instance, for some cases of air-water flow, we may consider (a) the pressure \( p \) in the air to depend only on time and not on space [through, say, some function \( p_{\text{air}}(t) \)] and (b) the viscous stresses in the air to be negligible. The whole-domain forms, Equations 9 or 14, are no longer available and Form 18 must be used. The jump conditions become boundary conditions on the border of the liquid domain:

\[
(-p + 2\mu n \cdot D \cdot n)|_S = p_{\text{air}} + 2\sigma \kappa
\]  

(19)
Figure 4  Interface reconnection through sheet breakup. This reconnection may occur in a hyperbolic region of the flow, in two-dimensional as well as in three-dimensional flow. The computation of the final phase of reconnection requires the estimation of microscopic forces.

and

\[ \mathbf{t}^{(k)} \cdot \mathbf{D} \cdot \mathbf{n} \big|_S = 0. \]  

(20)

It may be noted that the last condition, which results from the nullity of tangential stresses, is purely kinematic: It does not involve material properties at all. For this reason it has interesting consequences for the value of the vorticity on a free surface (Batchelor 1967, Longuet-Higgins 1998).

3. SPECIAL CASES: PARTICULATE AND GRID-FREE METHODS

Arguably, the most important special case is inviscid flow. The Navier-Stokes equation degenerates into the Euler equation. A boundary integral formulation
then exists, in which the interface is both a free boundary between phases and a vortex sheet (Kane 1994). The boundary integral may at first view be solved more simply than the full Navier-Stokes or Euler equations. In a cubic domain of size $L$ and with a spatial grid size $h$, one needs $N = L/h$ points along each dimension. The discretization of the full two-dimensional problem would require $N^2$ grid points. If the interface is also of length $|S| \approx O(L)$, then the boundary integral may be discretized with $O(N)$ points, which is much less than what is needed for the full Euler equation. However, if there are many droplets or bubbles, or if the interface is very convoluted, then $|S| \gg L$. However, for many problems the boundary-integral method offers a substantial savings of computations and memory requirements.

The formulation of the Euler equation as a boundary-integral problem is somewhat tricky, especially when there is a density jump. The equations of vortex sheet evolution were derived in part by Zalosh (1976), with corrections indicated by Rottman & Olfe (1977). Many other formulations and numerical methods have been proposed (Baker et al 1982, 1984; Oğuz & Prosperetti 1990). Various applications to bubble and droplet flow may be found in the literature (Lundgren & Mansour 1988, 1991; Oğuz & Prosperetti 1993; Boulton-Stone & Blake 1993).

Creeping flow is another interesting special case. There is also a boundary integral formulation of the problem (Stone 1994, Tsai & Miksis 1994), which is predominantly used for creeping flows with interfaces. When the Reynolds number vanishes, lattice-gas (Rothman & Zaleski 1994, 1997) and Boltzmann lattice-gas (Benzi et al 1992) methods are also a possibility. It was argued (Ladd 1994) that Boltzmann lattice-gas methods (and perhaps simple finite differences) may be more efficient than boundary-integral methods when the number of particles is large. Recent applications of lattice-gas methods to creeping multiphase flows may be found (Olson & Rothman 1997).

The lattice-gas and Boltzmann lattice-gas methods, despite their refreshing originality, are difficult to generalize beyond their domain of validity. Whenever either density or viscosity jump across the interface, the jump conditions of Equations 1 and 17 are not satisfied anymore.

One way to eliminate the problems posed by fixed or moving grids is to eliminate the grid, in part or completely. Partial elimination of the grid is achieved in the famous particle in cell (PIC) method (Harlow 1964). This method has evolved in a number of ways. Some versions retain coupling between particles and a mesh and others do not.

The domain is then traversed by a number of particles, with or without direct physical meaning. The smoothed particle hydrodynamics method (Monagahan 1992) is a general framework for solving differential equations using particles and smoothing kernels that define the intensity of interaction between particles,
depending on their mutual distance. The interaction between particles may be viewed either as a device to solve the differential equation or as an actual force between particles. When particles of different kinds (oil and water, to use a standard example) repel each other, phases may separate and an interface with surface tension may be established. By simply letting particles attract each other, Monaghan and coworkers were able to create a free surface (Monaghan et al 1994, Monaghan 1994), thus creating a realistic simulation of wave breaking. Phase separation may also be attained (Okuzono 1997).

An interesting review of developments up to 1989 may be found in Floryan & Rasmussen (1989). The statement in that reference, that “[t]he SPH method is relatively recent; it has been developed in the context of astrophysical hydrodynamics ... and seems to be hardly known in other areas of fluid dynamics” is, however, still quite accurate.

4. MOVING-GRID AND ADAPTIVE-GRID METHODS

Moving grid methods have been particularly successful for the study of the motion of small amplitude waves and weakly deformed bubbles. Curvilinear grids have been used for some time now to follow the motion of a rising bubble (Ryskin & Leal 1984a,b). The latter was a free-surface calculation and thus the fluid dynamics of the gas was not treated. A full calculation, with gas effects included, was performed by Dandy & Leal (1989). More recently, similar methods were used by Magnaudet et al (1995) and Cuenot et al (1997) with a quasiconformal mapping technique developed by Duraiswami & Prosperetti (1992). An example of an orthogonal grid is given in Figure 5.

