COMPUTATIONS OF DROP COLLISION AND COALESCENCE

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ABSTRACT

Computations of drops collisions, coalescence, and other problems involving drops are presented. The computations are made possible by a finite difference/front tracking technique that allows direct solutions of the Navier-Stokes equations for a multi-fluid system with complex, unsteady internal boundaries. This method has been used to examine the various collision modes for binary collisions of drops of equal size, mixing of two drops of unequal size, behavior of a suspension of drops in linear and parabolic shear flows, and the thermal migration of several drops. The key results from these simulations are reviewed. Extensions of the method to phase change problems and preliminary results for boiling are also shown.

INTRODUCTION

The presence of a free surface that is not constrained to be more or less flat due to the action of gravity is perhaps the most important aspect of fluid flow in microgravity. The absence of gravity generally makes surface tension effects important at much larger length scales than we are used to on earth. The large amplitude surface motion possible when gravity is small or absent is generally highly nonlinear and thus difficult to analyze by conventional means. Such surface motion is, nevertheless, to be expected in microgravity environment and it is necessary to understand it to be able to work with free surface systems. Experiments in microgravity are expensive, and usually difficult as well. It is therefore desirable to be able to predict the evolution of free surface systems numerically. Numerical simulations can replace experiments in some cases and complement experiments in other cases by providing information that are difficult to measure. Numerical simulations can also aid in the design of space experiments.

Numerical simulations of free surface flows have remained one of the frontiers of computational fluid dynamics since the beginning of large scale computations of fluid flow. Progress has however been much slower than for homogeneous flows and numerical simulations have not played the same role in multifluid and multiphase research as they have done for turbulence research, for example. Recently, however, a number of investigators have made considerable progress. We have been conducting simulations of multifluid and multiphase systems for several years and this paper reviews briefly those aspects of our work that are of particular relevance to microgravity fluid systems We start by a description of the numerical methodology, since it is critical to the success of our work, and then review a few applications.

NUMERICAL METHOD

The numerical method is based on writing one set of equations for the entire computational domain, independently of how many different fluids are involved. This is possible by allowing for different material properties in the formulation and adding singular terms at the phase boundaries to ensure that the correct boundary conditions are satisfied. The resulting "one-field" Navier-Stokes equations 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, and ρ and μ are the discontinuous density and viscosity fields, respectively. $\bar{f}$ is a body force that can be used to initiate the motion. The surface forces, F_σ act only on the interface between the different fluids and appears in the current formulation multiplied by a three-dimensional delta function, δ. The integral is over the entire front. 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. The momentum equation is supplemented by an equation of mass conservation, which for incompressible flows is simply

$$\nabla \cdot \bar{u} = 0$$

535

Combining this equation with the momentum equation leads to an elliptic equation for the pressure. Since the density and the viscosity are different for the different fluids, it is necessary to track the evolution of these fields by solving the equations of state which simply specify that each fluid particle retains it original density and viscosity:

$$\frac{\partial \rho}{\partial t} + \bar{u} \cdot \nabla \rho = 0; \quad \frac{\partial \mu}{\partial t} + \bar{u} \cdot \nabla \mu = 0$$

The momentum equation is discretized on a regular staggered grid using second order, centered finite differences for the spatial derivatives and a second order time integration scheme. The continuity equation, when combined with the momentum equation results in a pressure equation that is not separable as for homogeneous flow and is solved by a multigrid package (MUDPACK from NCAR). To advect the material properties, and to evaluate the surface tension term in the momentum equation, we track the interface between the different phases explicitly by using a moving grid of lower dimension than what we use for the conservation equations. This grid is usually referred to as a front. The one-field formulation used here is common to other techniques for multifluid flows such as the VOF (Volume of Fluid) and level set methods. In these methods, however, the phase boundary is not tracked explicitly, but reconstructed from a marker function. Explicitly tracking the interface avoids the difficulty of advecting such marker function and allows accurate evaluation of surface forces.

Computing surface tension accurately is one of the most difficult part of methods intended for simulations of multifluid flows. Our current algorithm, which appear to be very satisfactory, is based on computing directly the force on each element by

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

in a semi-implicit way. Here $\bar{t}$ is a tangent to the boundary of the surface element, $\bar{n}$ is the surface normal, and σ is the surface tension coefficient. By computing the surface 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 integral of surface tension forces 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.

