Direct Numerical Simulations of Gas–Liquid Multiphase Flows

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Accurately predicting the behavior of multiphase flows is a problem of immense industrial and scientific interest. Using modern computers, researchers can now study the dynamics in great detail, and computer simulations are yielding unprecedented insight. This book provides a comprehensive introduction to direct numerical simulations of multiphase flows for researchers and graduate students.

After a brief overview of the context and history, the authors review the governing equations. A particular emphasis is placed on the "one-fluid" formulation, where a single set of equations is used to describe the entire flow field and interface terms are included as singularity distributions. Several applications are discussed, such as atomization, droplet impact, breakup and collision, and bubbly flows, showing how direct numerical simulations have helped researchers advance both our understanding and our ability to make predictions. The final chapter gives an overview of recent studies of flows with relatively complex physics, such as mass transfer and chemical reactions, solidification, and boiling, and includes extensive references to current work.

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Preface

Progress is usually a sequence of events where advances in one field open up new opportunities in another, which in turn makes it possible to push yet another field forward, and so on. Thus, the development of fast and powerful computers has led to the development of new numerical methods for direct numerical simulations (DNS) of multiphase flows that have produced detailed studies and improved knowledge of multiphase flows. While the origin of DNS of multiphase flows goes back to the beginning of computational fluid dynamics in the early sixties, it is only in the last decade and a half that the field has taken off. We, the authors of this book, have had the privilege of being among the pioneers in the development of these methods and among the first researchers to apply DNS to study relatively complex multiphase flows. We have also had the opportunity to follow the progress of others closely, as participants in numerous meetings, as visitors to many laboratories, and as editors of scientific journals such as the *Journal of Computational Physics* and the *International Journal of Multiphase Flows*. To us, the state of the art can be summarized by two observations:

- Even though there are superficial differences between the various approaches being pursued for DNS of multiphase flows, the similarities and commonalities of the approaches are considerably greater than the differences.
- As methods become more sophisticated and the problems of interest become more complex, the barrier that must be overcome by a new investigator wishing to do DNS of multiphase flows keeps increasing.

This book is an attempt to address both issues.

The development of numerical methods for flows containing a sharp interface, as fluids consisting of two or more immiscible components inherently do, is currently a "hot" topic and significant progress has been made by a number of groups. Indeed, for a while there was hardly an issue of the *Journal of Computational Physics* that did not contain one or more papers describing such methods. In the present book we have elected to focus mostly on two specific classes of methods: volume of fluid (VOF) and front-tracking methods. This choice reflects our own background, as well as the fact that both types of method have been very successful and are responsible for some of the most significant new insights into multiphase flow dynamics that DNS has revealed. Furthermore, as emphasized by the first bullet point, the similarities in the different approaches are sufficiently great that

a reader of the present book would most likely find it relatively easy to switch to other methods capable of capturing the interface, such as level set and phase field.

The goal of DNS of multiphase flows is the understanding of the behavior and properties of such flows. We believe that while the development of numerical methods is important, it is in their applications where the most significant rewards are to be found. Thus, we include in the book several chapters where we describe the use of DNS to understand specific systems and what has been learned up to now. This is inherently a somewhat biased sample (since we elected to talk about studies that we know well – our own!), but we feel that the importance of these chapters goes beyond the specific topics treated. We furthermore firmly believe that the methods that we describe here have now reached sufficient maturity so that they can be used to probe the mysteries of a large number of complex flows. Therefore, the application of existing methods to problems that they are suited for and the development of new numerical methods for more complex flows, such as those described in the final chapter, are among the most exciting immediate directions for DNS of multiphase flows.

Our work has benefitted from the efforts of many colleagues and friends. First and foremost we thank our students, postdoctoral researchers and visitors for the many and significant contributions they have made to the work presented here. GT would like to thank his students, Drs. D. Yu, M. Song, S.O. Unverdi, E. Ervin, M.R. Nobari, C.H.H. Chang, Y.-J. Jan, S. Nas, M. Saeed, A. Esmaeeli, F. Tounsi, D. Juric, N.C. Suresh, J. Han, J. Che, B. Bunner, N. Al-Rawahi, W. Tauber, M. Stock, S. Biswas, and S. Thomas, as well as the following visitors and postdoctoral researchers: S. Homma, J. Wells, A. Fernandez, and J. Lu. RS would like to thank his students, Drs. E. Aulisa, L. Campioni, A. Cervone, and V. Marra, as well as his collaborators S. Manservisi, P. Yecko, and G. Zanetti. SZ would like to thank his students, Drs. B. Lafaurie, F.-X. Keller, J. Li, D. Gueyffier, S. Popinet, A. Leboissetier, L. Duchemin, O. Devauchelle, A. Bagué, and G. Agbaglah, as well as his collaborators, visitors, and postdoctoral researchers, G. Zanetti, A. Nadim, J.-M. Fullana, C. Josserand, P. Yecko, M. and Y. Renardy, E. Lopez-Pages, T. Boeck, P. Ray, D. Fuster, G. Tomar, and J. Hoepffner. SZ would also like to thank his trusted friends and mentors, Y. Pomeau, D.H. Rothman, and E.A. Spiegel, for their invaluable advice. We also thank Ms. Victoria Tsengué Ingoba for reading the complete book twice and pointing out numerous typos and mistakes. Any errors, omissions, and ambiguities are, of course, the fault of the authors alone.