There are many methods that use nonorthogonal grids. When the grid points move simply in a Lagrangian way, the grid may deform considerably (see Figure 6). It is more sensible in most cases to move the point in a mixed manner between the Lagrangian motion and the fixed Eulerian point of view (Hirt et al 1974). Frequent regridding or rezoning may, however, be necessary in both cases, with in some cases the additional complication of having to add and/or remove a few grid points. This is performed, for instance, in the free Lagrangian method (Fritts et al 1985, Fyfe et al 1988).

Recently, interesting applications of deforming finite elements to large interface deformation were made (Fukai et al 1993, 1995). Representations of the deforming grids may be found in Waldvogel et al (1996).

5. FIXED-GRID METHODS

In fixed-grid methods the grid used to solve the Navier-Stokes equation is entirely or quasi-entirely fixed. The grid may be quasi-entirely fixed when, for
Figure 5  An example of an orthogonal grid, used to compute oscillations of a bubble in a liquid. The bubble is axisymmetric. The bubble axis lies at the bottom of the figure. Only a fraction of the grid is shown. [Figure courtesy of J Magnaudet and coworkers.]

example, it is adaptive just for those cells cut by the interface, as in Figure 7 (Glimm et al 1986, 1987).

5.1 Marker Methods

In marker methods, tracers or marker particles are used in the algorithm to locate the phases. Interfacial or surface-marker methods use marker particles only on the interfaces. Volume-marker methods have marker particles in the whole domain.

For two-phase flow, surface markers are more accurate than volume markers because they track exactly the location of the interface. However, when there are more than two phases, it may become difficult to handle the complexity of triple lines (lines in three-dimensional space where three phases meet) and other effects associated with the presence of several phases. Volume markers afford a simple way of dealing with the problem. Volume markers become distorted as time goes by, just as does the Lagrangian grid of Figure 6.
Figure 6  In a grid that follows the fluid motion, a considerable distortion may appear even if the interface has undergone relatively mild deformation. [Redrawn after Figure 5 of McHyman (1984).]

An illustration of the surface-marker method, in two particular cases, is shown in Figures 8 and 9. One advantage of the use of surface markers is that it allows formation of very thin liquid bridges that do no break, as shown in Figure 8. However, this is a real gain only in some cases. The situation may be made clear by considering the spiraling wave of Figure 9. If both phases have

Figure 7  An example of local adaptation on an otherwise fixed grid. (Left) The undeformed finite element triangular grid; (Right) the thick line representing the interface is made up of sides of the new triangles.
Figure 8  An example of the use of surface markers on an underlying square grid. The use of surface markers allows maintenance of the thin layer shown in the figure. In other types of fixed-grid methods, this layer may break.

Figure 9  Another example of the use of surface markers: A vortical structure entrains the interface in a spiraling motion. Surface markers allow the capture of details of interface motion on scales much smaller than the grid spacing. However, as explained in the text, some small-scale detail of the hydrodynamics may be lost when scales much smaller than the grid are created.
the same viscosity and density and there is no surface tension, the interface is “transparent” to the fluid: The fluid, in a way, does not know that there is an interface. The phases are only distinguished by their “color” as an ideal passive scalar with zero diffusivity. In that case it makes sense to track details smaller than the grid.

On the other hand, if there is, for instance, a difference in density, there will be scales in the velocity and pressure fields much smaller than the grid, and these scales will not be well resolved using the uniform square grid of Figure 9.

Surface-marker methods have been used extensively by the Glimm group (Glimm et al 1986, 1987) and by the Tryggvason group (Tryggvason & Unverdi 1990; Unverdi & Tryggvason 1992a,b). Marker methods have other advantages, and an important one is the high degree of accuracy that may be achieved by representing the interface through high-order interpolation polynomials. This accuracy may improve the accuracy of surface tension calculations (Popinet & Zaleski 1998a,b).

5.2 Volume of Fluid Methods

As stated in the introduction, we consider in some detail VOF methods relative to two-dimensional incompressible flows, without mass transfer. Extension to compressible fluids can be found (Norman & Winkler 1986, Miller & Puckett 1996, Puckett & Saltzman 1992, Saurel & Abgrall 1998). Fluxes are defined on cell faces of a square mesh with constant grid spacing $h = \Delta x = \Delta y$. The generalization to three-dimensional domains and to nonuniform rectangular and parallelepipedic grids can be done with some extra conceptual effort, but it would unnecessarily complicate this presentation (Popinet et al 1997).

A discrete analog of the characteristic function $\chi$ used in Equation 7 is the scalar field $C_{ij}$, known as volume fraction or color function (it actually should be area fraction in two dimensions, but the standard appellation is volume fraction). The color function $C_{ij}$ represents the portion of the area of the cell $(i, j)$ filled with phase 1:

$$C_{ij}h^2 \approx \iint_{(i,j)} \chi(x, y) \, dx \, dy.$$

We have $0 < C < 1$ in cells cut by the interface $S$ and $C = 0$ or 1 away from it. An example of a color function corresponding to a circle arc is shown in Figure 10. In an incompressible flow, mass conservation is equivalent to conservation of volume and hence of the characteristic function $\chi$. There is a vast literature of numerical methods for conservation laws. However, an explicit account needs to be taken of the special nature of the problem, which is entirely concentrated on the interface $S$. Moreover, particular care has to be given to the
constraint $0 < C < 1$, because numerical errors in the estimation of the fluxes can lead to values of $C$ outside the physical range of validity.

