N95-14542

COMPUTATIONS OF DROP COLLISION AND COALESCENCE

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ABSTRACT

Computations of drops collisions and coalescence are presented. The computations are made possible by a recently developed 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 boundaries between the various collision modes for drops of equal size and two examples, one of a "reflective" collision and another of a "grazing" collision is shown. For drops of unequal size, coalescence can result in considerable mixing between the fluid from the small and the large drop. This problem is discussed and one example showed. In many cases it is necessary to account also for heat transfer along with the fluid mechanics. We show two preliminary results where we are using extensions of the method to simulate such problem. One example shows pattern formation among many drops moving due to thermal migration, the other shows unstable evolution of a solidification front.

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 predict its motion, or avoid it if necessary. Experiments in microgravity are at best expensive, and usually difficult as well. It is therefore desirable to be able to predict the evolution numerically. Such numerical simulations can, occasionally, replace experiments information that can not be measured. In other cases numerical simulations can complement experiments and aid in the design of 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. For an early work on drop collision, see ref. 3. Progress has however been much slower than for homogeneous flows and numerical simulations have not played the same role in multi-fluid and multiphase research as they have done for turbulence research, for example. Recently, however, a number of investigators have made considerable progress and this paper reviews briefly our effort in this area of relevance to microgravity fluid physics. 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 a hybrid between so called front capturing methods where a sharp front is resolved on a stationary grid and front tracking methods where the interface is followed by separate computational elements. We use a stationary regular grid for the fluid flow, just as front capturing methods, but track the interface by a separate grid of lower dimension. This grid is usually referred to as a front. However, unlike front tracking methods, we do not treat each phase separately, but work with the Navier-Stokes equations for the whole flow field. In a conservative form those are:

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

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 tension forces, F_σ act only on the interface between the fluid 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 above equation is discretized on a staggered grid using second order second order centered finite differences for the spatial derivatives and a second order time integration scheme for most of our computations. For short simulations, first and second order give very comparable results, but for long time simulations the higher order is a must. To monitor the accuracy we check, among other quantities, how well we conserve mass. While the finite difference method has good conservation properties, the front tracking is not inherently conservative. By using second order time integration and sufficiently fine resolution we always find that mass is well conserved. The momentum equation is supplemented by an equation of mass conservation, which for incompressible flows is simply

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

Combining this equation with the momentum equation leads to an elliptic equation for the pressure. Unlike the pressure equation for homogeneous flows, here it is nonseparable and fast methods used extensively for homogeneous flows (FISHPACK, for example) are not applicable. 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. 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:

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

In our front tracking code we do not solve these equations in this form, but use the front to determine the value at each grid point. This can be achieved efficiently by distributing the density gradient (or the jump) onto the grid and then reconstructing the density from its gradient. This allows two interfaces to lie close to each other so the gradient cancel. Usually it is only necessary to reset the density and viscosity of grid points next to the front.

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

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

where $\vec{t}$ is a tangent to the boundary of the surface element, $\vec{n}$ is the surface normal, and σ is the surface tension coefficient. 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 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.

Although by no means new, the formulation of two (or more) fluid problems in terms of one equation for the whole flow field is somewhat unusual. Furthermore, even though it is a rigorous approach, it is not immediately obvious that it will lead to an efficient computational method. We have therefore conducted extensive validation tests, not only to check the implementation, but also to assess its accuracy. We have compared the code with analytical solutions where available, such as the linear oscillations of a drop and the propagation of waves, with other computational work such as the simulations of Leal and coworkers (see, e.g. ref. X) and experimental results. 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 has other solutions we have found excellent agreement, even for modest resolutions. Examples of these validations are contained in various papers and dissertations, see ref. 5-9, 11, and 12.

RESULTS

We have investigated the head-on collisions of two drops in detail by axisymmetric computations and also done several fully three dimensional calculations of off-axis collisions. Figure 1 shows the head on collision of two drops from ref. 9. To move the drops toward each other we apply a body force on each drop that is turned off once the drops have reached the desired velocity and before the drops collide. In this case, the drop Weber number, $\rho dU^2/\sigma$, and the Reynolds number, $\rho Ud/\mu$, are 115 and 185, respectively. As the drops collide, they deform and once they are close enough, the film between them is ruptured so the drops coalesce into one drop. The kinetic energy is converted into surface tension energy as the drop is deformed into a disk-like shape, and once the it is nearly stationary the process is reversed and surface tension pulls the drop back into a spherical shape. In this particular case, the initial kinetic energy is sufficiently high and the dissipation sufficiently low that the drop actually splits into three. This evolution is observed experimentally, see ref. 2 and 4, for example, and is called reflective collision. For lower initial energy the drops do not separate again, but remain one. We have investigated the boundary between reflective collision and coalescing collisions (when the drops permanently become one drop) and found good agreement with experimental observations. For collisions close to the boundary there is a slight sensitivity to the exact time of rupture, but away from the boundary the evolution is not affected by the exact rupture time.