And last, but certainly not least, we would like to thank our families for unerring support, acceptance of long working hours, and tolerance of (what sometimes must have seemed) obscure priorities.

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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

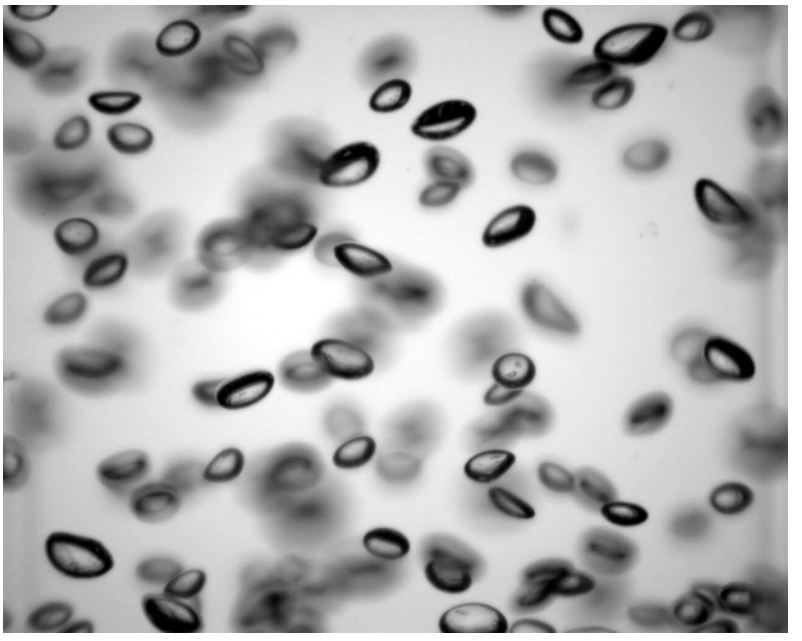

Fig. 1.1. A picture of many buoyant bubbles rising in an otherwise quiescent liquid pool. The average bubble diameter is about 2.2 mm and the void fraction is approximately 0.75%. From Bröder and Sommerfeld (2007). Reproduced with permission.

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.

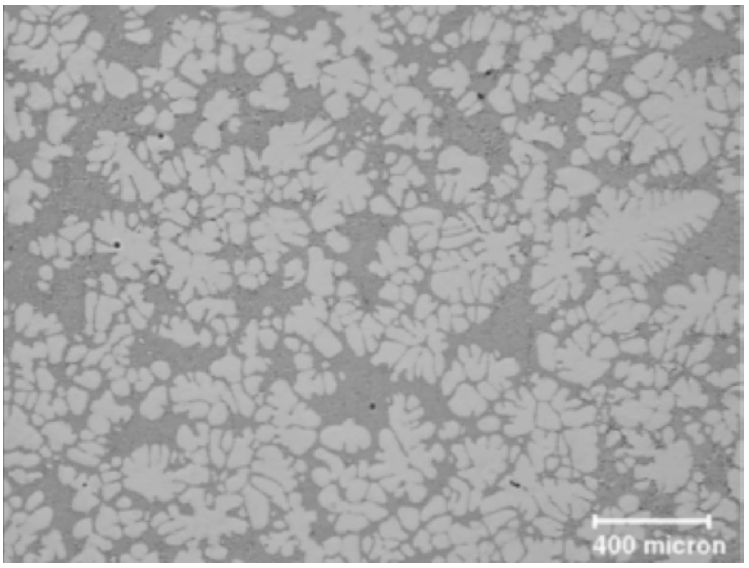

Fig. 1.5. Microstructure of an aluminum–silicon alloy. From D. Apelian, Worcester Polytechnic Institute. Reproduced with permission.

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”

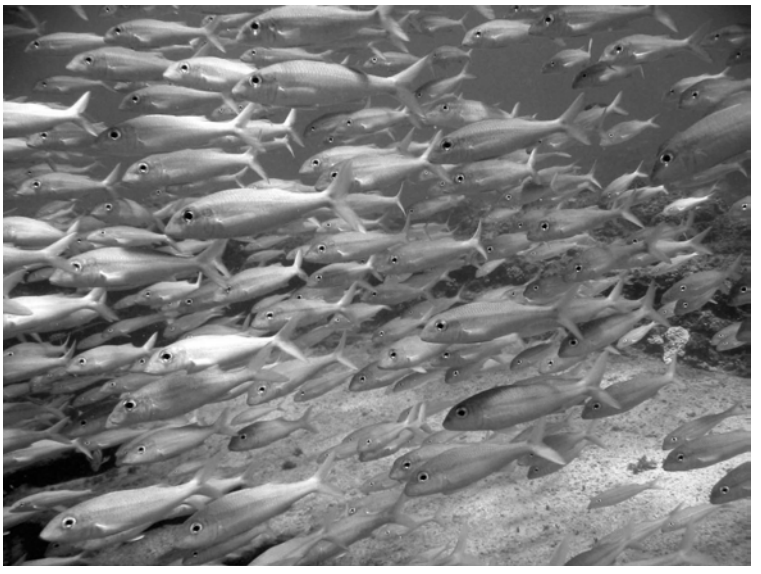

Fig. 1.6. A school of yellow-tailed goatfish (*Mulloidichthys flavolineatus*) near the Northwest Hawaiian Islands. Since self-propelled bodies develop a thrust-producing wake, their collective dynamics is likely to differ significantly from rising or falling bodies. From the NOAA Photo Library.

