1

Introduction

Gas–liquid multiphase flows play an essential role in the workings of Nature and the enterprises of mankind. Our everyday encounter with liquids is nearly always at a free surface, such as when drinking, washing, rinsing, and cooking. Similarly, such flows are in abundance in industrial applications: heat transfer by boiling is the preferred mode in both conventional and nuclear power plants, and bubble-driven circulation systems are used in metal processing operations such as steel making, ladle metallurgy, and the secondary refining of aluminum and copper. A significant fraction of the energy needs of mankind is met by burning liquid fuel, and a liquid must evaporate before it burns. In almost all cases the liquid is therefore atomized to generate a large number of small droplets and, hence, a large surface area. Indeed, except for drag (including pressure drops in pipes) and mixing of gaseous fuels, we would not be far off to assert that nearly all industrial applications of fluids involve a multiphase flow of one sort or another. Sometimes, one of the phases is a solid, such as in slurries and fluidized beds, but in a large number of applications one phase is a liquid and the other is a gas. Of natural gas–liquid multiphase flows, rain is perhaps the experience that first comes to mind, but bubbles and droplets play a major role in the exchange of heat and mass between the oceans and the atmosphere and in volcanic explosions. Living organisms are essentially large and complex multiphase systems.

Understanding the dynamics of gas–liquid multiphase flows is of critical engineering and scientific importance and the literature is extensive. From a mathematical point of view, multiphase flow problems are notoriously difficult and much of what we know has been obtained by experimentation and scaling analysis. Not only are the equations, governing the fluid flow in both phases, highly nonlinear, but the position of the phase boundary must generally be found as a part of the solution. Exact analytical solutions, therefore, exist only for the simplest problems, such as the steady-state motion of bubbles and droplets in Stokes flow, linear inviscid waves, and small oscillations of bubbles and droplets. Experimental studies of

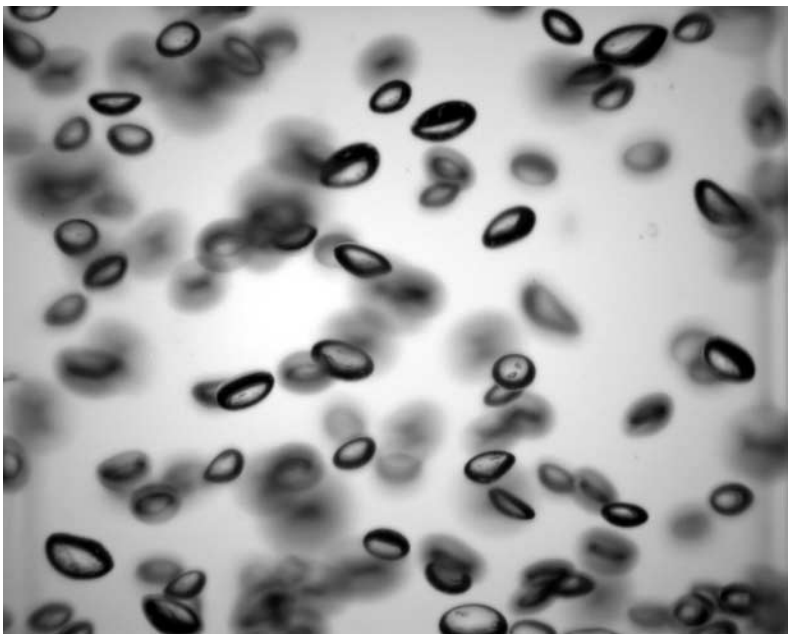

Fig. 1.1. A picture of many buoyant bubbles rising in an otherwise quiescent liquid pool. The average bubble diameter is about 2.2 mm and the void fraction is approximately 0.75%. From Bröder and Sommerfeld (2007). Reproduced with permission.

multiphase flows are not easy either. For many flows of practical interest the length scales are small, the time scales are short, and optical access to much of the flow is limited. The need for numerical solutions of the governing equations has, therefore, been felt by the multiphase research community since the origin of computational fluid dynamics, in the late fifties and early sixties. Although much has been accomplished, simulations of multiphase flows have remained far behind homogeneous flows where direct numerical simulations (DNS) have become a standard tool in turbulence research.