When the drops do not approach each other along the same axis, the evolution is fully three-dimensional. If the off-axis distance is small, the evolution is similar to a head on collision, but if the distance is large a new collision mode, usually called grazing collision, becomes possible. Figure 2 shows such a collision. The drops are initially accelerated toward each other by a body force. This force is turned off once the drops have reached the desired velocity and before they collide. As the drops collide, they deform, and once the film of ambient fluid between them is thin enough it is ruptured and the drops allowed to coalesce. If the offset is small, the coalescence is permanent for the Reynolds and Weber numbers used here, but when the offset is large, as is the case in figure 2, the drops tear apart again. We have compared the boundaries between permanent coalescence and grazing with experimental observations and find excellent agreement [see ref. 7 and 8 for details]. Both the axisymmetric and the three-dimensional computations have shed considerable light on the collision process and the role played by losses of surface tension energy during the actual coalescence when the thin film between the drops is ruptured.

Another problem that we have investigated in some detail is the coalescence and subsequent mixing of two, initially stationary drops of unequal size. This study was motivated by experiments conducted by Anilkumar, Lee and Wang (ref. 1) who brought two drops together slowly and made a video recording of the evolution after the film between them ruptures and surface tension forces pull the small drop into the larger one. For high viscosity drops the motion is quickly dissipated and the fluid from the small drop remains near the point where the drops touched. For lower viscosity, however, the fluid from the small drop is injected much more violently into the larger one, forming a jet that often reaches across the larger drop. In general, the penetration depth depends on the nondimensional viscosity and the size ratio of the drops, since for two drops of the same size, no jet formation occurs by symmetry. This problem requires a careful resolution of inertia, viscous and surface tension effects. We have investigated this problem in some detail and provided a reasonably complete picture of how the evolution depends on the parameters of the problem. Figure 3 shows the process. The initial configuration is shown on the left and the final configuration is on the right.

As the multi-fluid problem has been brought under control, we have moved toward more complex physics. A problem of a long standing interest to the microgravity community is the thermal migration of bubbles and drops. Here, two complications arise. First, we must solve for the temperature field and second, surface tension is now no longer a constant but depends on the temperature. We have dealt with variable surface tension before for problems involving surface active materials (or surfactants) so the added complication here is only the heat transfer part. Figure 4 shows a few frames from a two-dimensional calculation of the motion of six drops in a temperature gradient. The drop surface and isothermals are shown. The top and bottom boundaries are rigid walls at constant temperature, but the horizontal boundaries are periodic. The evolution seen here is typical for many drops at these parameter values. The drops line up across the channel until there is not room for more. The rest then forms a new line. If there are not

enough drops to fit across the channel, the drops position themselves as far apart from each other as possible. Preliminary simulations of fully three-dimensional drops indicate that the interactions are much weaker in three-dimensions, but we have not conducted a systematic study yet.

For material processing and thermal management the fluid mechanics is often, if not always going to be accompanied by phase changes. In preparation for simulations of fluid systems undergoing a change of phase such as during boiling or solidification, we have developed a method based on the same single domain formulation used for the fluid flow for solidification. Up to now we have only simulated solidification and figure 5 shows an example where an initially undercooled melt solidifies. We are currently combining this methodology with our fluid dynamics method.

CONCLUSIONS

We have discussed our development of numerical method suitable for the predictions of free surface flows in microgravity and the application of these methods to several problems. These applications 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. Our current *ad hoc* strategy seems to work well in some cases, but it is highly desirable to have a more general way of determining when the film ruptures. We believe that the rupture time is the most important information needed, and that for a large class of problems the details of the post rupture motion, including the formation of small drops can be safely ignored. In most cases the fluid motion is only a part of the process of interest and heat transfer and phase change must be dealt with in order to establish the understanding needed for a complete predictive capability. We have taken preliminary steps in this direction and examined the thermal migration of drops and solidification.

ACKNOWLEDGMENTS

This work has been supported under NASA grant NAG3-1317 and a NASA Graduate Student Fellowship NGT-51070 for D. Juric. We wish to thank Dr. D. Jacqmin at the NASA Lewis Research Center for many helpful discussions.