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

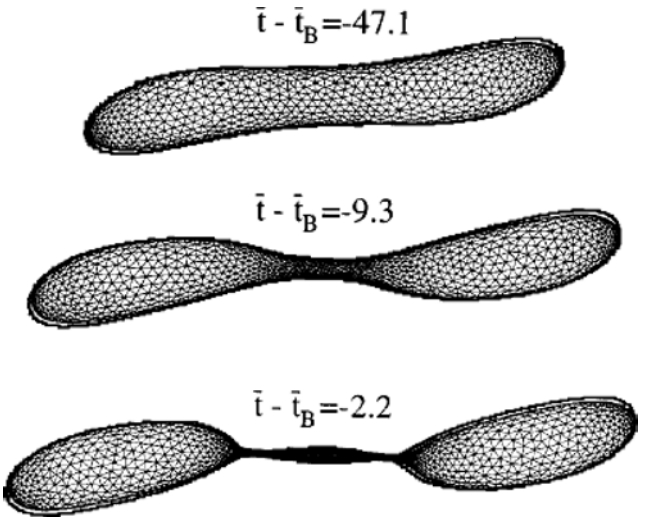

Fig. 1.7. A Stokes flow simulation of the breakup of a droplet in a linear shear flow. The barely visible line behind the numerical results is the outline of a drop traced from an experimental photograph. Reprinted with permission from Cristini *et al.* (1998). Copyright 2005, American Institute of Physics.

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.

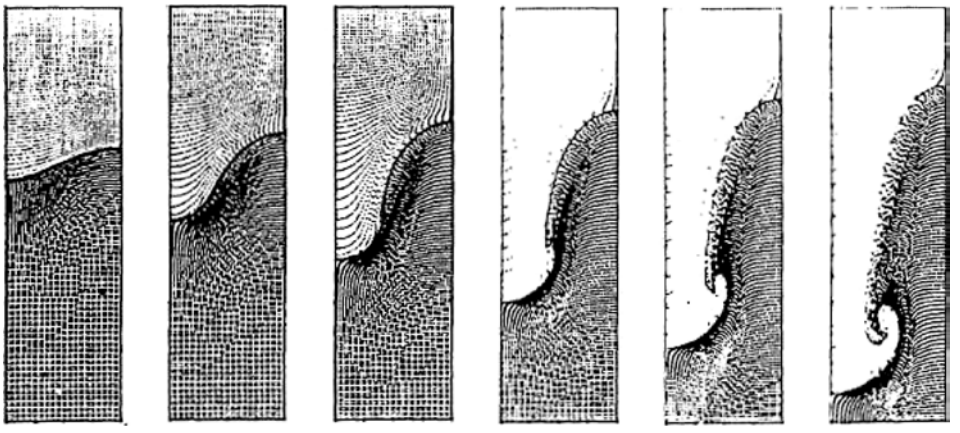

Fig. 1.8. The beginning of computational studies of multiphase flows. The evolution of the nonlinear Rayleigh–Taylor instability, computed using the two-fluid MAC method. Reprinted with permission from Daly (1969b). Copyright 2005, American Institute of Physics.

1.2.2 Finite Reynolds number flows

For intermediate Reynolds numbers it is necessary to solve the full Navier–Stokes equations. Nearly 10 years after Birkhoff's effort to simulate the inviscid Rayleigh–Taylor problem by a boundary integral technique, the marker-and-cell (MAC) method was developed at Los Alamos by Harlow and collaborators. In the MAC method the fluid is identified by marker particles distributed throughout the fluid region and the governing equations solved on a regular grid that covers both the fluid-filled and the empty part of the domain. The method was introduced in Harlow and Welch (1965) and two sample computations of the so-called dam breaking problem were shown in that first paper. Several papers quickly followed: Harlow and Welch (1966) examined the Rayleigh–Taylor problem (Fig. 1.8) and Harlow and Shannon (1967) studied the splash when a droplet hits a liquid surface. As originally implemented, the MAC method assumed a free surface, so there was only one fluid involved. This required boundary conditions to be applied at the surface and the fluid in the rest of the domain to be completely passive. The Los Alamos group realized, however, that the same methodology could be applied to two-fluid problems. Daly (1969b) computed the evolution of the Rayleigh–Taylor instability for finite density ratios and Daly and Pracht (1968) examined the initial motion of density currents. Surface tension was then added by Daly (1969a) and the method again used to examine the Rayleigh–Taylor instability. The MAC method quickly attracted a small group of followers that used it to study several problems: Chan and Street (1970) applied it to free-surface waves, Foote (1973)