VOF methods have been known for several decades and have gone through a continuous process of improvement. Their use and effectiveness are widespread, for several reasons:

1. They preserve mass in a natural way, as a direct consequence of the development of an advection algorithm based on a discrete representation of the conservation law (7).

2. No special provision is necessary to perform reconnection or breakup of the interface and in this sense the change of topology is implicit in the algorithm.

3. They can be relatively simply extended from two-dimensional to three-dimensional domains.

4. The scheme is local in the sense that only the $C$ values of the neighboring cells are needed to update the $C$ value in the cell $(i, j)$. For this reason, it is relatively simple to implement these algorithms in parallel, in particular within the framework of domain decomposition techniques.

In general, a VOF algorithm solves the problem of updating the volume fraction field $C$ given the fixed grid, the velocity field $u$, and the field $C$ at the previous step. In two dimensions, the interface is considered to be a continuous, piecewise smooth line; the problem of its reconstruction is that of finding an approximation to the section of the interface in each cut cell, by knowing only...
the volume fraction $C$ in that cell and in the neighboring ones. The simplest types of VOF-methods are the simple line interface calculation (SLIC) of Noh & Woodward (1976) or the SOLA-VOF algorithm of Hirt & Nichols (1981). These are first order, $O(h)$, in the accuracy of the reconstruction of the interface. Typically, the reconstructed interface is made up of a sequence of segments aligned with the grid, as shown in Figure 11a. The reconstruction is relatively crude, and its advection, even with simple velocity fields such as translations or solid body rotations, generates a large amount of flotsam. A few improvements have been made by several authors (Chorin 1980, Lafaurie et al 1994), but these features still remain.


To understand the reconstruction problem we have represented in each cell of Figure 12a possible distribution of the color function on the square grid. In Figure 12b, it is harder to determine the location of the interface, but a robust reconstruction method should be able to handle this case too without any ambiguity.

One of the critical simplifying features of VOF/PLIC algorithms is that one does not attempt to reconstruct the interface as a chain of joined segments (a continuous chain of segments) but rather as a discontinuous chain with however asymptotically small discontinuities.

Whenever the curvature is small (i.e. the radius of curvature is large with respect to the grid size) the method will be accurate. However, it is robust in the sense that it does not have a catastrophic behavior when the curvature increases or even becomes infinite, for instance at reconnection. Specifically,
Figure 12  Representing the color function as shaded squares of size proportional to the fractional volumes may help to explain the reconstruction problem. (a) A well-behaved distribution of the color function, corresponding to a smooth circular arc. (b) A more confused distribution.

When the curvature is small, the jumps in interface position at discontinuities are of order \( \|\|x\|\| \simeq O(\kappa h^2) \). When the curvature is large, we lose all details at scales smaller than the grid size \( h \).

A VOF/PLIC algorithm is divided into two parts: a reconstruction step and a propagation step. (This splitting also occurs in the numerical resolution of conservation laws.) We now describe these two components.

5.2.1 RECONSTRUCTION  The key part of the reconstruction step is the determination of the orientation of the segment. This is equivalent to the determination of the unit normal vector \( \mathbf{n} \) to the segment. Then, the normal vector \( \mathbf{n} \) and the volume fraction \( C \) uniquely determine the straight line.

A typical reconstruction is shown in Figure 11b. Several algorithms have been developed for the calculation of the normal vector (Puckett & Saltzman 1992, Parker & Youngs 1992). Here, we briefly review two of them. In the first one (Li 1995), a normal (nonunit) vector \( \mathbf{m} \) is estimated by a finite-difference formula:

\[
\mathbf{m}^h = \nabla^h C. \tag{21}
\]

This vector \( \mathbf{m} \) is cell-centered and it is approximated by first evaluating the cell-corner values of \( \mathbf{m} \), for example at position \((i + 1/2, j + 1/2)\):

\[
m_{x,i+1/2,j+1/2} = \frac{1}{2h}(C_{i+1,j} - C_{i,j} + C_{i+1,j+1} - C_{i,j+1}), \tag{22}
\]

\[
m_{y,i+1/2,j+1/2} = \frac{1}{2h}(C_{i,j+1} - C_{i,j} + C_{i+1,j+1} - C_{i+1,j}). \tag{23}
\]

The required cell-centered value is obtained by averaging:

\[
\mathbf{m}_{ij} = \frac{1}{4}(\mathbf{m}_{i+1/2,j-1/2} + \mathbf{m}_{i-1/2,j-1/2} + \mathbf{m}_{i+1/2,j+1/2} + \mathbf{m}_{i-1/2,j+1/2}). \tag{24}
\]
This estimation of the normal is sometimes called the Parker and Youngs approach (PY). In two dimensions, the discrete gradient $\nabla h C$ is constructed from the volume fraction values of a $3 \times 3$ block of cells centered at $(i, j)$.