Since the boundary between the fluids (the front) usually undergoes considerable deformation during each run, it is necessary to modify the surface mesh dynamically during the course of the computations. The surface mesh is an unstructured grid consisting of points that are linked by 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 by minimum effort. This is usually considered a major difficulty in implementing methods that explicitly track the front, but we have shown that with the right data structure these tasks become relatively straight forward. Although topology changes are easily done from a programming point of view, the physics is far from trivial. In reality, drops bounce off each other if the time when the drops are close is shorter than the time it takes to drain the film. Usually the film becomes very thin before it breaks and it would require excessive grid refinement to resolve the draining fully. At the moment we are dealing with this issue in a rather *ad hoc* way by simply changing the topology of the front at a prescribed time. However, considerable analytical work has been done on film draining and rupturing and we are currently exploring the possibility of combining such a model with our simulations.

The method has been implemented for two- and three-dimensional flows on regular grids and for axisymmetric geometries using stretched grids to allow local grid refinement. It has been applied to a number of multifluid problems and tested and validated in a number of ways, not only to check the implementation, but also to assess its accuracy. Those tests include comparisons with analytical solutions for simple problems, other numerical computations, and experiments. The actual resolution requirement varies with the parameters of the problem. High Reynolds numbers, for example, generally require finer resolution than lower ones, as in other numerical calculations. We have also found that for problems where the surface tension varies, such as for contaminated bubbles and drops moving by thermal migration we generally require finer resolution than for flows where the surface tension is constant. However, in all cases have we found that the methods converges rapidly under grid refinement, and in those cases where we have other solutions we have found excellent agreement, even for modest resolutions. The method has also been extended in various ways to allow for simulations of heat transfer, surfactant effects, thermal migration, and phase changes. These effects can also be dealt with using the one-field formulation, thus allowing for a very efficient solution process. Examples of these validations are contained in various papers and dissertations listed at the end of theis paper. Our work on other physical systems, such as bubbly flows are also discussed in these references.

RESULTS

We have examined the collision and coalescence of two drops in considerable detail. The results of our investigation of the head-on collision of drops can be found in Nobari, Jan, and Tryggvason (1996). In this paper we examine how the collision modes changed as a function of Weber number, and how the exact time of coalescence, where the film between the drops ruptures, affected the outcome of the collision. Figure 1 shows one simulation from this paper. This work has now lead to a collaboration with Professor C.K. Law of Princeton University who has conducted extensive experimental studies of drop collisions and a detailed comparison between his experimental results and the simulations has shown excellent agreement. The interplay between experiments and simulations has also greatly improved our understanding of the boundaries between the various collision regimes. Three-dimensional simulations of off-axis collisions are described in Nobari and Tryggvason (1996). The results there show good agreement with experimental investigations, but the study is not yet as detailed as for the head-on collisions. For drops of unequal size, we have examined the coalescence of initially stationary drops that are driven together by surface tension. The results, which have been submitted for publication (Nobari and Tryggvason, 1994), show that considerable mixing can take place due to vorticity injected into the large drop by the smaller one.

With the collision of drops well under control, we have examined more complex problems. These include both large scale simulations of many drops as well as problems where additional physical effects have to be accounted for, such asheat transfer, thermal migration of drops, and phase changes. For isothermal drops we have examined the behavior of many drops in wall driven and pressure driven shear flows. In normal gravity such situations occur frequently in emulsions, for example, where the density of the drops is comparable with the continuous fluid. In microgravity, there is no restriction on the density difference and for finite Reynolds number flows we can expect significant effect due to the inertia of the drops. This investigation also has relevance to high pressure sprays where there are strong interactions between the drops and the continuous phase. In figure 2 we show several frames from a fully three-dimensional simulation of twelve drops in a periodic channel. The domain simulated is resolved by a 64^3 grid and the simulations are carried out for sufficiently long time so the drop distribution reaches an approximately steady state. Using both three-dimensional simulations with a models number of drops and two-dimensional simulations with larger number, the effect of the various governing parameters has been explored. The simulations generally show that the drops migrate away from walls, forming a denser core near the centerline. A single drop, however, generally takes up a position approximately half way between the wall and the centerline (the so-called Segre-Silberg effect) and for dilute distributions we find local maximum in the concentration at this position.

