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MULTISCALE ISSUES IN DNS OF MULTIPHASE FLOWS*

Dedicated to Professor James Glimm on the occasion of his 75th birthday

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Abstract Direct numerical simulations (DNS) have now become a well established tool to examine complex multiphase flows. Such flows typically exhibit a large range of scales and it is generally necessary to use different descriptions of the flow depending on the scale that we are examining. Here we discuss multiphase flows from a multiscale perspective. Those include both how DNS are providing insight and understanding for modeling of scales much larger than the "dominant scale" (defined where surface tension, viscous forces or inertia are important), as well as how DNS are often limited by the need to resolve processes taking place on much smaller scales. Both problems can be cast into a language introduced for general classes of multiscale problems and reveal that while the classification may be new, the issues are not.

Key words direct numerical simulations; multiphase flow; multiscale problems
2000 MR Subject Classification 76T10

1 Introduction

The importance of understanding and controlling the behavior of multiphase fluid systems cannot be overstated. Multiphase flows are intrinsically linked to energy conversion and many (possibly most) studies of multiphase flow have been motivated by energy, in one way or another. Combustion of liquid fuels is the primary means of power generation for most land, sea, and air based vehicles. To burn the liquid it is essential to break it up into as fine drops as possible to increase the surface area and the atomization remains still the major weakness in modeling of sprays. The importance of the initial drop generation has stimulated the invention of a large number of atomizers and a large body of literature devoted to the study of such devices (see, for example [1], and [2]). Similarly, research into boiling has always been driven by "big" needs. Steam power marks the beginning of the industrial age and early boiler explosions played a major role in the establishments of industrial codes and standards. Research in the latter half of the twentieth century was originally driven by the needs of the nuclear industry

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and then by space exploration. More recently, interest in boiling has been driven by cooling of electronic components. As the power density increases, cooling is rapidly becoming one of the most important design constraints and the possibilities of single phase cooling are rapidly being exhausted. Thus it is clear that phase change increasingly must be used. In the chemical industry, bubbly columns, ranging in size from tens to hundreds of cubic meters, are used for a large number of critical processes, including partial oxidation of ethylene to acetaldehyde, isobutene separation, wet oxidation of heavily polluted effluent, and the production of synthetic liquid fuel from synthetic gas [3]. In many cases the liquid also contains suspended solid particles, such as catalysts. The absence of any moving parts and their relatively simple construction makes bubble columns particularly attractive for large-scale operations [4]. Their operation is, however, usually dependent of the size of the vessel and the difficulty of scaling up small pilot models makes numerical predictions importance.

Direct Numerical Simulations (DNS), where the time dependent flow field is computed for a system that is sufficiently small so that it can be fully resolved, but large enough so that non-trivial scale interactions are captured, are starting to transform our understanding of multiphase flows. Yet, such studies are still in their infancy and the rapidity by which they will lead to significant scientific breakthroughs and economic gains will depend on the availability of suitable computational tools and how easily they are adopted by new investigators. Given the many millions of tons of chemical products produced annually in bubble columns and the huge volume of liquid fuels that must be atomized, for example, even a small improvement in efficiency could translate into significant savings. For extended discussion of the role of numerical simulations, ranging from DNS to the average modeling of industrial systems, see [5].

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. The origin of the current surge of activities in multiphase flow simulations goes back to the late eighties and early nineties, when significant improvements in methods that use fixed grids (as used in the MAC and the VOF method) took place. Fixed grids offer great flexibility in the geometric complexity of the multiphase flow under investigation, combined with the efficiency inherent in the use of regular structured grids. Capturing of fluid shocks and interfaces was pioneered by Glimm and co-authors (see [6, 7, 8, 9, 10, 11] and a more recent review in [12]). Other advances included the introduction of the continuous surface force (CSF) method to compute surface tension in VOF methods [13], the level set method [14], phase field method [15] and the CIP method [16], for example, as well as the front tracking method of Unverdi and Tryggvason [17]. 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 has, for example, hardly been an issue of the Journal of Computational Physics recently 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 sim-

ulations 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. The overwhelming majority of studies that have been done so far have been concerned with disperse multiphase flows, where one phase is continuous and the other one appears as bubbles or drops. These investigations are already yielding new and exciting results for flows of scientific interest and technological importance. However, as more and more complex flows are examined, new challenges continue to emerge. Below we discuss some of those successes and challenges but before we do so, we will give a very brief overview of the so-called one-fluid formulation of the governing equations.