An alternate approach is a least-square method (Puckett 1991). The same block of cells is considered, but now the interface is approximated by a straight line in the whole block, with the constraint that the volume fraction of the central cell is always the true value $C$. By changing the slope of the line, one can minimize the discrete error between the true value $C$ and the value $\tilde{C}$ given by the linear approximation. For example, the discrete error $E$ in $L^2$ norm at cell $(i, j)$ is given by the expression

$$E(m) = \left( \sum_{k,l=-1}^{1} (\tilde{C}_{i+k,j+l}(m) - C_{i+k,j+l})^2 \right)^{\frac{1}{2}}. \quad (25)$$

More recently, the ELVIRA approach was proposed (Pilliod & Puckett 1997). In ELVIRA the slope is chosen among six “candidates” given by the backward, central, and forward differences of the column sums of the volume fractions done along the $x$ and the $y$ directions, respectively. The candidate that yields the lowest value of the error in Equation 25 wins.

The ELVIRA approach reconstructs exactly (with machine precision) a straight line interface. This method is thus truly second order, $O(h^2)$, unlike PY, which is intermediate between first and second order (Pilliod & Puckett 1997). Numerical experiments show, however, that at low-to-medium resolution it does not always give better results than PY, but as the resolution increases, ELVIRA gives the best results, as should be expected. This typically occurs when there are more than 20 grid points along the bubble diameter.

In the second part of the reconstruction, a linear interface that divides the computational cell into two parts containing the proper area of each fluid must be found. In general, the “forward” problem of finding the area within a square on each side of a given linear interface is more straightforward than the “inverse” problem of obtaining the equation for the linear interface, given the fraction of area contained on each side and the normal direction. Both are needed in the reconstruction and propagation steps of PLIC. We achieve this by deriving an explicit expression that relates the “cut” area to a parameter $\alpha$, which fully defines the straight line (Gueyffier et al 1998).

In two dimensions, the problem can be stated as follows. Given a square cell of side $h$ in the $(x, y)$ plane and a straight line (such as EH in Figure 13) with normal vector $\mathbf{m}$, find the area of the region below the line that also lies within the square cell. This corresponds to the area $ABFGD$ in Figure 13. To obtain an expression for this area, let us suppose that the components $m_x$ and $m_y$ of the normal $\mathbf{m}$ are both positive (this can always be arranged by a simple coordinate
transformation); in case one of the components vanishes, the calculation of the area becomes trivial. The most general equation for a straight line in the \((x, y)\) plane with normal \(m\) is
\[ m_x x + m_y y = \alpha, \tag{26} \]
where \(\alpha\) is a parameter. The area of the region contained below this line within the square cell \((i, j)\) (ABCD of Figure 13) is given by
\[
C_{ij} = \frac{\alpha^2}{2m_x m_y} \left[ 1 - H(\alpha - m_x h) \left( \frac{\alpha - m_x h}{\alpha} \right)^2 
- H(\alpha - m_y h) \left( \frac{\alpha - m_y h}{\alpha} \right)^2 \right]. \tag{27}
\]
The prefactor \(\alpha^2/2m_x m_y\) on the right-hand side of this equation is simply the area of the triangle \(AEH\). In case points \(E\) and \(H\) lie within the original square, this is the desired area. When \(\alpha > m_x h\), point \(E\) is to the right of point \(B\) and we must subtract the area of the small triangle \(BEF\) to obtain the proper area. Since triangle \(BEF\) is geometrically similar to triangle \(AEH\), the ratio of their areas is equal to the square of the ratio of the sides \(BE\) to \(AE\), given by
\[
\frac{\text{Area of } BEF}{\text{Area of } AEH} = \left( \frac{\alpha - m_x h}{\alpha} \right)^2.
\]
This corresponds to the second term within the square brackets on the right-hand side of Formula 27, which also contains the Heaviside step function $H(\alpha - m_x h)$, since the area of the triangle $BEF$ is only subtracted if $E$ is to the right of $B$. Similarly, the third term within the square brackets in the formula subtracts the area of the triangle $DGH$ when $\alpha > m_y h$ and point $H$ lies above point $D$. The single Formula 27 thus provides the area of the region below the straight line (Equation 26), which lies in the original square of side $h$ for all possible cases. The area is a continuous, one-to-one, monotonically increasing function of $\alpha$. It ranges from zero, when $\alpha = 0$, to $h^2$, when $\alpha$ reaches its maximum value of $(m_x + m_y)h$. There are two critical values of $\alpha$, corresponding to the zeros of the arguments of the Heaviside step functions in Formula 27, at which the function changes form. This occurs when the straight line (Equation 26) passes through the corners $B$ and $D$ of the square, i.e. when $\alpha = m_x h$ or $\alpha = m_y h$.

