A front tracking method for direct simulations of multi-phase flows

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Abstract

A finite difference/front tracking method for direct simulations of multiphase flows is described. A few examples of both two- and three-dimensional simulations are presented.

Background

Multi-phase flows are central to many industrial processes. Heat transfer by boiling is the preferred mode in most power plants and bubble driven circulation systems are used in metal processing operations such as steal making, ladle metallurgy and the secondary refining of aluminum and copper. In combustion of liquids the fuel is usually introduced as a spray, and sprays are central to most painting and coating processes. Similarly, many natural processes involve bubbles and drops. Rain is perhaps the most common example, but bubbles also play a major role in the air/ocean interaction, for example. Prediction and optimization of industrial processes requires reliable mathematical description. In fluid mechanics direct numerical solutions of the Navier-Stokes equations have become a standard research tool. Multiphase flows still remains outside of this activity, for the most part. The need is widely recognized by the community, but the computational complexity has limited most investigations to relatively simple

systems. Here, we describe a relatively new method that we are currently using to conduct direct simulations of multiphase flows.

In the limit of high and low Reynolds numbers, it is sometimes possible to simplify the flow description considerably by either ignoring inertia completely (Stokes flow) or by ignoring viscous effects completely (inviscid, potential flow). Most success has been achieved where the particles are undeformable spheres where, in both these limits, it is possible to reduce the governing equations to a system of coupled ordinary differential equations for the particle positions. For Stokes flow see Brady (1993) for a review. For inviscid flows, see Sangani and Prosperetti (1993), for example. For both Stokes flows as well as inviscid flows, problems with deformable boundaries can be simulated with boundary integral techniques. For Stokes flow, Zhou and Pozrikidis (1993, 1994) have simulate the unsteady motion of 12 two-dimensional drops both in a shear flow and in a channel where the flow is driven by a pressure gradient. Fully three-dimensional boundary integral computations of the interaction of two drops have recently been presented by Manga and Stone (1993), and Kennidy, Posrikidiz, and Skalak (1994) have examined the deformation of a drop in a shear flow. Chahine and collaborators (see Chahine, 1990, for example) have computed the interactions of a few inviscid cavitation bubbles.

For intermediate Reynolds numbers it is necessary to solve the full Navier-Stokes equations. The steady rise of buoyant, deformable, axisymmetric bubbles were simulated by Ryskin and Leal (1984) in a landmark paper that has had a major impact on subsequent development. Kang and Leal (1987) extended the methodology to axisymmetric, unsteady motion. Several other two-dimensional and axisymmetric computations of the unsteady motion of one or two bubbles or drops have appeared recently. Fukai et al. (1993) have computed the deformation of an axisymmetric drop colliding with a rigid wall and Shopov *et al* (1990) as well as Sussman, Smereka, and Osher (1994) have followed the initial deformations of a buoyant bubble, for example. The unsteady motion of a few two-dimensional solid cylinders has been simulated by Feng, Hu, and Joseph (1994) for several Reynolds numbers.

Numerical Method

Our method is properly described as a hybrid between a front capturing and a front tracking technique. We use a stationary regular grid for the fluid flow, but

also track the interface by a separate grid of lower dimension. This grid is usually referred to as a front, but unlike in front tracking methods, we do not treat each phase separately, but write only one set of Navier-Stokes equations for the whole flow field. In a conservative form those are:

$$\frac{\partial \rho \bar{u}}{\partial t} + \nabla \cdot \rho \bar{u}\bar{u} = -\nabla p + \bar{f} + \nabla \cdot \mu\left(\nabla \bar{u} + \nabla \bar{u}^T\right) + \int_F F_s \delta\left(\bar{x} - \bar{x}_f\right) da$$

Here, $\bar{u}$ is the velocity vector, p the pressure, ρ and μ the discontinuous density and viscosity field, respectively, and $\bar{f}$ is a body force. The surface tension force, F_σ, act only on the interface between the fluid and is therefore multiplied by a three-dimensional delta function, δ. The integral is over the entire boundary.