2 The One-Fluid Formulation

Simulations of multiphase flows have proceeded along two main tracks. In one approach, the governing equations are written down separately for each phase and the solutions matched through jump conditions across the interface. In the other approach, a single set of governing equations is written down for all the phases involved. The different fluids are identified by an indicator function χ as shown in Figure 1. The "one-fluid" approach is the basis for most of the methods currently used for DNS of multiphase flows, including VOF methods, the level set method [14], and the front tracking method of Unverdi and Tryggvason [17]. In the one-fluid formulation a single set of equations is written for all the phases involved, and the phase boundary is treated as an imbedded interface by adding the appropriate source terms to the conservation laws. These source terms are in the form of delta-functions localized at the interface and are selected in such a way as to satisfy the correct matching conditions at the phase boundary. For incompressible flows, the "one-fluid" Navier-Stokes equations are:

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho\nabla\mathbf{u}\mathbf{u} = -\nabla p + \nabla\cdot\mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T) + \sigma\kappa\mathbf{n}\delta(n). \tag{1}$$

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, κ is twice the mean curvature and $\mathbf{n}$ is a unit vector normal to the front. In most cases the flow is assumed to be incompressible so equation (1) is supplemented by

$$\nabla\mathbf{u} = 0. \tag{2}$$

When combined with the momentum equation, equation (2) leads to an elliptic equation for the pressure.

The single field formulation naturally incorporates the correct mass, momentum and energy balances across the interface. Integration of the conservation equations across the interface directly yields the standard jump conditions (see, for example [18]). The momentum equation, for example, becomes:

$$[[-p\mathbf{I} + \mu\cdot(\nabla\mathbf{u} + \nabla\mathbf{u}^T)]]\cdot\mathbf{n} = \sigma\kappa\mathbf{n}, \tag{3}$$

where the brackets denote the jump across the interface.

Equations (1) and (2) can be solved by a variety of numerical schemes, usually based on a finite volume projection method. The difference between the various methods is how the discontinuous density and viscosity (and other material fields) are advected and how surface

tension is computed. For a detailed description of the various numerical methods to handle the interface, see [19], for example.

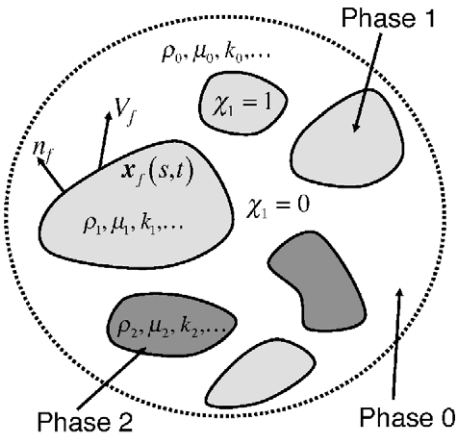

Fig. 1 The "one-fluid" description of multiphase flows. The different fluids are identified using an indicator function, χ, used to compute the different material properties and surface forces.

3 Need for Multiscale Descriptions

In spite of the enormous information and understanding that DNS are providing for relatively complex flows, real systems provide challenges that still limit the range of situations that can be simulated, even when we limit our studies to systems well described by continuum theories. The problem is, as one might expect, one of scale. Generally the smallest length scale of the flow has to be resolved by $O(10)$ grid points or so, and as the number of grid points available increases, the range of scales that can be resolved goes up. Current computer power makes it possible to simulate two fluid systems in domains resolved by several hundred grid points in each spatial direction (for thousands of time steps) relatively routinely and simulations of systems resolved by over 1000^3, or billion grid points, are becoming possible. Simulations of this size do obviously offer the opportunities to span scales whose ratios span over two orders to magnitude. This is, however, often not enough. The "natural" or a dominant small-scale in many multiphase fluid-fluid systems is set by the balance of surface tension and viscosity and inertia. For the breakup of a jet, for example, this scale determines the average droplet size. In most cases, this scale corresponds to roughly where the appropriately chosen nondimensional numbers, such as Weber, Capillary, Ohnsorge, and Reynolds, are $O(1)$ (and the key word here is obviously "appropriately"). Unfortunately, however, this is often not the only length scale that exists and frequently the flow exhibits both much larger and much smaller features.