In practice, not only does one need the “forward” Formula 27 between the cut area and the parameter $\alpha$, but the method also requires the “inverse” problem of determining the $\alpha$ that corresponds to a given cut area and normal direction in a computational cell. There are a number of ways to achieve this. One can simply use a standard root-finding approach to find the particular value of $\alpha$ at which the cut area has the desired value, for instance, an iterative method may be found in Rider & Kothe (1998). Another option is as follows: Corresponding to each critical value of $\alpha$ for which the interface passes through one of the corners of the square, there exists a critical value of the cut area. In between any two critical values, the function on the right hand side of Formula 27 is a known polynomial in $\alpha$ whose roots can be evaluated analytically. Thus, to resolve the inverse problem, we first identify which two critical values bound it on either side and then obtain the root of the correct polynomial in $\alpha$ in that range.

5.2.2 PROPAGATION The second step of the VOF algorithm is propagation. Once the interface has been reconstructed, its motion by the underlying flow field must be modeled by a suitable advection algorithm. Here, we describe in some detail the fractional step or operator split method, which updates the volume fraction $C$ by advecting the interface along one spatial direction at a time. Intermediate $C$ values are calculated during this process, and the final $C$ field is obtained only after advection of the interface along all coordinate directions.

One oft-used way to calculate fluxes along the $x$ direction is shown in Figure 14, where all the fluid to the right of the dashed line will cross the right boundary during time $\tau$. In our calculations (Gueyffier et al 1998) we use a Lagrangian approach; that is, we compute directly the motion of the interface segments (Figure 15). We have found this scheme to be more robust. Because
A simple scheme for the split computation of the fluxes. As in the upwind differencing scheme, the whole block of fractional volume in a band of width $u \tau$ is transferred from the upwind cell to the downwind cell. No account, however, is taken of the change of shape of the interface during the time step.

In practice, the time-stepping is performed separately in each spatial direction, we only describe the advection of the interface along one spatial coordinate, say $x$.

For each cell, three contributions are calculated: the area fluxes $\phi^-$ and $\phi^+$ entering the cell $(i, j)$, respectively, from cells $(i - 1, j)$ and $(i + 1, j)$ and the

A Lagrangian propagation step. The advection of the reconstructed segment is computed, defining a new segment that straddles two cells. From that new segment, fluxes are calculated.
area $\phi^0$ of the fluid contained at the beginning of the step in the control cell that remains there. The updated volume fraction in each cell after the fractional step along the $x$ direction is then given by

$$C_{i,j}^{(x)} = \left[\phi_{i,j} + \phi_{i,j}^0 + \phi_{i,j}^+\right].$$

(28)

Then, the overall fractional-step procedure requires two reconstructions of the interface and an advection step along each one of the two coordinate directions. The Lagrangian advection method allows us to take into account the stretching or compression of the interface during each single fractional step. The procedure can be made second-order accurate by alternating the advection directions at each time step.

Unsplit algorithms are geometrically more complex because they also need to take into account fluxes along the transverse direction, for example from cell $(i, j)$ to cell $(i+1, j+1)$. First-order and second-order accurate algorithms have been developed by several authors (Collela 1990, Bell et al 1990, LeVeque 1996, Puckett et al 1997, Rider & Kothe 1998). The results they present indicate that for a given order of accuracy of the advection model, the unsplit algorithm shows better resolution, especially near regions of high variation of the derivatives, such as corners. Moreover it is less prone to asymmetries in the numerical solution.

We conclude with a few remarks about possible developments on interface reconstruction. Several schemes can be devised to reduce the discontinuities at the cell faces present in the PLIC representation. We may calculate an average curvature at cell $(i, j)$ using the PLIC reconstruction in a $3 \times 3$ block of cells centered at cell $(i, j)$ with a least-square procedure. We then calculate two new intersections of the fitted circle with the faces of the cell and add an extra internal point to approximate the given curvature and to conserve area. Preliminary results (Manservisi et al 1998) indicate that this reconstruction of the interface is consistently better than in any other scheme we considered. Several other groups (DB Kothe, private communication) are also considering third-order reconstruction. Propagation of the interface with this approach is under development.

6. IMPLEMENTATION OF SURFACE TENSION

The surface tension term in the Navier-Stokes equation creates the most obvious difficulties, since it is a singular term. In several implementations of the method, these difficulties are manifest in both numerical instabilities and/or noise, and in poor accuracy of capillary effects.

On adaptive grids such as those of Figures 6 and 7, surface tension may, however, be easily represented as a jump condition for the pressure shown in
Equation 16 from one element to the next, or as a boundary condition for the pressure shown in Equation 19.

On fixed grids, there are two options:

1. Smoothing the capillary force: Surface tension is implemented in a simple, albeit approximate way, by distributing it over neighboring grid points.

2. Accurate finite volume balance of surface tension forces as realized in Popinet & Zaleski 1998a: This option has been used only for two-dimensional calculations because of the complexity of the geometric considerations involved.

In the following section we only describe the first option.