In this book we use DNS to mean simulations of unsteady flow containing a non-trivial range of scales, where the governing equations are solved using sufficiently fine grids so that all continuum time- and length-scales are fully resolved. We believe that this conforms reasonably well with commonly accepted usage, although we recognize that there are exceptions. Some authors feel that DNS refers exclusively to fully resolved simulations of turbulent flows, while others seem to use DNS for any computation of fluid flow that does not include a turbulence model. Our definition falls somewhere in the middle. We also note that some authors, especially in the field of atomization – which is of some importance in this book – refer to unresolved simulations without a turbulence model as LES. We also

Fig. 1.2. A photograph of an atomization experiment performed with coaxial water and air jets reproduced from Villermaux *et al.* (2004). Reproduced with permission. Copyright American Physical Society.

prefer to call such computations DNS, especially as a continuous effort is made in such simulations to check the results as the grid is refined. While it is not surprising that DNS of multiphase flows lags behind homogeneous flows, considering the added difficulty, the situation is certainly not due to lack of effort. However, in the last decade and a half or so, these efforts have started to pay off and rather significant progress has been accomplished on many fronts. It is now possible to do DNS for a large number of fairly complex systems and DNS are starting to yield information that are likely to be unobtainable in any other way. This book is an effort to assess the state of the art, to review how we came to where we are, and to provide the foundation for further progress, involving even more complex multiphase flows.

1.1 Examples of multiphase flows

Since this is a book about numerical simulations, it seems appropriate to start by showing a few "real" systems. The following examples are picked somewhat randomly, but give some insight into the kind of systems that can be examined by direct numerical simulations.

Bubbles are found in a large number of industrial applications. For example, they carry vapor away from hot surfaces in boiling heat transfer, disperse gases and provide stirring in various chemical processing systems, and also affect the propagation of sound in the ocean. To design systems that involve bubbly flows it is necessary to understand how the collective rise velocity of many bubbles depends

Fig. 1.3. The splash generated when a droplet hits a free surface. From A. Davidhazy. Rochester Institute of Technology. Reproduced with permission.

on the void fraction and the bubble size distribution, how bubbles disperse and how they stir up the fluid. Figure 1.1 is a picture of air bubbles rising through water in a small bubble column. The average bubble diameter is about 2.2 mm and the void fraction is approximately 0.75%. At these parameters the bubbles rise with an average velocity of roughly 0.27 m/s, but since the bubbles are not all of the same size they will generally rise with different velocities.

To generate sprays for combustion, coating and painting, irrigation, humidification, and a large number of other applications, a liquid jet must be atomized. Predicting the rate of atomization and the resulting droplet size distribution, as well as droplet velocity, is critical to the successful design of such processes. In Fig. 1.2, a liquid jet is ejected from a nozzle of diameter 8 mm with a velocity of 0.6 m/s. To accelerate its breakup, the jet is injected into a co-flowing air stream, with a velocity of 35 m/s. Initially, the shear between the air and the liquid leads to large axisymmetric waves, but as the waves move downstream the air pulls long filaments from the crest of the wave. The filaments then break into droplets by a capillary instability. See Marmottant and Villermaux (2001) and Villermaux *et al.* (2004) for details.