Most industrial multiphase flows of interest involve a very large number of bubbles or drops and length scales that are many times the dominant length scale. If we assume that we need $O(10)$ grid points to resolve a drop that is half a millimeter in diameter, then we need of the order of billion grid points to resolve a chamber that is ten centimeters cubed. Many industrial systems are much larger and many drops are much smaller. This is the classical

closure problems for multiphase flows. Equations for the average flow field can be derived by formal averaging of the governing equations but just as for single phase turbulent flows, the averaging results in unknown terms that need to be modeled.

Similarly, it is frequently found that multiphase flows also can generate features much smaller than the dominant flow scales, consisting of very thin films, filaments, and drops. Frequently there is a clear separation of scales between these features, usually inertia effects are relatively small for the local evolution, and in isolation these features are often well described by analytical models. While these features can, in principle, be captured by local, adaptive, grid refinement, doing so increases the complexity of the computations significantly and usually results in greatly increased computational time.

The multiscale aspects of multiphase flows can be put into a broader context by considering the classification recently proposed by E and Enquist [20] who divide multiscale problems into two broad categories:

- Type A Problems: Dealing with Isolated Defects
- Type B Problems: Constitutive Modeling Based on the Microscopic Models

In Figure 2 we shows the issues schematically for bubbly flow in an inclined channel. Problem B is the classical averaging encountered in turbulence and multiphase flow modeling. We desire to obtain a model that accurately captures the aspects of the flow that are of relevance to us, without having to compute the intricate details of the flow. Problem A is how to deal with unresolved thin films, threads and droplets that appear as the flow evolves.

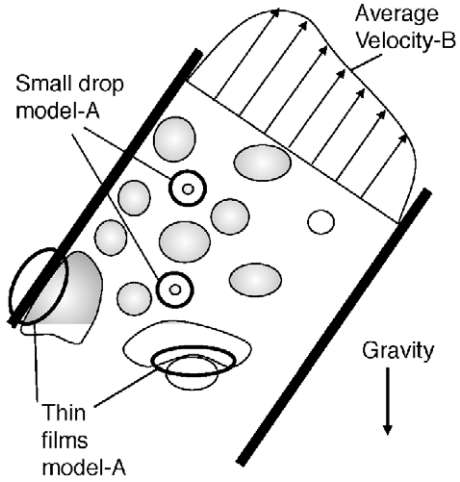

Fig. 2 The need for multiscale approaches for multiphase flows. DNS are particularly well suited to capture the motion of several bubbles and drops. We are often interested in the average motion at much larger scales. Similarly, DNS are often limited by the emergence of very small scales such as thin films and small drops that are too small to fully resolve.

4 The Average Flow at Large Scales: Type B Problems

Computational modeling of industrial scale systems generally relies on equations for the average flow. Reynolds Averaged Navier-Stokes (RANS) computations of homogeneous flows have

a long history, starting with the pioneering work of Launder and Spalding [21] and Harlow and collaborators (e.g. [22]). 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. This development can be found in, for example, [23, 24, 25]. 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 up 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 the lift, but for higher concentrations and deformable bubbles or drops the situation is more uncertain. The momentum equations for the continuous phase are always solved using an Eulerian approach, where the averaged equations are solved on a fixed grid, but the dispersed phase can be treated either using a Lagrangian or an Eulerian approach. In the Eulerian 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 the continuous phase is initially quiescent. These velocity fluctuations show up as Reynolds stresses in the averaged equations and are therefore called "pseudo turbulence." They are usually modeled using potential flow solutions for flow over a sphere and in turbulent flow 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 often do well and capture the main flow features, once the various parameters have been adjusted.

One of the most uncertain aspects of models for gas-liquid multiphase flow is the treatment of bubbles near solid boundaries. The existence of a bubble rich wall-layer in upflows containing nearly spherical bubbles has been known experimentally for many years [27, 28]. The lift force drives nearly spherical bubbles in upflow to the wall, resulting in a wall peak in the void fraction. At steady state the average liquid velocity in the core is uniform, with the increase in the liquid velocity taking place across the bubbly wall layer. In current models, bubbles that come close to a wall are usually prevented from going through the wall by the addition of a wall-force. Although the magnitude of the wall force has been estimated using results from a full numerical simulation of the flow around a sphere [29], in general, the correct magnitude of the wall-force is not known. The wall-force, however, does control the flow in some cases. When standard wall force models are used, the increase in velocity across the wall layer depends very sensitively on the magnitude of the wall force and since the velocity in the core depends on the velocity profile near the wall, the net result is that the total flow rate depends nearly entirely on the magnitude of the wall force.