6.1 Smoothing the Discontinuity of Capillary Forces

Several articles introduce what amounts in effect to distributing the surface tension over grid points neighboring the interface. Consider the phase-characteristic function \( \chi \). It may be smoothed by convolution with a kernel

\[
\tilde{\chi}(x) = \int_V \chi(x') H(x - x'; \epsilon) \, dx',
\]

(29)

where \( H(x; \epsilon) \) is an integration kernel verifying \( H \rightarrow \delta_S \), when \( \epsilon \rightarrow 0 \). The computation is based on the following remark: For a given value of \( c \) let \( S_c \) be the surface with \( \tilde{\chi}(x) = c \), \( \tilde{\kappa}(x) \) the curvature of \( S_c \) at \( x \), and \( m = \nabla \tilde{\chi} \). Then from Equation 11

\[
\tilde{\kappa}(x) = -\nabla \cdot \left( \frac{m}{2||m||} \right).
\]

(30)

When \( \epsilon \rightarrow 0, \tilde{\kappa} \rightarrow \kappa \) and one finds the “real” curvature. After Brackbill et al (1992), this method is sometimes called the continuous surface force (CSF) method. To implement the CSF method it is not necessary to perform a great deal of smoothing. We, as well as several authors with whom we had private communications, have directly implemented finite differences of \( \chi \) without smoothing or with very narrow kernels without any major problem. A discussion of the merits of better kernels may be found for instance in Aleinov & Puckett (1995). We (Lafaurie et al 1994) defined the finite filter

\[
[F(C)]_{ij} = \frac{1}{2} C_{ij} + \frac{1}{8} [C_{i,j-1} + C_{i,j+1} + C_{i-1,j} + C_{i+1,j}].
\]

(31)

The action of this filter may be repeated \( m_f \) times to yield an additional degree of smoothing \( \tilde{C} = F^{(m_f)}(C) \). The gradient \( m \) is then computed by finite differences, using for instance Expressions 22 and 23. We have found that one or two iterations of this filter were optimal.
It is possible to connect the use of a filtered surface tension with the idea of a thickened interface (Anderson et al. 1998). A thick interface occurs naturally in the Van der Waals-Cahn-Hilliard theory of interfaces. In this theory, matter is considered at an intermediate scale between the classical continuum mechanics scale at which interfaces are sharp and the molecular scale where matter is discontinuous. At this scale, continuous fields of density and velocity still exist and interfaces have a finite thickness. An example of a dynamical equation with thick interfaces for a one-species, liquid-vapor flow as well as numerical simulations of that model may be found in Nadiga & Zaleski (1996). For two incompressible phases, the Van der Waals-Cahn-Hilliard framework was used by Jacqmin (1996). An application to moving contact lines may be found in Seppecher (1996).

6.2 Momentum Conservation

The smoothing method makes it possible to find an approximation of the singular tensor defined in Equation 12,

\[ T = \sigma (I - n \otimes n) ||\nabla \tilde{\chi}||, \]  

(32)

where the unit normal \( n \) is

\[ n = \frac{\nabla \tilde{\chi}}{||\nabla \tilde{\chi}||}. \]  

(33)

The momentum-conserving formulation is a finite difference approximation of Equation 32. In practice, a 4- or 6-point approximation was used for the computation of the normals.

As in the method used by Brackbill et al. (1992), this approximation converges in theory toward the true normal as \( H \to \delta_s \). When the kernel \( H_\epsilon \) is narrowed one should keep \( m_f \) large in order to have \( h \ll \epsilon \). However, numerical experiences have shown that the best results are obtained when \( m_f = 1 \) or 2. Larger values of \( m_f \) increase the spurious currents.

6.3 Other Methods for Surface Tension

The direct measurement of normal vectors and their derivatives is possible when the interface is tracked by markers or when it is an element boundary.

We have tested a method of surface markers together with the MAC finite difference method (Popinet & Zaleski 1998a). The surface stresses were again computed and integrated over the boundary of a finite volume for the \( x \) and \( y \) momentum. When carefully implemented, this method makes it possible to considerably reduce the spurious currents.

6.4 Capillary Waves

The simulation of capillary waves is an important test for the interface simulation methods in general. It has been performed in detail by Fyfe et al. (1988) for
their free Lagrangian method. Their computations were carefully analyzed for possible errors coming from finite domain size, nonlinear effects, and viscous effects. High levels of accuracy were obtained for waves on planar interfaces, but the accuracy was less for capillary oscillations of cylinders (two-dimensional flows around circular patches). For the conservative method described above, tests were presented by Gueyffier et al (1998). For comparisons with the level-set method see Sussman et al (1994) and Sussman & Smereka (1997). For all these fixed-grid methods the accuracy is of the order of 1%. Marker methods with smoothed surface tension also give comparable results (Nobari et al 1996). However, somewhat more accuracy, of the order of 0.5%, may be obtained by an accurate finite-volume balance (Popinet & Zaleski 1998a).

6.5 Spurious Currents

A major difficulty with many methods of interface calculations is the existence of the so-called spurious or parasite currents. These currents are vortices appearing in numerical simulations in the neighborhood of interfaces despite the absence of any external forcing. They are observed with many surface tension simulation methods, including the CSF method, the conservative method of Lafaurie et al (1994), and the lattice-Boltzmann method (Gunstensen 1992), in which they were first discovered. They result in a limitation of the range of parameters that may be accessed by the model.

