Direct Numerical Simulations of Bubbly Flows

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Abstract. The status of direct numerical simulations of bubbly flows is reviewed and a few recent results are presented. The development of numerical methods based on the one-field formulation has made it possible to follow the evolution of a large number of bubbles for a sufficiently long time so that converged statistics for the averaged properties of the flow can be obtained. In addition to extensive studies of homogeneous bubbly flows, recent investigations have helped give insight into drag reduction due to the injection of bubbles into turbulent flows and two-fluid modeling of laminar multiphase flows in channels.

1 Introduction

Boiling heat transfer, cloud cavitation, aeration and stirring of reactors in water purification and waste water treatment plants, bubble columns and centrifuges in the petrochemical industry, cooling circuits of nuclear reactors, propagation of sound in the ocean, the exchange of gases and heat between the oceans and the atmosphere, and explosive volcanic eruptions, are just a few examples of multiphase bubbly flows occurring in both industrial and natural processes. As these examples show, understanding the evolution and properties of bubbly flows is therefore of major technological as well as scientific interest.

Although Direct Numerical Simulations (DNS) of bubbly flows have come into their own only in the last few years, computational studies of multiphase flow date back to the beginning of computational fluid dynamics, when the MAC method of Harlow and collaborators was used for simulations of the Rayleigh–Taylor instability, splats due to impacting droplets, and other problems involving a free surface or a fluid interface. Although the MAC method, and its successor the VOF method, slowly gained popularity, in the late seventies and the early eighties, serious computational studies relied mostly on boundary integral methods and body fitted grids for intermediate Reynolds numbers [23]. The current surge of activities in multiphase flow simulations goes back to the beginning of the nineties, when significant improvements in methods that use fixed grids took place. Fixed grids offer great flexibility in the geometric complexity of the multiphase flow under investigation, com-

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bined with the efficiency inherent in the use of regular structured grids. The continuous surface force (CSF) method [4] to compute surface tension in VOF methods, the level set [24], the phase field, and the CIP [27] methods were all introduced at that time, along with the front tracking method of Unverdi and Tryggvason [30]. By now, a large number of refinement and new methods have been introduced and the development of numerical methods for multiphase flow is currently a "hot" topic. There is, for example, hardly an issue of the *Journal of Computational Physics* that does not have at least one paper in some way related to multiphase flow simulations.

The development of more efficient, accurate, and robust methods continues to be of considerable interest, as well as the extension of the various methods to handle more complex physics. It is, however, the use of numerical methods to conduct direct numerical simulations of complex multiphase flows that is sure to have the greatest impact in the future. Such simulations are already yielding unprecedented insight, even though DNS have only been used to examine a tiny fraction of the systems that can be explored with current capabilities. Those studies that have been done have focused mostly on suspensions of solid particles and bubbly flows. Here we will discuss the current status of DNS of bubbly flows.

2 Numerical method

For non-dilute disperse multiphase flows at intermediate Reynolds numbers, it is necessary to solve the full unsteady Navier–Stokes equations. Most methods currently in use for DNS of multiphase flows are based on writing one set of the governing equations for the whole flow field by allowing the density and viscosity fields to be discontinuous across the phase boundary and by including a singular term representing the surface forces. The momentum equation is:

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\nabla\cdot\mathbf{uu} = -\nabla P + \nabla\cdot\mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T) + \sigma\int_F \kappa_f \mathbf{n}_f \delta(\mathbf{x}-\mathbf{x}_f)\,\mathrm{d}A_f. \quad (1)$$

Usually both fluids are assumed to be incompressible:

$$\nabla\cdot\mathbf{u} = 0. \quad (2)$$

Here, $\mathbf{u}$ is the velocity, P is the pressure, and ρ and μ are the discontinuous density and viscosity fields, respectively. δ is a three-dimensional delta-function constructed by repeated multiplication of one-dimensional delta-functions. κ is twice the mean curvature. $\mathbf{n}$ is a unit vector normal to the front. Formally, the integral is over the entire front, thereby adding the delta-functions together to create a force that is concentrated at the interface, but smooth along the front. $\mathbf{x}$ is the point at which the equation is evaluated and $\mathbf{x}_f$ is the position of the front.