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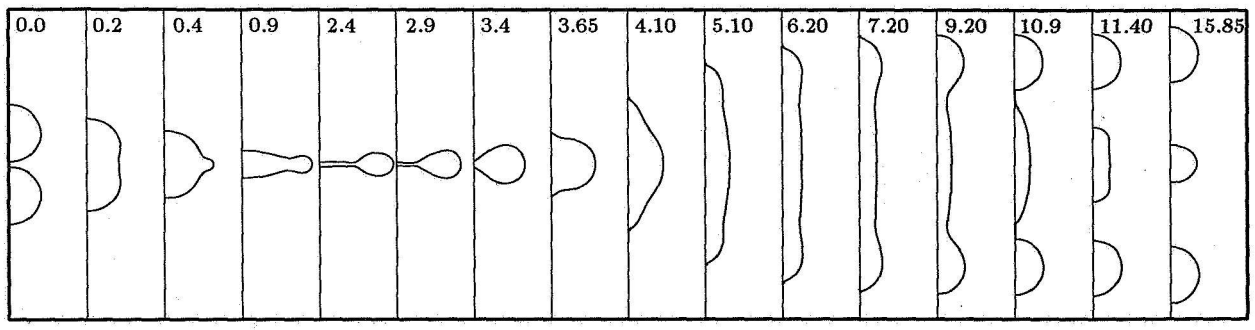

Figure 1. The head on collision of two drops computed by an axisymmetric version of our method. Here We=115 and Re=185. The drops are sufficiently energetic so they break up again after initial coalescence.

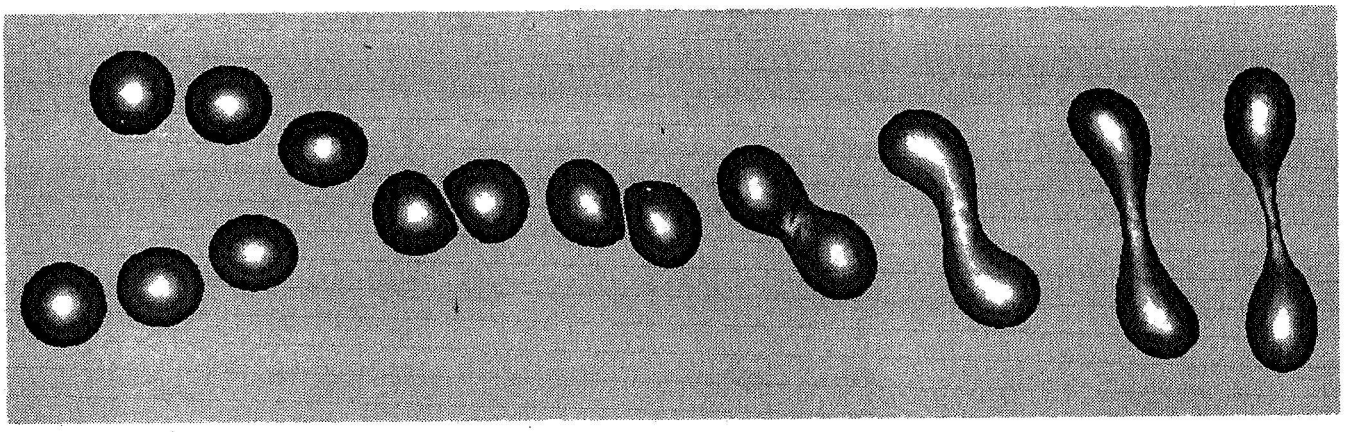

Figure 2. Fully three-dimensional grazing collision of two drops. Here, We = 23 and Re = 68. The line along which each drops moves are separated by 0.825 drop diameters.