It is important to note that this equation contain no approximations beyond those in the usual Navier-Stokes equations. In particular, it contains implicitly the proper stress conditions for the fluid interface. If we integrate over a small volume containing the interface, most of the terms go to zero as we shrink the integration volume, and in the limit of infinitesimal volume we end up with

$$\left[\left[-p\bar{n} + \mu\left(\nabla \bar{u} + \nabla \bar{u}^T\right) \cdot \bar{n}\right)\right] = \sigma \kappa \bar{n}$$

where the brackets denote the jump across the interface. These are, of course, the usual conditions imposed on a fluid boundary. Integrating the mass conservation equation across the interface shows that continuity of normal velocities is also satisfied. To discretize the above equation, we use a staggered grid. The spatial derivatives are approximated by a second order centered finite differences and for most of our computations we use a second order time integration scheme. This results in a method that has excellent conservation properties.

The momentum equations are supplemented by the incompressibility conditions, which, when combined with the momentum equations leads to an elliptic equation for the pressure. We used a simple SOR for many of our early computations (in the so-called Black and Red form for computations on the CRAY), but now a multigrid package (MUDPACK from NCAR) is used for most of our computations. Within each phase we take density and viscosity to be constant. These fields are updated at every time step after the front has been moved, see Unverdi and Tryggvason (1992) for details.

The surface tension force, which is computed from the front configuration is, perhaps, the most difficult part of the algorithm. Therefore, we have spent considerable time on that and explored various alternatives. The current

algorithm, which appear to be very satisfactory, is based on computing directly the force on each element by a line integral over the boundary of each surface element:

$$\bar{F}_\sigma = \oint_{elem} \sigma \bar{n} \times \bar{t} ds$$

Here, $\bar{t}$ is a tangent to the boundary of the surface element and $\bar{n}$ is the surface normal. By computing the surface tension forces this way, we explicitly enforce that the integral over any portion of the surface gives the right value, and for closed surfaces, in particular, we enforce that the net force on the surface is zero. This is particularly important for long time simulations where a failure to enforce this constrain can lead to unphysical motion of bubbles and drops.

The surface mesh is an unstructured grid consisting of points and elements. Both the points and the elements are arranged in a linked list, so it is relatively easy to change the structure of the front, including adding and deleting points and elements. Topological changes, such as when bubbles coalesce or drops break in two can also be accomplished.

The computational technique described above has been used to simulate several multi-fluid problems. Among those are head-on collisions of drops presented by Nobari, Jan and Tryggvason (1993) and three-dimensional collisions shown in Nobari and Tryggvason (1994). Unverdi and Tryggvason (1992) simulated the collision of fully three dimensional bubbles; Esmaeeli, Ervin, and Tryggvason (1994) discuss the lift of deformable bubbles rising in a shear flow; Jan and Tryggvason (1992) examined the effect of contaminants on the rise of buoyant bubbles and Nobari and Tryggvason (1994) followed the coalescence of drops of different sizes. Nas and Tryggvason (1992) presented simulation of thermal migration of many two dimensional bubbles.

In figures 1-3 we show a few examples. In figure 1 a single frame from a computation of four buoyant bubbles rising in a doubly periodic box are shown. Here the Reynolds number is moderate (around 40) and the deformation of the bubbles is small. We have done a number of both two- and three-dimensional computations of several bubbles to examine the evolution of dense bubble clouds. For low Reynolds numbers and two-dimensions, we have computed the evolution of over three-hundred bubbles for a relatively long time. Figure 2 shows one frame from a two-dimensional computation of the resuspension of drops in a shear flow. Initially the drops are all next to the lower wall, but here they have spread across the channel, mainly due to collisions with each other.

We have also examined the effect of heat transfer and variable surface tension, and figure 3 shows one frame from a three-dimensional simulation of the thermal migration of two bubbles due to a temperature dependent surface tension.