Droplets impacting solid or liquid surfaces generally splash, often disrupting the surface significantly. Rain droplets falling on the ground often result in soil erosion,

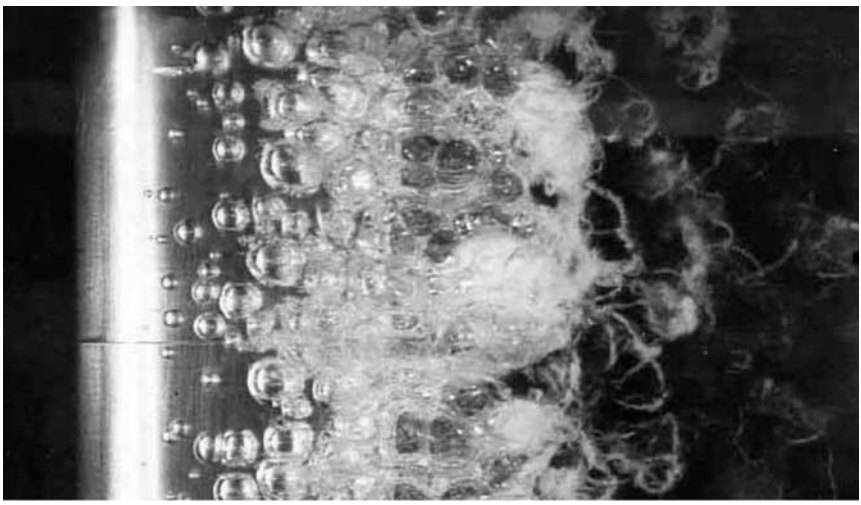

Fig. 1.4. Massive cavitation near the maximum thickness of an airfoil. The flow is from the left to right. In addition to volume change due to phase change, the compressibility of the bubbles is often important (see Section 11.1.5). From Kermeen (1956). Reproduced with permission.

for example. But droplet impact can also help to increase the heat transfer, such as in quenching and spray cooling, and rain often greatly enhances the mixing at the ocean surface. Figure 1.3 shows the splash created when a droplet of a diameter of about 3 mm, released from nearly 0.5 m above the surface, impacts a liquid layer a little over a droplet-diameter deep. The impact of the droplet creates a liquid crater and a rim that often breaks into droplets. As the crater collapses, air bubbles are sometimes trapped in the liquid.

While bubbles are often generated by air injection into a pool of liquid or are formed by entrainment at a free surface, such as when waves break, they also frequently form when a liquid changes phase into vapor. Such a phase change is often nucleated at a solid surface and can take place either by heating the liquid above the saturation temperature, as in boiling, or by lowering the pressure below the vapor pressure, as in cavitation. Figure 1.4 shows massive cavitation near the maximum thickness of an airfoil submerged in water. The chord of the airfoil is 7.6 cm, the flow speed is 13.7 m/s from left to right, and the increase in the liquid velocity as it passes over the leading edge of the airfoil leads to a drop in pressure that is sufficiently large so that the liquid "boils." As the vapor bubbles move into regions of higher pressure at the back of the airfoil, they collapse. However, residual gases, dissolved in the liquid, diffuse into the bubbles during their existence, leaving traces that are visible after the vapor has condensed.

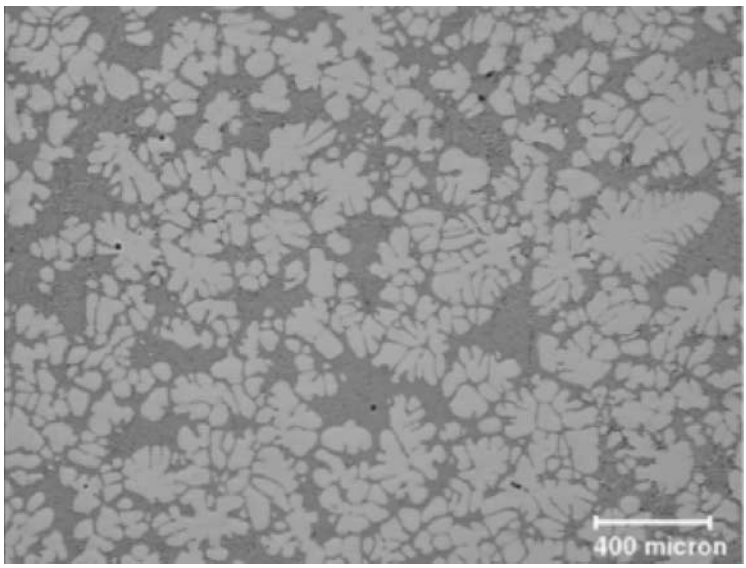

Fig. 1.5. Microstructure of an aluminum–silicon alloy. From D. Apelian, Worcester Polytechnic Institute. Reproduced with permission.