It is difficult to give a systematic expression for the amplitude of spurious currents because they often fluctuate in time, but direct measurements (Lafaurie et al 1994) yield approximately

$$ u_p \simeq 0.01 \frac{\sigma}{\mu}. $$

(34)

These currents were also measured around droplets in the connected marker method of Tryggvason and coworkers. There spurious currents appear to be of the order

$$ u_p \sim 10^{-5} \frac{\sigma}{\mu} $$

(Tryggvason, unpublished lecture notes).

6.6 Problems with Large Surface Tension

The simulation methods for flows with interfaces are limited in the range of dimensionless numbers that may be reached. The situation is analogous to that of direct numerical simulations of homogeneous flows, where there is an upper limit for the Reynolds number that grows like a power of the number of grid points.

For interface methods, calculations often become difficult when the surface tension becomes large and the density jump is also large. This may happen for bubbles or droplets of small radius $R$, when surface tension is large compared
with viscosity. This means that either the capillary number \( \text{Ca} = \frac{\mu U}{\sigma} \) is small or that the Laplace number \( \text{La} = \frac{\sigma \rho R}{\mu^2} \) is large. Numerical experiments show that at small \( \text{Ca} \), but moderate \( \text{La} \), no catastrophic instability occurs, and that the only troublesome effects are the spurious currents. However, at large \( \text{La} \), parasite currents may grow and become large enough to destroy the interface. This may be easily explained by the connection between \( \text{La} \) and Reynolds numbers of spurious currents given by Equation 34,

\[
\text{La} = 100 \text{Re}_p, \tag{35}
\]

where \( \text{Re}_p = \frac{u_p R}{\nu} \). In practice, computations become difficult when \( \text{La} \sim 10^6 \). This is approximately the value for a 1-cm droplet or bubble. Thus, this droplet size represents the borderline for current-day simulations.

For larger droplets and Reynolds numbers, one needs to compare surface tension and inertia. At small Weber numbers, \( \text{We} = \frac{U^2 \rho R}{\sigma} \), capillary tension dominates inertial phenomena. Since this happens for smaller \( R \), it may explain why several articles and private communications report difficulties with smaller particles.

### 6.7 Problems with Small Surface Tension

At large Weber numbers, problems also occur because the computed objects (droplets, bubbles, filaments) become very small. In this situation, the breakup phenomenon tends to create smaller structures until the Weber number becomes small enough, at around \( \text{We} = 10 \). If and when these structures reach sizes smaller than the mesh, a loss of accuracy occurs.

First-order methods, such as the SOLA-VOF method (Hirt & Nichols 1981), are numerically unstable in the absence of surface tension. The interface is progressively destroyed by the generation of flotsam, and surface tension is the only way to keep the interface well defined. On the other hand, PLIC methods (Li 1995) and other more accurate methods such as front tracking avoid this numerical instability. The small structures created at large Weber numbers are often well resolved and have physical meaning.

Moreover, at low Reynolds numbers, small surface tension implies large \( \text{Ca} \). This is equally catastrophic, since viscous flow may create cusps in the interface.

### 7. TESTS AND APPLICATIONS

#### 7.1 A Reconnection Test: Sessile Droplets

Sessile droplets are created by letting the liquid flow very slowly out of a crank. A pendant drop forms and remains attached to the crank only through a thin liquid bridge, which eventually pinches in several places.
This problem was studied in an inviscid framework by Schulkes (1994) and Oguz & Prosperetti (1993) using a boundary-integral method. Eggers & Dupont (1994) obtained an approximation of the full Navier-Stokes equation, which is in part a lubrication approximation valid in the limit of slowly varying thickness $R(z)$. It is a lubrication approximation only in part because it includes a surface-tension term that is exact, and thus the Eggers-Dupont equation is also valid for static shapes with arbitrary slopes of $R(z)$, such as droplets. Both approaches (Schulkes 1994, Eggers & Dupont 1994) were found to be in very good agreement with the experiments of Peregrine (Peregrine et al 1990). More recently, full three-dimensional and two-dimensional axisymmetric viscous simulations have been carried out for this physical situation using the VOF method by Gueyffier et al (1998) and the results show an excellent agreement with the pictures of Peregrine et al (1990).

7.2 Sedimentation of Droplet Arrays in Creeping Flow

The asymptotic fall velocity of a droplet is given by the classic Hadamard-Rybczynski expression (Batchelor 1967)

$$U_{HR} = \frac{2}{3\mu_{out}} (\rho_{out} - \rho_{drop}) a^2 \frac{1 + K}{2 + 3K} g,$$

(36)

where $\mu_{out}$ and $\rho_{out}$ are the dynamical viscosity and density of the outer fluid and $K = \mu_{out}/\mu_{drop}$ is the ratio between the dynamic viscosities of the two fluids. Sangani (1987) found solutions to the Stokes equation for periodic arrays of droplets. The ratio between the sedimentation velocity of the array of drops $U$ and Hadamard-Rybczynski velocity for a single drop $U_{HR}$ only depends on the viscosity ratio $K$ and on the volume fraction between drops and the outer fluid $c$.

These theoretical results were compared with three-dimensional calculations with our VOF/PLIC method. The results are shown in Figure 16. The error increases with $K$. This is due to the manner in which viscosity is averaged in cut cells. This creates $O(h)$ errors in the viscous stresses. This problem was addressed by Coward et al (1997).