We have recently used DNS of bubbly flow in a vertical tube to examine how bubbles behave near walls. In [30] we examined this in some detail, comparing DNS results with predictions of the model of [31] as well as the analysis in [32]. The results showed that at steady-state the flow of nearly spherical bubbles consists of two regions: a core where the void fraction is such

that the weight of the mixture exactly matches the imposed pressure gradient, including the hydrostatic one, and a wall layer that is free of bubbles for downflow and bubble rich for upflow. The thickness of the wall layer for downflow and the void fraction for upflow depends on the how much the void fraction in the core has to be changed to reach hydrostatic equilibrium [33, 34]. The lateral migration of bubbles to and from the wall is due to the lift force on the bubbles and as bubbles increase in size and become more deformable, the magnitude of the lift force is reduced (sometimes becoming negative, pushing the bubbles away from the wall for upflow). Lu and Tryggvason [26] examined the motion of a single bubble (as well as many bubbles) in turbulent upflow and determined the approximate deformability beyond which bubbles are no longer pushed to the wall for one set of parameters. Figure 3 shows results from two simulations of bubbles rising in a turbulent flow in a vertical channel. In the frame on the left the bubbles are nearly spherical and the flow is characterized by several bubbles hugging the walls. On the right, where the bubbles are more deformable, the bubbles stay in the middle of the channel. The void fraction is shown in the graph in the bottom of the figure and it is clear that the distribution is completely different. For details see [26]. These simulations have shown that while averaged models capture the void fraction distribution reasonably well, particularly in the bulk away from wall, the models do very poorly in describing the velocity in the wall layer. Since the velocity in a bubbly upflow in a pipe is completely determined by what happens in the wall layer, accurate prediction of the wall layer velocity profile is obviously of major importance. We should contrast this situation with downflow, where the wall layer is generally free of bubbles and averaged models do a very good job at predicting the overall flow rate. The difficulty of accurately including the observed mechanisms in averaged models [35] argue for the importance of examining new ways to include bubble rich wall layers. The wall layer is usually very thin and limited to about a bubble diameter (1–2 mm for air bubbles in water). For large scale simulations of industrial size systems, this layer cannot be resolved and even if it could, the evidences suggest that it needs to be treated by models that are different than those used for the flow in the bulk, such as by the introduction of a wall function, as often used in the modeling of turbulence in single phase flows [36]. We are currently examining this possibility further. For other investigations of how to use DNS to help with modeling of the average flow, see [37, 38], for example.

In addition to helping develop closure laws for standard models of multiphase flows, such as the two-fluid model, DNS are also making it clear that the data currently available calls for more sophisticated models. As for turbulent flow of single-phase fluids, it is usually found that in addition to relatively universal small-scale turbulence, multiphase flows also contains larger scale structures that are highly dependent on the problem geometry. Thus, Large Eddy Simulations (LES), where the large-scale structures are captured by solving the governing equations but the small-scale behavior is modeled, should be as useful in multiphase flows as for turbulence n a single-phase flow. While several authors have tracked particles using LES models for the fluid, attempts to derive a more rigorous formalism for LES of multiphase flows are just starting. Little has yet been done along those lines (see [39]) and it seems safe to conclude that the development of averaged descriptions of multiphase flows that go beyond the two-fluid models is likely to be one of the exciting developments in the modeling of multiphase flow in the near future.