The approach taken for the fluid flow, works also for heat flow and phase changes. In Juric and Tryggvason (1994) we developed a method to simulate phase changes in a pure material in the absence of any fluid motion. With these assumptions we have only to solve one heat conduction equation:

$$\frac{\partial \rho c T}{\partial t} = \nabla \cdot k \nabla T + \int_F \dot{q} \delta(\bar{x} - \bar{x}_F) da$$

where $\dot{q}$ is adjusted in such a way that the temperature of the interface is given by the Gibbs-Tompson conditions

$$T_F = T_M \left(1 - \frac{\sigma \kappa}{L}\right)$$

Here, T_M is the melt temperature, T_F is the temperature at the front, k is the conductivity, and L is the volumetric latent heat. Additional terms can be added to the right hand side to account for surface tension anisotropy, for example. We have compared the method with exact solutions for stable solidification and found excellent agreement for relatively coarse resolution. We have also used it to simulate the evolution of fairly complex unsteady solidification problems as shown in Figure 4 where the evolution of an unstable solidification front into an undercooled melt is computed.

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References

J.F. Brady. Stokesian Dynamics Simulation of Particulate Flows. In: M.C. Roco (editor). Particulate Two-Phase Flow. Butterworth. (1993), 912-950.

Chahine, G.L. Numerical modeling of the dynamic behavior of bubbles in nonuniform flow field, Numerical Methods For Multiphase Flows 91 (1990), pp. 57-64

Esmaeeli, A., Ervin, E. A., & Tryggvason, G. Numerical simulations of rising bubbles, (Ed: J.R. Blake), Proc. IUTAM Conference on Bubble Dynamics and Interfacial Phenomena (1994).

Feng, J., Hu, H.H. & Joseph, D.D. Direct simulation of initial value problems for the motion of solid bodies in a Newtonian fluid. Part 1. Sedimation. J. Fluid Mech. **261** (1994), 95-134.

Fukai, J., Zhao, Z., Poulikakos, D., Megaridis, C.M. & Miyatake, O. Modeling of the deformation of a liquid droplet impinging upon a flat surface. Phys. Fluids A **5** (1993), 2588-2599.

Jan, Y.-J., & Tryggvason, G. Computational Studies of Contaminated Bubbles. Submitted for publication (1993).

Juric, D. & Tryggvason, G. A Front Tracking Method for Dentritic Solidification. Submitted for publication (1994).

Kang, I.S. & Leal, L. G. Numerical solution of axisymmetric, unsteady free-boundary problems at finite Reynolds number. I. Finite-Difference scheme and its applications to the deformation of a bubble in a uniaxial straining flow. Phys. Fluids **30** (1987), 1929-1940.

Kennedy, M.R. Pozrikidis, C. & Skalak, R. Motion and Deformation of Liquid Drops, and the Rheology of Dilute Emulsions in Simple Shear Flows. Computers Fluids **23** (1994), pp. 251-278.

Nas, S. & Tryggvason, G. Computational investigation of the thermal migration of bubbles and drops", *Proc. ASME Winter Annual Meeting* FED-175 (1993), 71-83

Nobari, M.R., Jan, Y.-J. & Tryggvason G. Head-on collisions of drops-a numerical investigation", Submitted for publication (1994).

Nobari, M.R. & Tryggvason, G. Numerical simulations of drop collisions. AIAA 94-0835.

Manga, M. & Stone, H.A. Buoyancy-driven interactions between deformable drops at low Reynolds numbers. J. Fluid Mech. **256** (1993), 647-683.

Ryskin, G. & Leal, L.G. Numerical solution of free-boundary problems in fluid mechanics. part 2. Buoyancy-driven motion of a gas bubble through a quiescent liquid, J. Fluid Mech. 148 (1984), pp. 19-35

Sangani, A.S. & Prosperetti, A. . Numerical Simulation of the Motion of Particles at Large Reynolds Numbers. In: M.C. Roco (editor). Particulate Two-Phase Flow. Butterworth (1993). 971-998.