In many multiphase systems one phase is a solid. Suspensions of solid particles in liquids or gases are common and the definition of multiphase flows is sometimes extended to cover flows through or over complex stationary solids, such as packed beds, porous media, forests, and cities. The main difference between gas–liquid multiphase flows and solid–gas or solid–liquid multiphase flows is usually that the interface maintains its shape in the latter cases, even though the location of the solid may change. In some instances, however, that is not the case. Flexible solids can change their shape in response to fluid flow, and during solidification or erosion the boundary can evolve, sometimes into shapes that are just as convoluted as encountered for gas–liquid systems. When a metal alloy solidifies, the solute is initially rejected by the solid phase. This leads to constitutional undercooling and an instability of the solidification front. The solute-rich phase eventually solidifies, but with a very different composition than the material that first became solid. The size, shape, and composition of the resulting microstructures determine the properties of the material, and those are usually sensitively dependent on the various process parameters. A representative micrograph of an Al–Si alloy prepared by metallographic techniques and etching to reveal phase boundaries and interfaces is shown in Fig. 1.5. The light gray phase is almost pure aluminum and solidifies first, but constitutional undercooling leads to dendritic structures of a size on the order of a few tens of micrometers.

Living systems provide an abundance of multiphase flow examples. Suspended blood cells and aerosol in pulmonary flow are obvious examples at the "body"

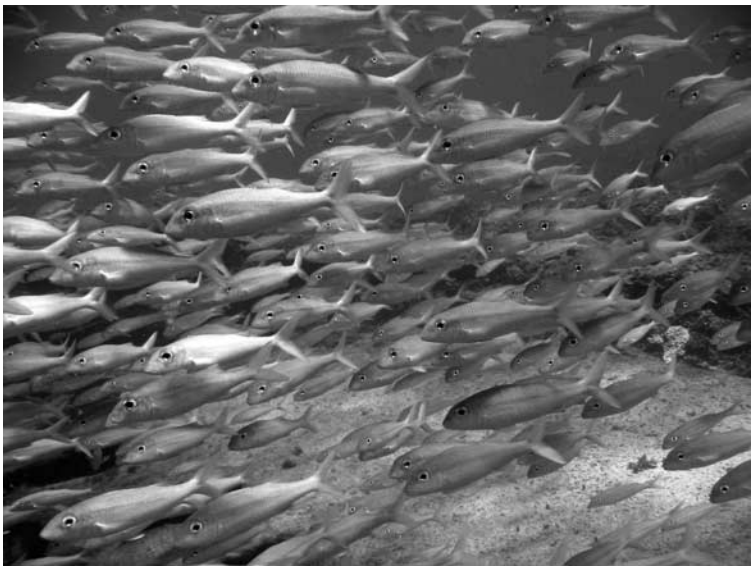

Fig. 1.6. A school of yellow-tailed goatfish (*Mulloidichthys flavolineatus*) near the Northwest Hawaiian Islands. Since self-propelled bodies develop a thrust-producing wake, their collective dynamics is likely to differ significantly from rising or falling bodies. From the NOAA Photo Library.

scale, as are the motion of organs and even complete individuals. But even more complex systems, such as the motion of a flock of birds through air and a school of fish through water, are also multiphase flows. Figure 1.6 show a large number of yellow-tailed goatfish swimming together and coordinating their movement. An understanding of the motion of both a single fish and the collective motion of a large school may have implication for population control and harvesting, as well as the construction of mechanical swimming and flying devices.

1.2 Computational modeling

Computations of multifluid (two different fluids) and multiphase (same fluid, different phases) flows are nearly as old as computations of constant-density flows. As for such flows, a number of different approaches have been tried and a number of simplifications used. In this section we will attempt to give a brief but comprehensive overview of the major efforts to simulate multi-fluid flows. We make no attempt to cite every paper, but hope to mention all major developments.