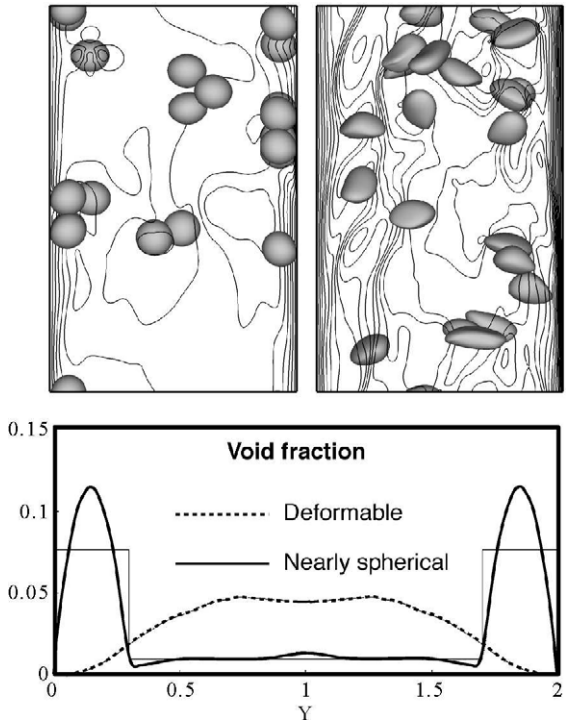

Fig. 3 Two frames from simulations of turbulent bubbly upflow in a vertical channel. The bubble distribution and iso-contours of the vertical velocity in the middle plane of the channel are shown. In the frame on the left the bubbles are nearly spherical, resulting in a prominent wall-peak in the bubble distribution. On the right the bubbles are much more deformable and stay in the middle of the channel. In the bottom frame, the average void fraction is shown. For details see [26].

5 Capturing Unresolved Thin Threads, Films and Drops: Type A Problems

While there has been considerable focus on using DNS to help develop predictive methods for flow scales much larger than the "dominant scales," multiphase flows often generate features much smaller than the dominant scales, consisting of very thin films, filaments, and drops. Consider, for example, the relatively tame problem of the collision of two droplets that are a few hundred micrometers in diameters. As the drops collide, they deform and trap air in a thin film between them. The air drains out of the film and if the drops stay in contact long enough, the film ruptures. It is, however, generally believed that the film thickness must get down to just about few hundred Angstroms before it ruptures. 100 A = 10 nm = 0.01 μm, so if the drops are 500 μm in diameter, the range of scales, from the thickness of the film to the diameter of the drop is 10^4. It is, at least in principle, possible to capture this motion for very simple situations (such as the head-on collision of two drops, where the motion could be resolved by unevenly spaced grid points using axisymmetry to reduce the computations effort). However, for more complex systems of several drops moving arbitrarily, fully resolved simulations are essentially

impossible at the present time. The small scale flow is, however, often relatively simple. High surface tension limits the geometric complexity and high viscosity limits the complexity of the flow. Thus, these features can often be accurately described by analytical or semi-analytical models. The representation of small-scale features in multiphase flow using simplified models is perhaps best demonstrated by the point particle approximations. For very small drops, that are smaller than the smallest flow scales (and whose Stokes number is smaller than unity) several investigators have carried out simulations where the flow away from the particles is fully resolved but the particles are approximated as points. Although the flow is not resolved by the computational grid, there are good reasons to believe that the accuracy of these models can be very high and when the Reynolds number of the particle is low enough, analytical results for the forces between the particle and the fluid eliminates any empirical adjustments. Another example of a multiscale approach in multiphase flow simulations is the near field correction used in simulations of multi particle systems in the Stokes flow limit, where either a lubrication approximation or an analytical solution are used to resolve the flow between nearly touching solids. Even when it is possible to use adaptive grid refinement to capture small-scale features, modeling them—when that is possible—can reduce the computational cost significantly.

We have recently started to develop thin film models to capture regions in multiphase flow that are difficult to resolve without excessive grid refinement. Figure 4 shows one example of the use of multiscale modeling to allow us to capture under-resolved features in a flow where "most" of the flow is well resolved [40]. Here we use a thin film model to describe the flow in the film under a drop falling onto and sliding down a sloping wall. The drop itself is easily resolved using about twenty grid points per its diameter (the coarse grid), but as it slides down the wall the film between the drop and the wall becomes very thin. For the case examined in the figure, we have selected the governing parameters in such a way that we can produce a fully resolved solution using unevenly spaced grid points and by comparing the results from the fully resolved simulation and the results for a coarser grid, we see that not resolving the film results in a significant error. In the simulations with the thin film model, we apply the usual no-slip boundary conditions at the wall, except where the film is. There we find the shear stress using the film model and apply shear stress boundary conditions. The flow in the film is driven by the pressure gradient found from the full fluid solution. Obviously the use of the model produces results that are relatively close to the fully converged solution. For more details, see [40]. In these simulations we used a very simple film model but for more complex problems and higher accuracy, we expect that more sophisticated film models [41, 42, 43] will be necessary.