Shopov, P.J., Minev, P.D., Bazhekov, I.B. & Zapryanov, Z.D. Interaction of a deformable bubble with a rigid wall at moderate Reynolds numbers, J. Fluid Mech. **219** (1990), 241-271

Sussman, M., Smereka, P. & Osher, S. A Level Set Approach for Computing Solutions to Incompressible Two-Phase Flows. J. Comput. Phys. **114** (1994), 146-159.

Unverdi, S.O. & Tryggvason, T. A front-tracking method for viscous, incompressible, multi-fluid flows, J. Comput. Phys. **100** (1992), 25-37

Unverdi, S.O. & Tryggvason, G. Computations of multi-fluid flows, Physica D **60** (1992), 70-83

Zhou, H. & Pozrikidis, C. Pressure-Driven Flow of Suspensions of Liquid Drops. Phys. Fluids **6** (1994), 80-94.

Zhou, H. & Pozrikidis, C. The flow of ordered and random suspensions of two-dimensional drops in a channel. J. Fluid Mech. **255** (1993), 103-127.

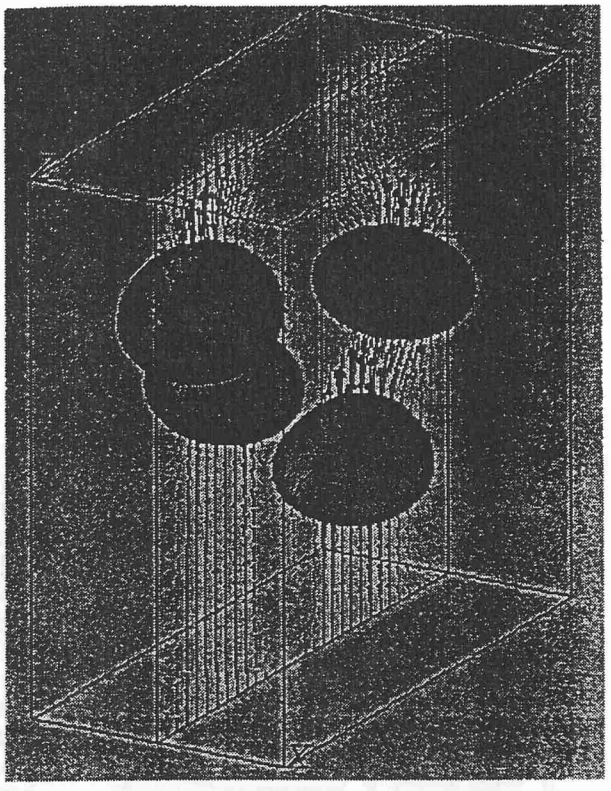

Figure 1. One frame from a three-dimensional computation of the motion of four bubbles in a doubly periodic domain. Here the Morton number is 10^{-5} and the Eotvos number is 3, giving a Reynolds number of about 40 for a single bubble in unbounded fluid. The computations are done on a 64^3 grid.

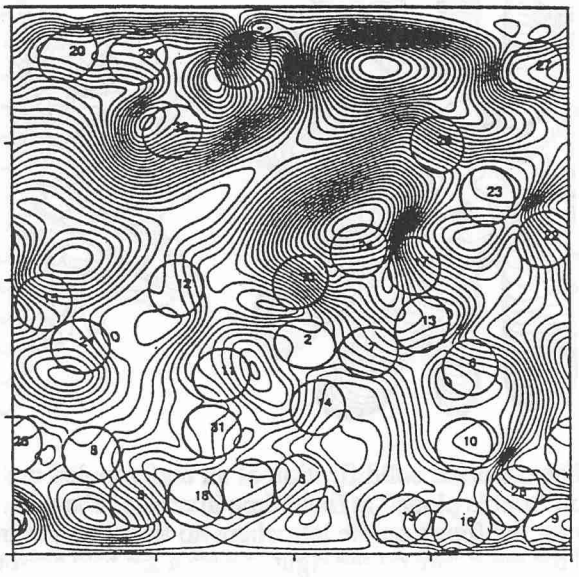

Figure 2. One frame from a two-dimensional computation of the resuspension of several drops in a shear flow. The drops were initially near the bottom wall but have spread across the channel at this time, mainly due to collisions with each other. Here, the shear Reynolds number is 20 and a 288 by 288 grid was used.