Numerical implementations of Equations (1) and (2) include the Volume of Fluid, the Level Set, and the CIP methods as well as the Front-Tracking/Finite Volume method of Unverdi and Tryggvason [30]. The front-tracking method is used for the simulations presented here. In all these methods, the governing equations are solved

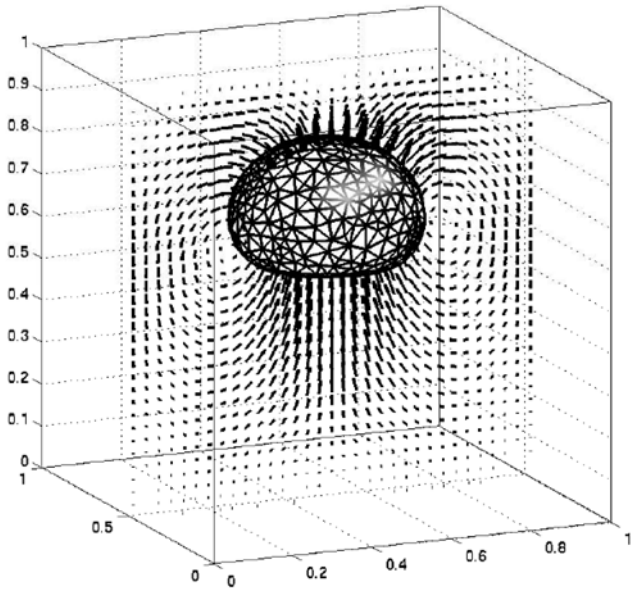

Fig. 1. The computational setup. The conservation equations are solved on a regular structured grid, but the phase boundary is tracked by a moving unstructured triangular grid.

by a projection method on a fixed grid. The way the phase boundary is tracked is, however, different. In most cases a marker function that identifies the different fluids is advected by the flow. In the method of Unverdi and Tryggvason, however, the phase boundary is tracked by connected marker points (the "front") and the marker function reconstructed from the location of the "front". This keeps the boundary between the phases sharp, and allows the accurate computation of the surface tension. The front points are advected by the flow velocity, interpolated from the fixed grid. As the front deforms, surface markers are dynamically added and deleted. The surface tension is represented by a distribution of singularities (delta-functions) located at the front. The gradients of the density and viscosity become delta functions when the change is abrupt across the boundary. To transfer the front singularities to the fixed grid, the delta functions are approximated by smoother functions with a compact support on the fixed grid. At each time step, after the front has been advected, the density and the viscosity fields are reconstructed by integration of the smooth grid-delta function. The surface tension is then added to the nodal values of the discrete Navier–Stokes equations. Finally, an elliptic pressure equation is solved by a multigrid method to impose a divergence-free velocity field. For a detailed description of the original method, including various validation studies, see [29, 30]. Figure 1, where the velocity field computed on a fixed grid is shown along with the tracked surface for a single buoyant bubble, summarizes the computational approach.

The original method of Unverdi and Tryggvason [30] has been extremely successful for relatively complex multiphase flows at modest Reynolds numbers. As it

has been applied to more challenging problems, such as higher Reynolds numbers and large properties ratios, a number of improvements have been implemented. The development include improved regridding procedures for the tracked front, conservative techniques to compute the surface tension, high order upwind methods for the advection terms, the use of non-conservative form of the advection terms to eliminate spurious oscillations for high density ratios, and non-uniform grids. The basic method has, however, remained the same, confirming that robustness of direct tracking of the interface.

3 Results

Below we review briefly the status of our studies of bubbly flows, using direct numerical simulations. We have examined a large number of cases, but until recently we have mostly focused on homogeneous flows, modeled by fully periodic domains.

3.1 Homogeneous bubbly flows

The interactions of two bubbles in a periodic domain was examined briefly in [30]. The motion of many nearly spherical bubbles at moderate Reynolds numbers was studied by Esmaeeli and Tryggvason [10] for a case where the average rise Reynolds number of the bubbles remained relatively small (1–2) and Esmaeeli and Tryggvason [11] looked at another case where the Reynolds number was 20–30. Bunner and Tryggvason [5, 6] simulated a much larger number of three-dimensional bubbles using a parallel version of the method used by Esmaeeli and Tryggvason. Their largest simulations followed the motion of 216 three-dimensional buoyant bubbles per periodic domain for a relatively long time. The simulations showed, among other things, that modest Reynolds bubbles generally interact through "drafting, kissing, and tumbling" collision [13] and that the probability of finding horizontal bubble pairs increases with the Reynolds numbers. While "low order" statistical quantities like the rise velocity of the bubbles converged rapidly as the size of the system increases, other quantities like the dispersion coefficients converge slower. Esmaeeli et al. [12] briefly examined bubbles that settle down into periodic wobbling and showed that the bubbles slow down significantly once they start to wobble. Göz et al. [14] examined higher Reynolds number bubbles and found what looked like chaotic motion at high enough Reynolds numbers. The effect of deformability was studies by Bunner and Tryggvason [7] who found that relatively modest deformability could lead to a streaming state where bubbles gathered in a stream or a chimney. Other studies of the motion and interactions of many bubbles have been done by several Japanese authors. Early work, using the VOF method to compute the motion of a single two-dimensional bubble can be found in [28] and more recent work on bubble interactions, using both VOF and the Lattice Boltzman Method, is presented in [25, 26]. The various simulations that have been done for bubbly flows suggest that we are well on our way to understand elementary behavior of homogeneous bubbly flow when the Reynolds number is relatively low.