Capturing the draining of thin films is particularly important for accurate modeling of topology changes, where two drops or bubbles coalesce into one, or one drop breaks into two. Topology changes take place in two ways, thin films that rupture and thin threads that snap. Thin threads appear to be—by far—the more easier to deal with. There are good reasons to believe that the Navier-Stokes equations describe how their diameter becomes zero in a finite time and simulations suggest that the overall results are relatively insensitive to how they are treated. In front tracking computations we often simply do nothing and are left with a very thin string of points, representing a filament of essentially zero thickness. For very accurate treatment of this filament, we should keep track of how it breaks into small drops and represent the resulting drops as point particles. The tracking of the draining of thin films and their

rupture is much more critical to the overall accuracy of simulations where topology changes take place. For clean interfaces that are fully mobile, we generally find that we capture well their evolution even if they are poorly resolved (not surprising since to the rest of the flow the film is simply a membrane), with the exception of its thickness. Thickness is critical for predictions of rupture and the main goal of tracking the film accurately is to be able to predict when it can rupture. In the front tracking method that we use, where the fluid interface is explicitly marked by connected markers, the film never ruptures by default but in simulations where the different fluids are followed by the advection of a marker function, such as in VOF or level set methods, the film would always rupture once the film is thinner than a grid spacing or so. Both methods can, of course, be modified to behave differently and we have conducted a number of simulations where we rupture films either when they are thin enough or at given times. Not capturing rupture correctly can prevent results computed using marker functions from converging since finer grids postpone the rupture. Relatively little has been done yet to combine accurate multipscale models of the draining of thin films with algorithms to do the actual topology change.

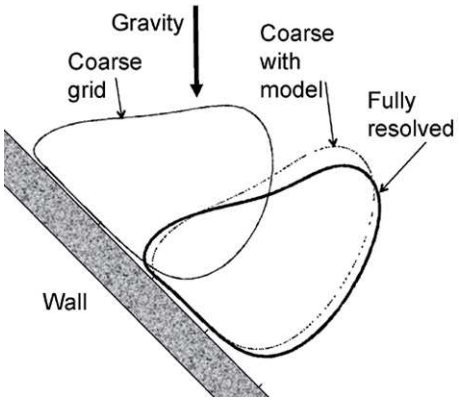

Fig. 4 Results from the use of a thin film model to capture the motion of a drop sliding down an inclined wall. The solid dark line shows a fully resolved drop, computed using an unevenly spaced grid with a large number of points used to resolve the film between the drop and the wall. Using a thin film model yields a coarse grid solution in relatively close agreement with the fully resolved results. For details, see [40]

As we go to smaller and smaller scales, we eventually reach a point where it is no longer fully justified to assume that the usual continuum hypothesis is accurate. It is then necessary to either change the modeling approach completely by, for example, using molecular simulations or possibly something like the dissipative particle dynamics approach, or work with modified continuum formulations designed to account for small scale effects. The second approach leads to phase field models where a thermodynamically consistent model is derived for the transition zone. Phase field models have been widely used for simulations of solidification where a properly selected energy function leads to the proper surface tension anisotrophy and kinetic effects. For multifluid systems Jacqmin [15] has used a phase field method to study the dynamics of a moving contact line and the the draining and rupturing of thin films has been examined in [44]. Such modeling should integrate well with the approach described above.

6 Conclusions

Multiphase flows are important for energy production, manufacturing and chemical processes, wastewater treatment, agriculture, and many other industries. Specific problems range from the cooling of high energy density electronic component to the production of synthetic fuel, for example. The initial motivation for the development of DNS was, to a large extend, the desire to develop closures for equations describing the average large-scale flows. However, as the use of DNS for multiphase flow studies has increased and it has been applied to an increased number of problems, it has become clear that in many situations the formation of small-scale features such as thin films or drops require excessive resolution. Here we look at DNS of multiphase flows from a multiscale perspective, and cast these challenges in a multiscale terminology. Multiscale computations often imply situations where it is necessary to go beyond the continuum scale. However, even within the realms of the continuum assumptions there are scales that need to be bridged and here we use "multiscale" more generally to imply any large range of scales that needs to be accommodated and treated differently. Using the classification proposed by E and Enquist [20] we find that multiphase flows provides examples of both type A and type B problems. While the developments of closure is a classical B-type problem, the use of simple analytical models to capture features that are not resolved by a grid appropriate for the rest of the flow is an A-type problem. The emergence of thin films, threads, and drops is a ubiquitous feature of multiphase flows and the development of a methodology that allows us to capture those features using multiscale approaches that do not increases the resolution requirement will greatly extend the range of problems that can be examined using DNS.

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