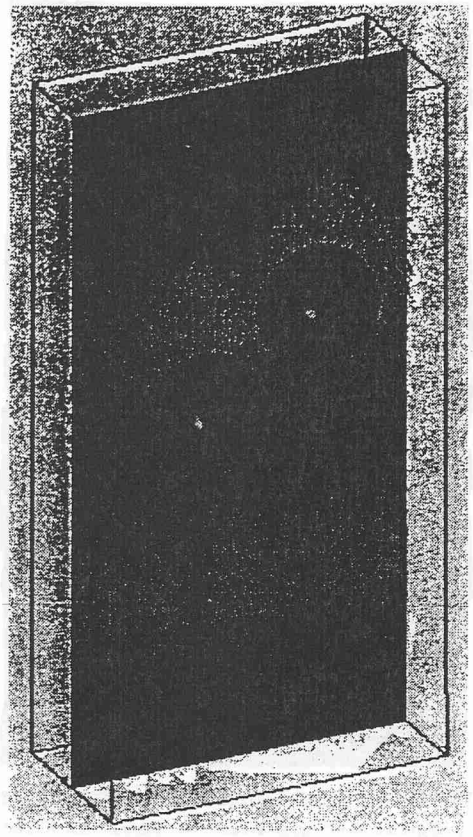

Figure 3. One frame from a three-dimensional computation of the thermal migration of two bubbles. The top wall is hot and the bottom wall is cold and the energy equation is solved in addition to the Navier Stokes equations. The bubbles migrate toward the hot wall due to temperature dependent surface tension. The Marangoni number here is 20 and the grid is 64 by 32 by 128 grid points.

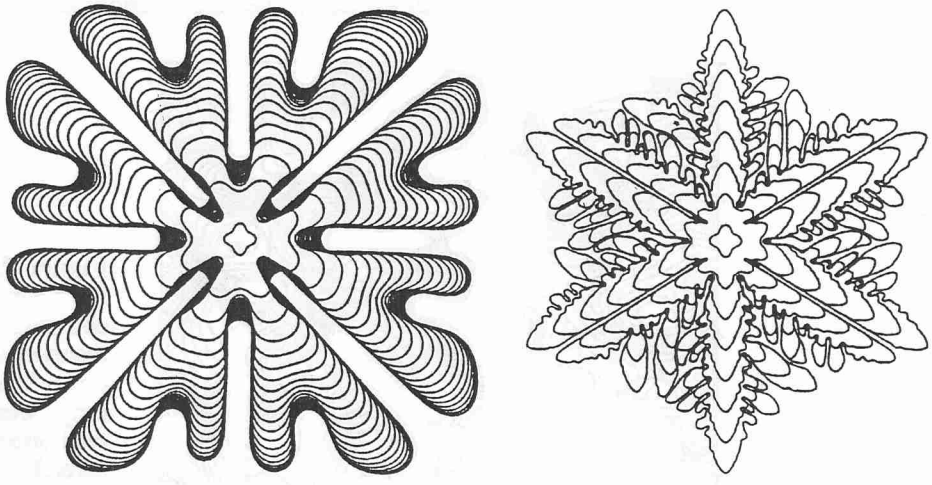

Figure 4. The dendritic solidification of an undercooled melt. The solidification front is plotted at fixed time intervals. The grid resolution is 200 by 200 for the figure on the left where no anisotropy is included, and 800 by 800 for the figure on the right, where a six fold anisotropy is used.