When gravity is absent, other effects, such as variable surface tension can dominate the dynamics. While thermal migration, where surface tension variations are brought about by variable temperature field, has been extensively studied for a single bubble or a drop, little is known about the interactions of many drops, particularly at finite Reynolds and Marangoni numbers. Figure 3 show an example of a fully three-dimensional simulation of two drops on a 32 by 64 by 128 grid. The drop surface and the temperature field in the centerplane are shown. The top and bottom boundaries are rigid walls at constant temperature, but the horizontal boundaries are periodic. This simulation, along with several two-dimensional ones of several drops show that the drops tend to form layers perpendicular to the temperature gradient. The simulations also show that even though surface tension is relatively low, the drops generally do not deform to any significant degree as they move.

The methodology used for the problems discussed above can be extended to much more complex physics in a relatively straight forward way. Application to the relatively simple problem of solidification of pure material in the absence of flow is discussed in Juric and Tryggvason (1995) where validation studies for simple problems and applications to the growth of dendrites can be found. Extension to binary alloys where it is necessary to follow the composition of the material can be found in Juric (1996). For full multiphase problems where fluid flow, heat transfer, and phase change are taking place simultaneously, we combine the method for the energy equation used for the solidification problems with the method for the Navier-Stokes equations. The resulting code has allowed us to simulate several boiling problems and in figure 4 we show a simulation of the growth of a vapor bubble in superheated fluid. The domain, which is resolved by a 100 by 100 grid, is open at the top, allowing fluid to escape as the bubble grows. The bubble shape is perturbed slightly at time zero and as the bubble expands, these perturbations grow. The bubble shape at time zero and several subsequent times is shown in the frame to the left. The right frame shows the bubble shape and temperature contours at an intermediate time. A simplified version of this method has also been used to simulate solidification of drops colliding with a wall in the case where the density of the melt and the solid are the same.

CONCLUSIONS

We have discussed a numerical methodology to simulate multifluid and multiphase flows in microgravity and shown a few application of these methods. These simulations have already lead to a better understanding of some aspects of drop collisions and coalescence and also demonstrate the versatility of the method. Overall, it seems reasonable to state that the fluid problem is under good control with the exception of how to handle the rupture of thin films, although our current *ad hoc* strategy seems to work well in some cases. In most cases the fluid motion is only a part of an engineering application and heat transfer and phase change must be dealt with in order to establish the understanding needed for a completely predictive capability. We have taken preliminary steps in this direction and examined the thermal migration of drops and various phase change problems. The capability to examine the detailed evolution of boiling fluids, for example, promises to yield a dramatic new insight and understanding.

ACKNOWLEDGMENTS

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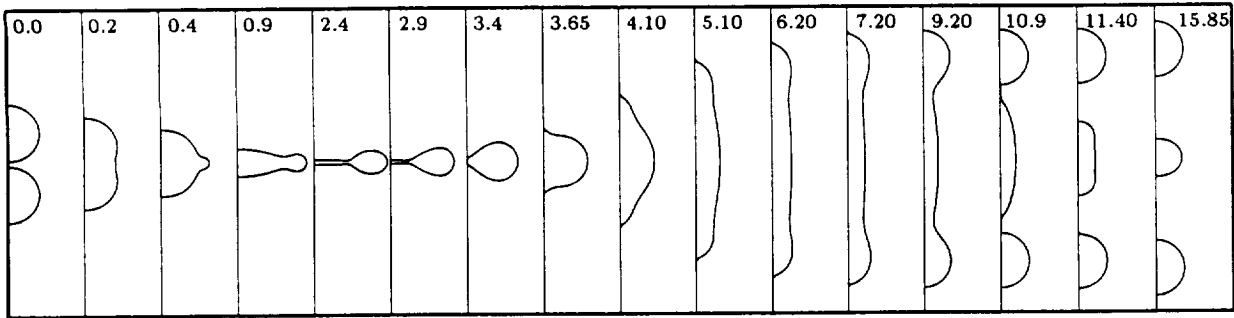D. Juric and G. Tryggvason, "Direct Numerical Simulations of Flows with Phase Change," AIAA 96-0857eeting, (1996).