7.3 Breakup of Liquid Jets and Kelvin-Helmholtz Instability

The phenomenon of droplet peeling on the surface of liquid jets has been abundantly studied (Hoyt & Taylor 1977, Reitz & Bracco 1982). These jets are often produced in engine nozzles. The mechanism for the breakup of the jet is complex and difficult to observe because of the very small space- and timescales involved. Numerical simulation is therefore well placed to deal with this problem. Breakup of liquid jet has been studied using VOF methods at relatively low We by Richards et al (1993, 1994). For fluids of interest in combustion studies
Figure 16  Ratio between sedimentation velocity of an infinite array of drops and Stokes velocity for a single drop.

(such as liquid-oxygen/hydrogen or hydrocarbon/air mixtures), the principal difficulties occur from the very large values of the capillary number $Ca$. This number is about 0.25 in a typical water jet in air at 10 m/s water velocity, whereas it can reach the value 10 in hydrocarbons or cryogenic fluids. Figure 17 shows an example of such a peeling obtained for $Ca = 0.02$, whereas Figure 18 shows an example for $Ca = 1$. The simulations give different results. In the second case, structures of very small size are formed because of the systematic stretching of a thin filament of liquid. The precision of the calculation is limited by the formation of these very small structures. Our three-dimensional simulations analyze the response to spanwise perturbations of the above two-dimensional base-flow (Zaleski et al 1996). The pinching mechanism by which liquid droplets detach from the edges of sheets in two-dimensional flow is not necessarily the realistic three-dimensional regime. We have been able so far to distinguish two scenarios by which three-dimensional flow sets in. For small three-dimensional perturbations, the simulation remains two-dimensional until the sheet breaks and a cylinder pinches off. Subsequently, the capillary instability of jets gives three-dimensional structure to the flow. In this case, the two-dimensional simulations are useful for predicting the evolution of the flow and the droplet size.
In contrast, for higher three-dimensional perturbations, a different scenario is observed, as shown in Figure 19 (this simulation took about 48 h to complete on an IBM RS6000/370). The rim-like edge concentrates in a protruding finger that will be subject to the capillary instability. However, the unstable cylinder is now streamwise. The formation of streamwise filaments or fingers is observed in real experiments on shear layers (Raynal et al 1995) and it is also reminiscent of the crown formation in droplet impact experiments (Yarin & Weiss 1995).

7.4 Other Applications
Although the surface-wave problem has been studied for a long time using boundary-integral methods for inviscid flow, it is only recently that several
Figure 18  Droplet formation at higher capillary and Weber numbers. The intermediate steps are not shown. The level lines of the vortices are omitted in (b) to avoid overcrowding the plot.
Figure 19  Breakup of the interface through a secondary instability of the sheet. $\rho_L/\rho_G = 10$, $Re = 1000$, and $We = 300$. 

authors have attempted to solve the full Navier-Stokes equations. The dissipation of surface waves was studied by Yang & Tryggvason (1998). Wave breaking and the mixing of the fluid from the plunging jet was studied by Abadie & Caltagirone (1998). Breaking waves with plunging jets and several splash-ups were simulated by Chen et al (1998).

Applications of surface marker methods to biology are a promising area of research. One example in this direction is Agresar et al (1998). Boiling flow is also a new application of surface-tracking methods (Juric & Tryggvason 1998).

Finally, bubbly flow with a large number of bubbles has been intensively studied both in two and three dimensions by several groups (see Esmaeeli & Tryggvason 1996, 1998a,b; Tomiyama 1998).
Of great importance for modeling multiphase flow is the study of single bubbles in various configurations. Three-dimensional numerical simulation is required for the study of asymmetric flow such as bubbles in shear flows (Ervin & Tryggvason 1997).

8. CONCLUSION

In our opinion, the main progress witnessed over the past 10 years is the advent of many three-dimensional calculations. Two-dimensional calculations have also matured, producing either highly accurate results or calculations over impressively large grids.

The one new method that appeared is level sets. It is seducing by its simplicity but has not yet produced the wide range of results, especially in three-dimensions, achieved by older methods. The VOF method has been considerably improved by the systematic use in the scientific literature of the higher order piecewise linear interface calculation method.

Important calculations have not yet been done. For instance, there is no three-dimensional calculation of a falling drop or rising bubble in the difficult air/water conditions and in the nontrivial regimes where axial symmetry does not hold. Many complex flows, such as atomizing jets, splashing droplets, or breaking waves, have been studied only in a preliminary way. Finally, for some flows, quantitative results are difficult to get, in particular, agreement between simulations and linear theory for shear flow instabilities.

For engineering applications, new methods need to be developed that could adapt to complex geometries, such as combustors and nozzles, to cite just two of a whole world of examples.

It is our opinion that these difficulties should soon be resolved. This would allow these methods to connect directly with scientific problems and engineering applications in multiphase flow. From there the simulation of interfaces could move on to incorporate more complex physics, such as models of intermolecular forces, complex surface rheology, and the transport and effects of tensio-active molecules.

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