and Foote (1975) simulated the oscillations of an axisymmetric droplet and the collision of a droplet with a rigid wall, respectively, and Chapman and Plesset (1972) and Mitchell and Hammitt (1973) followed the collapse of a cavitation bubble. While the Los Alamos group did a number of computations of various problems in the sixties and early seventies and Harlow described the basic idea in a *Scientific American* article (Harlow and Fromm, 1965), the enormous potential of this newfound tool did not, for the most part, capture the fancy of the fluid mechanics research community. Although the MAC method was designed specifically for multifluid problems (hence the M for markers!), it was also the first method to successfully solve the Navier–Stokes equation using the primitive variables (velocity and pressure). The staggered grid used was a novelty, and today it is a common practice to refer to any method using a projection-based time integration on a staggered grid as a MAC method (see Chapter 3).

The next generation of methods for multifluid flows evolved gradually from the MAC method. It was already clear in the Harlow and Welch (1965) paper that the marker particles could cause inaccuracies, and of the many algorithmic ideas explored by the Los Alamos group, the replacement of the particles by a marker function soon became the most popular alternative. Thus, the volume-of-fluid (VOF) method was born. VOF was first discussed in a refereed journal article by Hirt and Nichols (1981), but the method originated earlier (DeBar, 1974; Noh and Woodward, 1976). The basic problem with advecting a marker function is the numerical diffusion resulting from working with a cell-averaged marker function (see Chapter 4). To prevent the marker function from continuing to diffuse, the interface is "reconstructed" in the VOF method in such a way that the marker does not start to flow into a new cell until the current cell is full. The one-dimensional implementation of this idea is essentially trivial, and in the early implementation of VOF the interface in each cell was simply assumed to be a vertical plane for advection in the horizontal direction and a horizontal plane for advection in the vertical direction. This relatively crude reconstruction often led to large amount of "floatsam and jetsam" (small unphysical droplets that break away from the interface) that degraded the accuracy of the computation. To improve the representation, Youngs (1982), Ashgriz and Poo (1991), and others introduced more complex reconstructions of the interface, representing it with a line (two dimensions) or a plane (three dimensions) that could be oriented arbitrarily in such a way as to best fit the interface. This increased the complexity of the method considerably, but resulted in greatly improved advection of the marker function. Even with higher order representation of the fluid interface in each cell, the accurate computation of surface tension remained a major problem. In his simulations of surface tension effects on the Rayleigh–Taylor instability, using the MAC method, Daly (1969b) introduced explicit surface markers for this purpose. However, the premise behind the

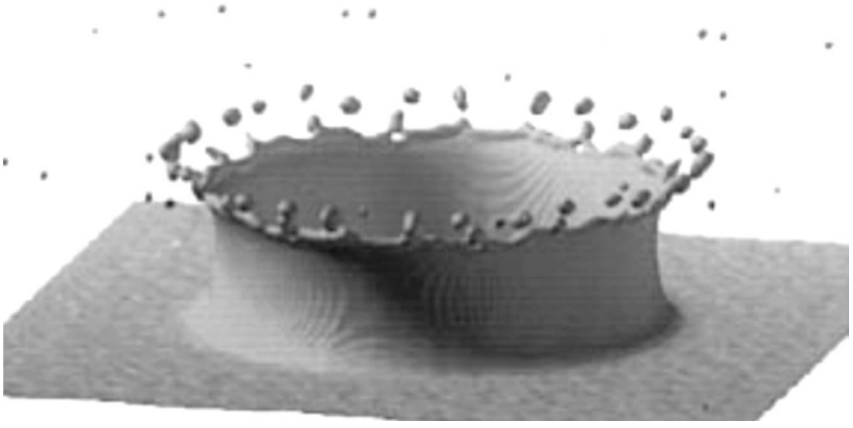

Fig. 1.9. Computation of a splashing drop using an advanced VOF method. Reprinted from Rieber and Frohn (1999) with permission from Elsevier.

development of the VOF method was to get away from using any kind of surface marker so that the surface tension had to be obtained from the marker function instead. This was achieved by Brackbill *et al.* (1992), who showed that the curvature (and hence surface tension) could be computed by taking the discrete divergence of the marker function. A "conservative" version of this "continuum surface force" method was developed by Lafaurie *et al.* (1994). The VOF method has been extended in various ways by a number of authors. In addition to better ways to reconstruct the interface (Rider and Kothe, 1998; Scardovelli and Zaleski, 2000; Aulisa *et al.*, 2007) and compute the surface tension (Renardy and Renardy, 2002; Popinet, 2009), more advanced advection schemes for the momentum equation and better solvers for the pressure equation have been introduced (see Rudman (1997), for example). Other refinements include the use of sub-cells to keep the interface as sharp as possible (Chen *et al.*, 1997a). VOF methods are in widespread use today, and many commercial codes include VOF to track interfaces and free surfaces. Figure 1.9 shows one example of a computation of the splash made when a liquid droplet hits a free surface, done by a modern VOF method. We will discuss the use of VOF extensively in later chapters.