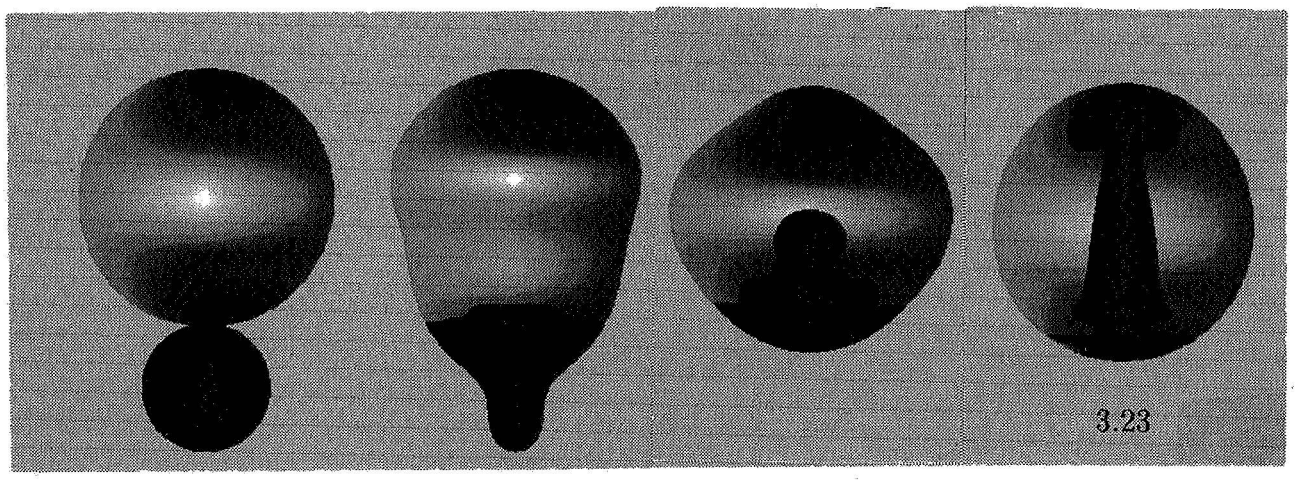

Figure 3. Coalescence and mixing of two stationary drops of unequal size.

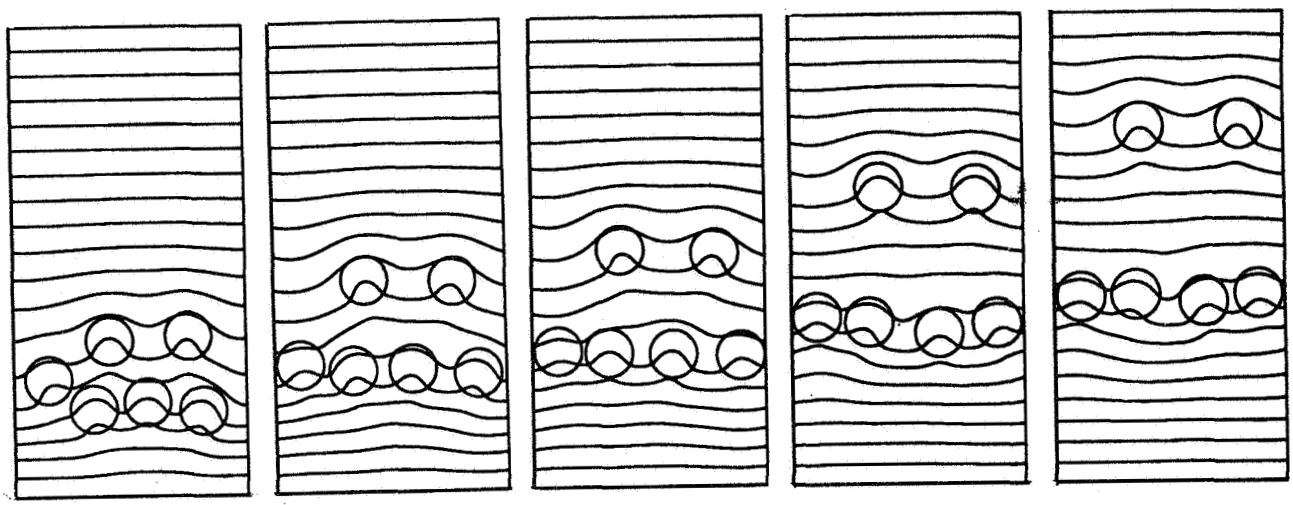

Figure 4. The thermal migration of several two-dimensional drops. The initial conditions are to the left. The drops and the isotherms are shown.

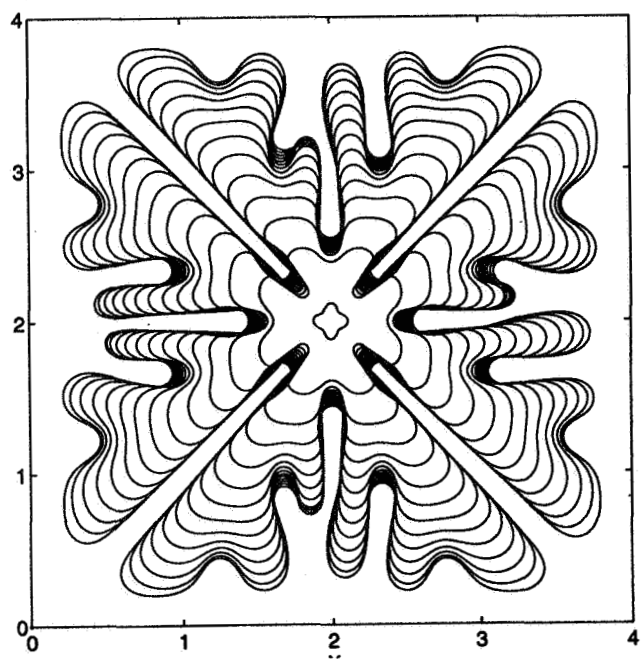

Figure 5. The evolution of an unstable solidification front. The front is shown at several times as it advances into the undercooled melt.