1.2.1 Simple flows ($Re = 0$ and $Re = \infty$)

In the limit of either very large or very small viscosity (as measured by the Reynolds number, see Section 2.2.6), it is sometimes possible to simplify considerably the

flow description by either ignoring inertia completely (Stokes flow) or by ignoring viscous effects completely (inviscid flow). For inviscid flows it is usually further necessary to assume that the flow is irrotational, except at fluid interfaces. Most success has been achieved for disperse flows of undeformable spheres where, in both these limits, it is possible to reduce the governing equations to a system of coupled ordinary differential equations (ODEs) for the particle positions. For Stokes flow the main developer was Brady and his collaborators (see Brady and Bossis (1988) for a review of early work) who have investigated extensively the properties of suspensions of particles in shear flows, among other problems. For inviscid flows, Sangani and Didwania (1993) and Smereka (1993) simulated the motion of spherical bubbles in a periodic box and observed that the bubbles tended to form horizontal clusters, particularly when the variance of the bubble velocity was small.

For both Stokes flows and inviscid potential flows, problems with deformable boundaries can be simulated with boundary integral techniques. One of the earliest attempts was due to Birkhoff (1954), where the evolution of the interface between a heavy fluid initially on top of a lighter one (the Rayleigh–Taylor instability) was followed by a method tracking the interface between two inviscid and irrotational fluids. Both the method and the problem later became a staple of multiphase flow simulations. A boundary integral method for water waves was presented by Longuet-Higgins and Cokelet (1976) and used to examine breaking waves. This paper had enormous influence and was followed by a large number of very successful extensions and applications, particularly for water waves (e.g. Vinje and Brevig, 1981; Baker *et al.*, 1982; Schultz *et al.*, 1994). Other applications include the evolution of the Rayleigh–Taylor instability (Baker *et al.*, 1980), the growth and collapse of cavitation bubbles (Blake and Gibson, 1981; Robinson *et al.*, 2001), the generation of bubbles and droplets due to the coalescence of bubbles with a free surface (Oguz and Prosperetti, 1990; Boulton-Stone and Blake, 1993), the formation of bubbles and droplets from an orifice (Oguz and Prosperetti, 1993), and the interactions of vortical flows with a free surface (Yu and Tryggvason, 1990), just to name a few. All boundary integral (or boundary element, when the integration is element based) methods for inviscid flows are based on following the evolution of the strength of surface singularities in time by integrating a Bernoulli-type equation. The surface singularities give one velocity component and Green's second theorem yields the other, thus allowing the position of the surface to be advanced in time. Different surface singularities allow for a large number of different methods (some that can only deal with a free surface and others that are suited for two-fluid problems), and different implementations multiply the possibilities even further. For an extensive discussion and recent progress, see Hou *et al.* (2001). Although continuous improvements are being made and new applications continue

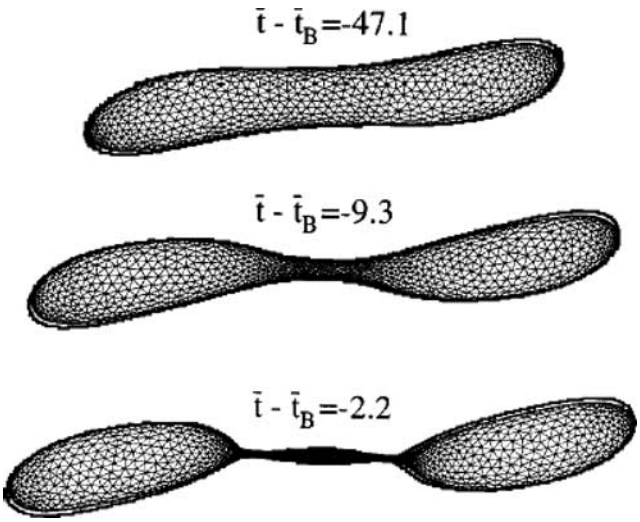

Fig. 1.7. A Stokes flow simulation of the breakup of a droplet in a linear shear flow. The barely visible line behind the numerical results is the outline of a drop traced from an experimental photograph. Reprinted with permission from Cristini *et al.* (1998). Copyright 2005, American Institute of Physics.