| 0.0 | 0.2 | 0.4 | 0.9 | 2.4 | 2.9 | 3.4 | 3.65 | 4.10 | 5.10 | 6.20 | 7.20 | 9.20 | 10.9 | 11.40 | 15.85 |

Figure 1. The head-on collision of two drops computed by an axisymmetric version of our method. Here We=115 and Re=185. The drops are sufficiently energetic so they break up again after initial coalescence.
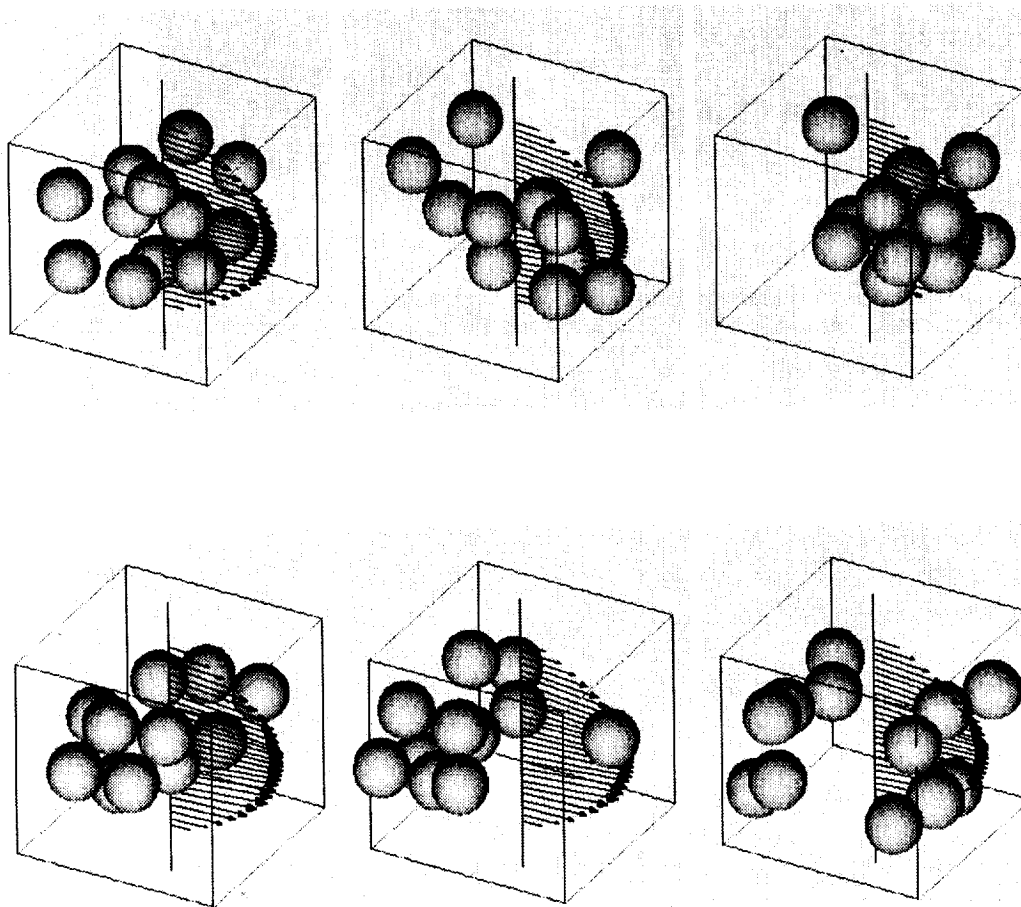
Figure 2. Simulation of the motion of twelve drops in a wall bounded/periodic pressure driven flow. Re=20, We=0.125 and the computational domain is resolved by a 64^3 grid.