The basic ideas behind the MAC and the VOF methods gave rise to several new approaches in the early nineties. Unverdi and Tryggvason (1992) introduced a front-tracking method for multifluid flows where the interface was marked by connected marker points. The markers are used to advect the material properties (such as density and viscosity) and to compute surface tension, but the rest of the computations are done on a fixed grid as in the VOF method. Although using

connected markers to update the material function was new, marker particles had already been used by Daly (1969a), who used them to evaluate surface tension in simulations with the MAC method, in the immersed-boundary method of Peskin (1977) for one-dimensional elastic fibers in homogeneous viscous fluids and in the vortex-in-cell method of Tryggvason and Aref (1983) for two-fluid interfaces in a Hele–Shaw cell, for example. The front-tracking method of Unverdi and Tryggvason (1992) has been very successful for simulations of finite Reynolds number flows of immiscible fluids and Tryggvason and collaborators have used it to explore a large number of problems.

The early nineties also saw the introduction of the level-set, the CIP, and the phase-field methods to track fluid interfaces on stationary grids. The level-set method was introduced by Osher and Sethian (1988), but its first use to track fluid interfaces appears to be in the work of Sussman *et al.* (1994) and Chang *et al.* (1996), who used it to simulate the rise of bubbles and the fall of droplets in two dimensions. An axisymmetric version was used subsequently by Sussman and Smereka (1997) to examine the behavior of bubbles and droplets. Unlike the VOF method, where a discontinuous marker function is advected with the flow, in the level-set method a continuous level-set function is used. The interface is then identified with the zero contour of the level-set function. To reconstruct the material properties of the flow (density and viscosity, for example) a marker function is constructed from the level-set function. The marker function is given a smooth transition zone from one fluid to the next, thus increasing the regularity of the interface over the VOF method where the interface is confined to only one grid space. However, this mapping from the level-set function to the marker function requires the level-set function to maintain the same shape near the interface and to deal with this problem, Sussman *et al.* (1994) introduced a reinitialization procedure where the level-set function is adjusted in such a way that its value is equal to the shortest distance to the interface at all times. This step was critical in making level-sets work for fluid-dynamics simulations. Surface tension is found in the same way as in the continuous surface force technique introduced for VOF methods by Brackbill *et al.* (1992). The early implementation of the level-set method did not conserve mass very well, and a number of improvements and extensions followed its original introduction. Sussman *et al.* (1998) and Sussman and Fatemi (1999) introduced ways to improved mass conservation, Sussman *et al.* (1999) coupled level-set tracking with adaptive grid refinement and a hybrid VOF/level-set method was developed by Sussman and Puckett (2000), for example.

The constrained interpolated propagation (CIP) method introduced by Takewaki *et al.* (1985) has been particularly popular with Japanese authors, who have applied it to a wide variety of multiphase problems. In the CIP method, the transition from one fluid to another is described by a cubic polynomial. Both the marker function

and its derivative are then updated to advect the interface. In addition to simulating two-fluid problems, the method has been used for a number of more complex applications, such as those involving floating solids; see Yabe *et al.* (2001).

In the phase-field method the governing equations are modified in such a way that the dynamics of the smoothed region between the different fluids is described in a thermodynamically consistent way. In actual implementations the thickness of the transition is, however, much larger than it is in real systems and the net effect of the modification is to provide an "antidiffusive" term that keeps the interface reasonably sharp. While superficially there are considerable similarities between phase-field and level-set methods, the fundamental ideas behind the methods are very different. In the level-set method the smoothness of the phase boundary is completely artificial and introduced for numerical reasons only. In phase-field methods, on the other hand, the transition zone is real, although it is made much thicker than it should be for numerical reasons. It is not clear, at the time of this writing, whether keeping the correct thermodynamic conditions in an artificially thick interface has any advantages over methods that start with a completely sharp interface. The key drawback seems to be that since the propagation and properties of the interface depend sensitively on the dynamics in the transition zone, it must be well resolved. For the motion of two immiscible fluids, that are well described by assuming a sharp interface, this adds a resolution requirement that is more stringent than for other "one-fluid" methods. The phase-field approach was originally introduced to model solidification (see Kobayashi (1992, 1993)) and has found widespread use in such simulations. With the exception of the modeling of solidification in the presence of flows (Beckermann *et al.*, 1999; Tonhardt and Amberg, 1998), its use for fluid dynamic simulations is relatively limited (Jacqmin, 1999; Jamet *et al.*, 2001). The main appeal of the phase-field methods appears to be for problems where small-scale physics must be accounted for and it is difficult to do so in the sharp interface limit.