3.2 Using DNS to validate and develop models

For industrial systems DNS are generally not practical and it is necessary to use models that predict the average behavior of the system. Reynolds Averaged Navier–Stokes (RANS) computations of homogeneous flows have a long history, starting with the pioneering work of Launder and Spalding [20] and Harlow and collaborators (e.g. [2]). For multiphase flows, several averaged models have been developed, ranging from simple mixture models to more sophisticated two-fluid models. Considerable effort has, in particular, been devoted to the development of two-fluid models for disperse flows (see, for example, [8, 9, 31]. The averaging leads to an equation for the void fraction and separate momentum equations for each phase. It also results in the usual Reynolds stresses and the force between the phases as the terms that must be modeled. The force is usually split into several parts, including the steady-state drag and lift, added mass, Basset force, wall drag and wall-repulsion, and dispersion force. These terms are modeled using a combination of analytical solutions for Stokes flow and empirical correlations/corrections to account for higher Reynolds numbers. For a spherical isolated particle the forces are reasonably well understood, with the exception of lift, but for higher concentrations and deformable bubbles the situation is more uncertain. The momentum equation for the continuous phase is always solved using an Eularian approach, where the averaged equations are solved on a fixed grid, but the dispersed phase can be treated either using a Lagrangian or an Eularian approach. In the Eularian approach the momentum equation for the averaged particle velocity is solved in the same way as for the continuous phase, but in the Lagrangian approach the dispersed phase is represented by point particles that are tracked through the flow domain. As the particles move, they generate velocity disturbances in the continuous phase, even if it is initially quiescent. These velocity fluctuations show up as Reynolds stresses in the averaged equations and are usually modeled using potential flow solutions for flow over a sphere. In turbulent flows they are simply added to the Reynolds stresses generated by the fluid turbulence. For well-behaved flows, such as flows in pipes and ducts, current two-fluid models generally do well and capture the main flow features.

We have recently started to look at two-fluid models by comparing results from direct numerical simulations with the predictions of the model of Antal et al. [1] for laminar bubbly flow. The primary goal of this study is simply to find out what kind of domain sizes are needed to produce results with well-converged averages. The simulations were done assuming a two-dimensional flow so we had to adjust the model parameters slightly. We did, however, find that once we adjusted the parameters for one flow, other situations were well predicted by the same model parameters. For steady-state flow, where the slip velocity between the bubbles and the continuous phase is given by an algebraic relation, there is no question of ill-posedness and the model converged rapidly when the grid is refined. We are currently in the progress of doing fully three-dimensional simulations that will allow us to do a more thorough term-by-term assessment of the closure models and to explore their sensitivity to a distribution of bubble sizes, bubble deformability, and so on. We have also done a low resolution preliminary simulation of bubbles in a turbulent channel flow (similar

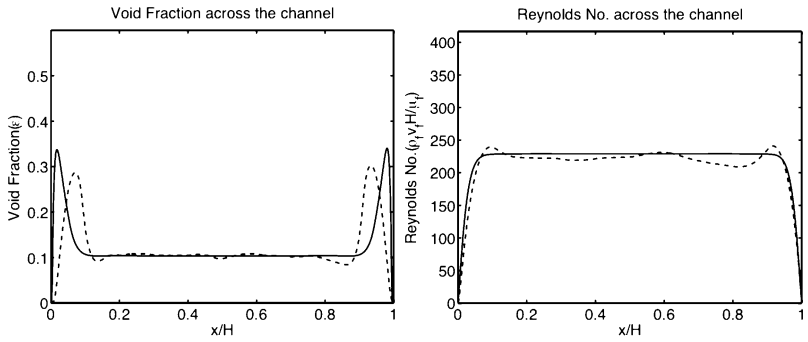

Fig. 2. Comparison of the average velocity and void fraction profile from a simulation of 64 bubbles and the two-flluid model of Antal et al. [1]. While the model does not capture completely the location of the wall peaks in void fraction, the overall agreement is good.