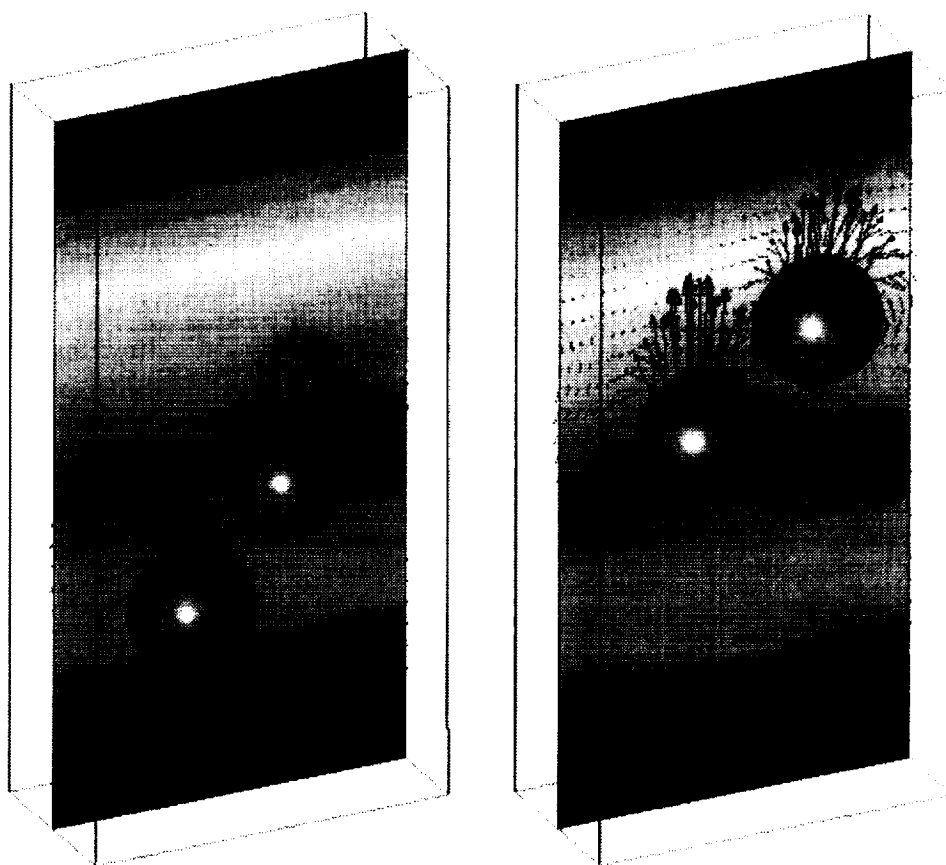
Figure 3. The thermal migration of several two three-dimensional drops simulated on a 64 by 32 by 128 grid. Here, Ca=20 and Re=60. The initial conditions are to the left. The drops and the isotherms are shown.
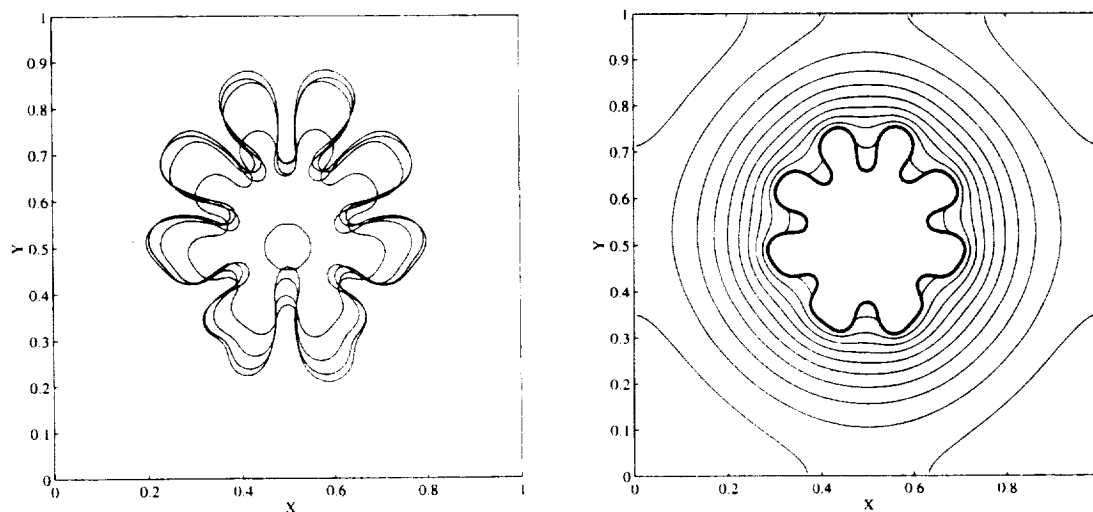

Figure 4. The evolution of a bubble groving in superheated liquid. The bubble surface at several different times is shown in the frame to the left. The bubble surface and several isotherms at an intermidiate time are shown on the right.