In the "one-fluid" methods described above, where a single set of governing equations is used to describe the fluid motion in both fluids, the fluid motion is mostly computed on regular structured grids and the main difference between the various methods is how a marker function is advected (and how surface tension is found). The thickness of the interface varies from one cell in VOF methods to a few cells in level-set and front-tracking methods, but once the marker function has been found, the specific scheme for the interface advection is essentially irrelevant for the rest of the computations. While these methods have been enormously successful, their accuracy is generally somewhat limited. There have, therefore, recently been several attempts to generate methods that retain most of the advantages of these methods but treat the interface as "fully sharp." The origin of these attempts can be traced to the work of Glimm and collaborators (Glimm *et al.*, 1981; Glimm

and McBryan, 1985; Chern *et al.*, 1986), who used grids that were modified locally near an interface in such a way that the interface coincided with a cell boundary, and more recent "cut-cell" methods for the inclusion of complex bodies in simulations of inviscid flows (Quirk, 1994; Powell, 1998). In their modern incarnation, sharp interface methods include the ghost fluid method, the immersed-interface method and the method of Udaykumar *et al.* (2001). In the "ghost fluid" method introduced by Fedkiw *et al.* (1999) the interface is marked by advecting a level-set function, but to find numerical approximations to derivatives near the interface, where the finite difference stencil involves values from the other side of the interface, fictitious values are assigned to those grid points. The values are obtained by extrapolation, and a few different possibilities for doing so are discussed by Glimm *et al.* (2001), for example. The "immersed-interface" method of Lee and LeVeque (2003), on the other hand, is based on modifying the numerical approximations near the interface by explicitly incorporating the jump across the interface into the finite difference equations. While this is easily done for relatively simple jump conditions, it becomes more involved for complex situations. Lee and LeVeque (2003) thus found it necessary to limit their development to fluids with the same viscosity. In the method of Udaykumar *et al.* (2001), complex solid boundaries are represented on a regular grid by merging cells near the interface and using polynomial fitting to find field values at the interface. This method, which is related to the "cut-cell" methods used for inviscid compressible flows (Powell, 1998), has so far only been implemented for solids and fluids, including solidification (Yang and Udaykumar, 2005), but there seems to be no reason why the method cannot be used for multifluid problems. For an extension to three dimensions, see Marella *et al.* (2005).

While the original "one-fluid" methods require essentially no modification of the flow solver near the interface (except allowing for variable density and viscosity), the sharp interface methods all require localized modifications of the basic scheme. This results in considerably more complex numerical schemes, but is also likely to improve the accuracy. That may be important for extreme values of the governing parameters, such as large differences between the material properties of the different fluids and low viscosities. The sharp interface approach may also be required for flows with very complex interface physics. However, methods based on a straightforward implementation of the "one-fluid" formulation of the governing equations, coupled with advanced schemes to advect the interface (or marker function), have already demonstrated their usefulness for a large range of problems, and it is likely that their simplicity will ensure that they will continue to be widely used.

In addition to the development of more accurate implementations of the "one-fluid" approach, many investigators have pursued extension of the basic schemes to problems that are more complex than the flow of two immiscible liquids. More

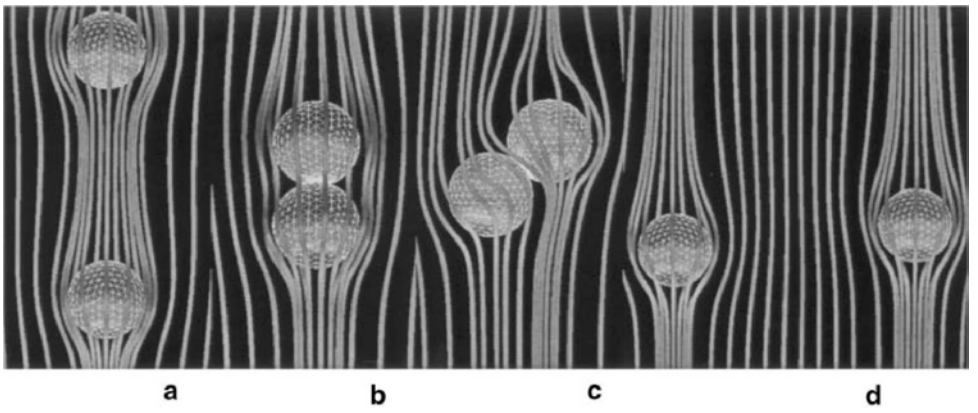

Fig. 1.10. The interaction of two falling spheres. The spheres are shown at four different times, going from left to right. Reprinted from Hu *et al.* (2001), with permission from Elsevier.

complex physics has been incorporated to simulate contaminated interfaces, mass transfer and chemical reactions, electrorheological effects, boiling, solidification, and the interaction of solid bodies with a free surface or a fluid interface. We will briefly review such advanced applications at the very end of the book, in Chapter 11.

While methods based on the "one-fluid" approach were being developed, other techniques were also explored. Hirt *et al.* (1970) describe one of the earliest use of structured, boundary-fitted Lagrangian grids. In this approach a logically rectangular structured grid is used, but the grid points move with the fluid velocity, thus deforming the grid. This approach is particularly well suited when the interface topology is relatively simple and no unexpected interface configurations develop. In a related approach, a grid line is aligned with the fluid interface, but the grid away from the interface is generated using standard grid-generation techniques, such as conformal mapping, or other more advanced elliptic grid-generation schemes. The method was used by Ryskin and Leal (1984) to compute the steady rise of buoyant, deformable, axisymmetric bubbles. They assumed that the fluid inside the bubble could be neglected, but Dandy and Leal (1989) and Kang and Leal (1987) extended the method to two-fluid problems and unsteady flows. Several authors have used this approach to examine relatively simple problems, such as the steady-state motion of single particles or moderate deformation of free surfaces. Fully three-dimensional simulations are relatively rare (see, though, Takagi *et al.* (1997)), and it is probably fair to say that it is unlikely that this approach will be the method of choice for very complex problems such as the three-dimensional unsteady motion of several particles.