to our study of drag reduction described below, but with bubbles rising due to buoyancy) and we plan to use the results to shed some light on the interaction of bubble induced velocity fluctuations and the already existing turbulence. Figure 2 shows a comparison of the simulated void fraction and velocity profiles, averaged over the entire computational domain, and profiles predicted using the two-fluid model of Antal et al. [1]. Except for the location of the wall-peak, the model captures the simulated results reasonably well. The results also show that the bubbles are pushed to the wall until the flow in the center of the channel is in hydrostatic equilibrium and essentially homogeneous. For details, see [3].

3.3 Drag reduction due to bubble injection

In addition to providing data and insight for modeling, DNS studies can help explain complex interactions between the bubbles and the flow. Sometimes such interactions involve very subtle effects. Figure 3 shows one frame from a simulation of bubbles in a turbulent channel flow with a Reynolds number of 4000. In addition to the bubbles, isocontours of spanwise vorticity are shown, with different shading indicating positive and negative vorticity. The wall shear on the bottom wall is also shown. The goal of this investigation is to cast some light on the mechanisms underlying drag reduction due to bubble injection and to provide data to help with the modeling of such flows. Experimental studies (see [17, 19, 22], for a review) show that the injection of a relatively small amount of bubbles into a turbulent boundary layer can result in a significant drag reduction. While the general belief seems to be that the bubbles should be as small as possible (a few wall units in diameter), drag reduction is found experimentally in situations where the bubbles are considerably larger (order of 100 wall units).

We have examined the effect of bubbles on turbulent channel flow, mostly using simulations with sixteen bubbles in the so-called “minimum turbulent channel” of Jimenez and Moin [15]. The results, discussed in detail in [21], show that slightly

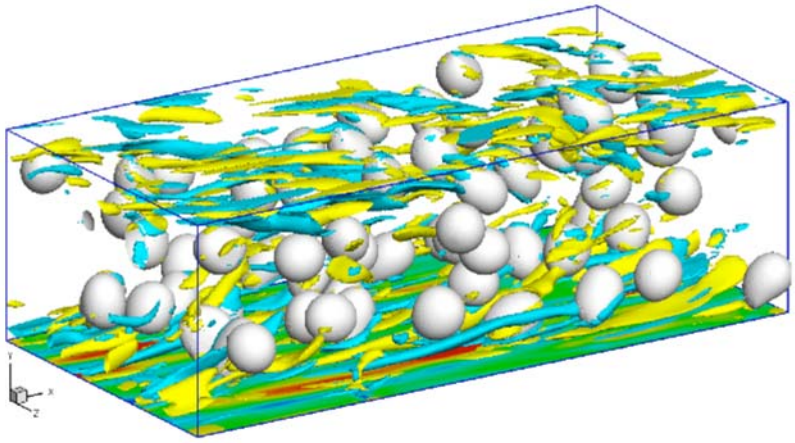

Fig. 3. One frame from a simulation of the effect of bubbles on the wall shear in a turbulent flow, at a relatively early time. The computational domain is $2\pi \times \pi \times 2$ in the streamwise, spanwise and wall-normal direction, respectively.

deformable bubbles can lead to significant reduction of the wall drag (up to 20%) by sliding over streamwise vortices and forcing them toward the wall where they are cancelled by the wall bound vorticity of the opposite sign. Spherical bubbles, on the other hand, often reach into the viscous sublayer where they are slowed down and lead to a increase in drag. This study has demonstrated powerfully the ability of DNS to explain very subtle effects that could probably not be understood in any other way. While the minimum turbulent channel flow is, admittedly, a somewhat special situation, preliminary simulations using larger channels (Figure 3), suggest that the evolution does not depend sensitively on the channel size. Kanai and Miyata [16] and Kawamura and Kodama [18] have also examined the motion of bubbles in turbulent channel flows, but did not see drag reduction.

4 Conclusions

The goal of numerical studies of multiphase flows is to obtain insight into the dynamics of the flow as well as quantitative data. Such data is essential for the modeling of industrial flows. Major progress has been made in using DNS to understand bubbly flows in the last few years, but much remains to be done. Very little has been done to examine the effect of different bubbles sizes and essentially noting for bubble breakup and coalescence. Similarly, the application of the results to help with the improvements of models is only beginning.

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