to appear, two-dimensional boundary integral techniques for inviscid flows are by now – more than 30 years after the publication of the paper by Longuet-Higgins and Cokelet – a fairly mature technology. Fully three-dimensional computations are, however, still rare. Chahine and Duraiswami (1992) computed the interactions of a few inviscid cavitation bubbles and Xue *et al.* (2001) have simulated a three-dimensional breaking wave. While the potential flow assumption has led to many spectacular successes, particularly for short-time transient flows, its inherent limitations are many. The lack of a small-scale dissipative mechanism makes those models susceptible to singularity formation and the absence of dissipation usually makes them unsuitable for the predictions of the long-time evolution of any system.

The key to the reformulation of inviscid interface problems with irrotational flow in terms of a boundary integral is the linearity of the potential equation. In the opposite limit, where inertia effects can be ignored and the flow is dominated by viscous dissipation, the Navier–Stokes equations become linear (the so-called Stokes flow limit) and it is also possible to recast the governing equations as an integral equation on a moving surface. Boundary integral simulations of unsteady two-fluid Stokes problems originated with Youngren and Acrivos (1976) and Rallison and Acrivos (1978), who simulated the deformation of a bubble and a droplet, respectively, in an extensional flow. Subsequently, several authors have

investigated a number of problems. Pozrikidis and collaborators have examined several aspects of suspensions of droplets, starting with a study by Zhou and Pozrikidis (1993) of the suspension of a few two-dimensional droplets in a channel. Simulations of fully three-dimensional suspensions have been done by Loewenberg and Hinch (1996) and Zinchenko and Davis (2000). The method has been described in detail in the book by Pozrikidis (1992), and Pozrikidis (2001) gives a very complete summary of the various applications. An example of a computation of the breakup of a very viscous droplet in a linear shear flow, using a method that adaptively refines the surface grid as the droplet deforms, is shown in Fig. 1.7.

In addition to inviscid flows and Stokes flows, boundary integral methods have been used by a number of authors to examine two-dimensional, two-fluid flows in Hele–Shaw cells. Although the flow is completely viscous, away from the interface it is a potential flow. The interface can be represented by the singularities used for inviscid flows (de Josselin de Jong, 1960), but the evolution equation for the singularity strength is different. This was used by Tryggvason and Aref (1983, 1985) to examine the Saffman–Taylor instability, where an interface separating two fluids of different viscosity deforms if the less viscous fluid is displacing the more viscous one. They used a fixed grid to solve for the normal velocity component (instead of Green's theorem), but Green's theorem was subsequently used by several authors to develop boundary integral methods for interfaces in Hele–Shaw cells. See, for example, DeGregoria and Schwartz (1985), Meiburg and Homsy (1988), and the review by Hou *et al.* (2001).

Under the heading of simple flows we should also mention simulations of the motion of solid particles, in the limit where the fluid motion can be neglected and the dynamics is governed only by the inertia of the particles. Several authors have followed the motion of a large number of particles that interact only when they collide with each other. Here, it is also sufficient to solve a system of ODEs for the particle motion. Simulations of this kind are usually called "granular dynamics." For an early discussion, see Louge (1994); a more recent one can be found in Pöschel and Schwage (2005), for example. While these methods have been enormously successful in simulating certain types of solid–gas multiphase flows, they are limited to a very small class of problems. One could, however, argue that simulations of the motion of particles interacting through a potential, such as simulations of the gravitational interactions of planets or galaxies and molecular dynamics, also fall into this class. Discussing such methods and their applications would enlarge the scope of the present work enormously, and so we will confine our coverage by simply suggesting that the interested reader consults the appropriate references, such as Schlick (2002) for molecular simulations and Hockney and Eastwood (1981) for astrophysical and other systems.