A much more general approach to continuously represent a fluid interface by a grid line is to use fully unstructured grids. This allows grid points to be inserted and deleted as needed and distorted grid cells to be reshaped. While the grid was moved with the fluid velocity in some of the early applications of this method, the more modern approach is either to move only the interface points or to move the interior nodes with a velocity different from the fluid velocity, in such a way that the grid distortion is reduced but adequate resolution is still maintained. A large number of methods have been developed that fall into this general category, but we will only reference a few examples. Oran and Boris (1987) simulated the breakup of a two-dimensional drop; Shopov *et al.* (1990) examined the initial deformation of a buoyant bubble; Feng *et al.* (1994, 1995) and Hu (1996) computed the unsteady two-dimensional motion of several particles and Fukai *et al.* (1995) followed the collision of a single axisymmetric droplet with a wall. Although this appears to be a fairly complex approach, Johnson and Tezduyar (1997) and Hu *et al.* (2001) have produced very impressive results for the three-dimensional unsteady motion of many spherical particles. Figure 1.10 shows an example of a simulation done using the arbitrary-Lagrangian–Eulerian method of Hu *et al.* (2001). Here, two solid spheres are initially falling in-line (left frame). Since the trailing sphere is sheltered from the flow by the leading one, it catches up and "kisses" the leading one. The in-line configuration is unstable and the spheres "tumble" (two middle frames). After tumbling, the spheres drift apart (right frame).

The most recent addition to the collection of methods to simulate finite Reynolds number multiphase flows is the lattice–Boltzmann method (LBM). It is now clear that LBM can be used to obtain results of accuracy comparable to more conventional methods. It is still not clear, however, whether the LBM is significantly faster or simpler than other methods (as sometimes claimed), but most likely these methods are here to stay. For a discussion see, for example, Shan and Chen (1993) and Sankaranarayanan *et al.* (2002). A comparison of results obtained by the LBM method and the front-tracking method of Unverdi and Tryggvason (1992) can be found in Sankaranarayanan *et al.* (2003). We will not discuss LBM in this book, but refer the reader to Rothman and Zaleski (1997) and Chapter 6 in Prosperetti and Tryggvason (2007).

1.3 Looking ahead

Direct numerical simulations of multiphase flows have come a long way in the last decade and a half or so. It is now possible to simulate accurately the evolution of disperse flows of several hundred bubbles, droplets, and particles for sufficiently long times so that reliable values can be obtained for various statistical quantities. Similarly, major progress has been achieved in the development of methods

for more complex flows, including those where a liquid solidifies or evaporates. Simulations of large systems undergoing boiling and solidification are therefore within reach.

Much remains to be done, however, and it is probably fair to say that the use of direct numerical simulations of multiphase flows for research and design is still in the embryonic state. The possibility of computing the evolution of complex multiphase flows – such as churn-turbulent bubbly flow undergoing boiling, or the breakup of a jet into evaporating droplets – will transform our understanding of flows of enormous economic significance. Currently, control of most multiphase flow processes is fairly rudimentary and almost exclusively based on intuition and empirical observations. Industries that deal primarily with multiphase flows are, however, multibillion dollar operations, and the savings realized if atomizers for spray generation, bubble injectors in bubble columns, and inserts into pipes to break up droplets, just to name a few examples, could be improved by just a little bit would add up to a substantial amount of money. Reliable predictions would also reduce the design cost significantly for situations such as space vehicles and habitats where experimental investigations are expensive. And, as the possibilities of manipulating flows at the very smallest scales by either stationary or free flowing microelectromechanical devices become more realistic, the need to predict the effect of such manipulations becomes critical.

While speculating about the long-term impact of any new technology is a dangerous thing – and we will simply state that the impact of direct numerical simulations of multiphase flows will without doubt be significant – it is easier to predict the near future. Apart from the obvious prediction that computers will continue to become faster and more available, we expect that the development of numerical methods will focus mainly on flows with complex physics. Although some progress has already been achieved for flows with variable surface tension, flows coupled to temperature and electric fields, and flows with phase change, simulations of such systems are still far from being commonplace. In addition to the need to solve a large number of equations, coupled systems generally possess much larger ranges of length and time scales than simple two-fluid systems. Thus, the incorporation of implicit time-integrators for stiff systems and adaptive gridding will become even more important. It is also likely, as more and more complex problems are dealt with, that the differences between direct numerical simulations – where everything is resolved fully – and simulations where the smallest scales are modeled will become blurred. Simulations of atomization where the evolution of thin films are computed by "subgrid" models and very small droplets are included as point particles are relatively obvious examples of such simulations (for a discussion of the point-particle approximation, see Chapter 9 in Prosperetti and Tryggvason (2007), for example). Other examples include possible couplings of continuum

approaches such as those described in this book with microscopic simulations of moving contact lines, kinetics effects at a solidifying interface, and reactions in thin flames. Simulations of non-Newtonian fluids, where the microstructure has to be modeled in such a way that the molecular structure is accounted for in some way, also fall under this category.

In addition to the development of more powerful numerical methods, it is increasingly critical to deal with the "human" aspect of large-scale numerical simulations. The physical problems that we must deal with and the computational tools that are available are rapidly becoming very complex. The difficulty of developing fully parallelized software to solve the continuum equations (fluid flow, mass and heat transfer, etc.), where three-dimensional interfaces must be handled and the grids must be dynamically adapted, is putting such simulations beyond the reach of a single graduate student. In the future these simulations may even be beyond the capacity of small research groups. It is becoming very difficult for a graduate student to learn everything that they need to know and make significant new progress in 4 to 5 years. Lowering the "knowledge barrier" and ensuring that new investigators can enter the field of direct numerical simulations of multiphase flow may well become as important as improving the efficiency and accuracy of the numerical methods. The present book is an attempt to ease the entry of new researchers into this field.

2

Fluid mechanics with interfaces

The equations governing multiphase flows, where a sharp interface separates immiscible fluids or phases, are presented in this chapter. We first derive the equations for flows without interfaces, in a relatively standard manner. Then we discuss the mathematical representation of a moving interface and the appropriate jump conditions needed to couple the equations across the interfaces. Finally, we introduce the so-called "one-fluid" approach, where the interface is introduced as a singular distribution in equations written for the whole flow field. The "one-fluid" form of the equations plays a fundamental rôle for the numerical methods discussed in the rest of the book.

2.1 General principles

The derivation of the governing equations is based on three general principles: the continuum hypothesis, the hypothesis of sharp interfaces, and the neglect of intermolecular forces. The assumption that fluids can be treated as a continuum is usually an excellent approximation. Real fluids are, of course, made of atoms or molecules. To understand the continuum hypothesis, consider the density or amount of mass per unit volume. If this amount were measured in a box of sufficiently small dimensions ℓ, it would be a wildly fluctuating quantity (see Batchelor (1970), for a detailed discussion). However, as the box side ℓ increases, the density becomes ever smoother, until it is well approximated by a smooth function ρ. For liquids in ambient conditions this happens for ℓ above a few tens of nanometers ($1\text{ nm} = 10^{-9}$ m). In some cases, such as in dilute gases, the discrete nature of matter may be felt over much larger length scales. For dilute gases, the average distance between molecular collisions, or the *mean free path* ℓ_{mfp}, is the important length scale. The gas obeys the Navier–Stokes equations for scales $\ell \gg \ell_{\text{mfp}}$. Molecular simulations, where the motion of many individual molecules is followed for sufficiently long times so that meaningful averages can be computed, show that

the fluid behaves as a continuum for a surprisingly small number of molecules. Koplik *et al.* (1988) found, for example, that under realistic pressure and temperature a few hundred molecules in a channel resulted in a Poiseuille flow that agreed with the predictions of continuum theory.

Beyond the continuum hypothesis, for multiphase flows we shall make the *assumption of sharp interfaces*. Interfaces separate different fluids, such as air and water, oil and vinegar, or any other pair of *immiscible* fluids and different thermodynamic phases, such as solid and liquid or vapor and liquid. The properties of the fluids, including their equation of state, density, viscosity and heat conductivity, generally change across the interface. The transition from one phase to another occurs on very small scales, as described above. For continuum scales we may safely assume that interfaces have vanishing thickness.

We also impose certain restrictions on the type of forces that are taken into account. Long-range forces between fluid particles, such as electromagnetic forces in charged fluids, shall not be considered. Intermolecular forces, such as van der Waals forces that play an important rôle in interface physics, are modelled by retaining their most important effect: capillarity. This effect, also called surface tension, amounts to a stress concentrated at the sharp interfaces.

The three assumptions above also reflect the fact that it would be nearly impossible, with the current state of the art, to describe complex droplet and bubble interactions while keeping the microscopic physics. For instance, simulating physical phenomena from the nanometer to the centimeter scale would require 10^7 grid points in every direction, an extravagant requirement for any type of computation, even with the use of cleverly employed adaptive mesh refinement, at least at present.

Beyond the three assumptions above, we mostly deal with incompressible flows in this book, although in the present chapter we derive the equations initially for general flow situations.

2.2 Basic equations

Expressing the basic principles of conservation of mass, momentum, and energy mathematically leads to the governing equations for fluid flow. In addition to the general *conservation* principles, we also need *constitutive* assumptions about the specific nature of each fluid. Here we will work only with Newtonian fluids.

2.2.1 Mass conservation

The principle of conservation of mass states that mass cannot be created or destroyed. Therefore, if we consider a volume V, fixed in space, then the mass inside this volume can only change if mass flows in or out through its boundary S. The