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International Journal of Multiphase Flow 29 (2003) 1089–1099

International Journal of Multiphase Flow

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Appendix 3: Report of study group on computational physics ☆

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Abstract

The great improvement of algorithms and computing hardware in the last few years must be ranked as one of the most important turning points in the history of multiphase flow research. After a brief review of some of this recent progress, it is pointed out that, besides its application to solving actual problems, computational physics plays other key roles: (1) As a tool to develop and understand basic physics and as a guide toward asking more penetrating questions; (2) As an aid in closing the averaged equations; (3) As a means to *learn to compute better*. Roadblocks toward greater effectiveness are the huge complexity of many of the necessary computational tasks but also, at a more practical level, the transmission of "computational knowledge" from one researcher to another, much in the same way as experimentalists can rely on readily available equipment (e.g., lasers, etc.), without having to build each item themselves. The solution to this problem will require a cultural shift—from a "cottage industry" to a "big science" mentality—which can be aided by a different attitude on the part of the funding agencies. Great synergism can be achieved by a closer integration of the multiphase computational physics enterprise with both Applied Mathematics and Computer Science.

Keywords: Computational multiphase flow; Direct numerical simulations; Numerical methods

1. Introduction

Since the early days at Los Alamos National Laboratory, four decades ago, theoretical work in multiphase flow has relied on computation. This trend has undergone a marked increase in the

☆ Members of the Study Group on Computational Physics in the Workshop on Scientific Issues in Multiphase Flow (May 7–9, 2002, Champaign-Urbana, IL) are Andrea Prosperetti (chair), Grétar Tryggvason (co-chair), S. Balachandar, Shiyi Chen, Lance Collins, Howard Hu, Martin Maxey, Olivier Simonin, Theo Theofanous.

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0301-9322/03/$ - see front matter
doi:10.1016/S0301-9322(03)00081-8

last few years, thanks to major developments in algorithms and computer power. As a consequence, the prediction of remarkable progress in this area in the coming few years is an easy one to make.

Computations of multiphase systems play many roles. First and foremost is the generation of basic understanding of the behavior of well-defined systems, not only through the simulation of the actual physical process, but also with the aid of computational "experiments." Multiphase flows are notorious for the difficulties in setting up fully controlled physical experiments. However, computationally, it is possible, for example, to include or neglect gravity, account for the effects of a well-characterized surfactant, and others. It is now possible to compute routinely the behavior of relatively simple systems, such as the capillary break-up of jets and the shape of bubbles. The next few years are likely to result in an explosion of results for such relatively simple systems where computations will help us gain a very complete picture of the relevant physics over a large range of parameters.

At the opposite end, one finds the great complexity of scales and phenomena of practical multiphase flows, where the behavior of the system is often exceedingly intricate (e.g., churn-turbulent, developing gas–liquid flows) or affected, at the large scales, by small-scale processes (e.g., nucleation, wetting, contact line motion, and others). The simulation of phenomena of the latter type must rely on effective computational methods for multiscale problems, which are still in their infancy. At a practical, industrial level, the simulation of phenomena of the former type must rely on an averaged description and closure models to account for the unresolved phenomena. In this sense, the situation here is similar to single-phase turbulent flows where, in the last two decades, simulations have played a major role, e.g., in developing large-eddy models. Simulations are starting to play a similar role for multiphase flow and it is already clear that the opportunities for major progress are enormous.

Next to the problem of dealing with scale integration, it is a remarkable development that the next challenge is perhaps not so much increasing the computational power as understanding how to best exploit the enormous amount of data generated by simulations. Our very thinking patterns, developed in an environment where analytical and experimental results were limited, are becoming inadequate tools to deal with the newfound abundance of data. It is of the utmost importance that progress in computation be paralleled by new theoretical frameworks that make sense of and condense the results. Computation has made theory more relevant.

The work of Magnaudet and Eames (2000) on the flow around a spherical bubble and that by Bagchi and Balachandar (2002) around spherical particles are typical examples of the role of computation in answering fundamental questions in multiphase flows. While these activities will undoubtedly increase, it must be recognized that such simulations are, in some sense, relatively straightforward extensions of what is currently possible. It is in the examination of very complex, very large-scale systems, where it is necessary to follow the complex evolution of an enormous range of scales for a long time, that the major challenges and opportunities lie. Such simulations, in which it is possible to get access to the complete data and to control accurately every aspect of the system, will not only revolutionize our predictive capability, but also open up new opportunities for controlling the behavior of such systems.

At the same time, the new insight offered by detailed simulations will be instrumental in developing better closures for averaged-equations models. While, for the foreseeable future, it is hard to imagine another form for practical engineering simulation tools, it must be recognized

that the classical two- (or multi-) fluid models suffer from several ills as well as limitations. Major new advances are envisaged which will capitalize on numerical capabilities and lead to farther-reaching modeling tools suitable for practical applications.

2. Numerical methods

Direct numerical simulations of multiphase flow, where the full continuum equations are solved on a computational grid sufficiently fine to resolve all continuum scales, date back to the origin of computational fluid dynamics at Los Alamos in the early and mid-1960s. The difficulty of following the deformation of an unsteady fluid interface separating phases of different properties, and limited computer power, restricted the complexity of the systems that could be examined. During the last decade, however, major progress has been made using a variety of numerical techniques. Before we discuss direct numerical simulations of multiphase flows (next section), here we will briefly review the methods that have been used for such simulations.

The oldest and still the most popular approach to compute multifluid and multiphase flows is to imbed the front directly on a regular, stationary grid. The marker-and-cell method, where marker particles are used to identify each fluid, and the volume-of-fluid (VOF) method, where a marker function is used, are the best-known examples. Traditionally, the main difficulty in using these methods has been the maintenance of a sharp boundary between the different fluids and the computation of the surface tension. A number of recent developments, including a technique to include surface tension developed by Brackbill et al. (1992) and the use of "level sets" (see, e.g., Sussman et al., 1994) to mark the fluid interface, have increased the accuracy and therefore the applicability of this approach. A review of the VOF method can be found in Scardovelli and Zaleski (1999). The level set method is reviewed by Osher and Fedkiw (2001) and by Sethian (2001). Recent additions to the collection of methods that capture fluid interfaces on a fixed grid include the CIP method of Yabe et al. (1997) and the phase field method of Jacqmin (1999); for reviews see Yabe et al. (2001) and Jamet et al. (2001). In these methods, one set of equations is used for the whole flow field and the various material properties form fields that change discontinuously across a phase boundary. Surface terms therefore have to be added as singularities at the interface. This "one fluid" approach has also been used by Tryggvason and collaborators (see Unverdi and Tryggvason, 1992; Tryggvason et al., 2001, for a review) to successfully simulate a number of multiphase systems. The difference between Tryggvason's approach and the "front-capturing" methods listed above is in the use of explicit marker points to follow the fluid interface. Since the one field approach is retained (unlike front tracking methods where each fluid is treated separately) the method is best described as a hybrid between front capturing and front tracking. The fictitious domain method of Glowinski et al. (2001), where solid body motion is enforced by Lagrangian multipliers also falls into this category.

The second class of methods, and the one that offers the potentially highest accuracy, uses separate, boundary fitted grids for each phase. The steady rise of buoyant, deformable, axisymmetric bubbles was simulated by Ryskin and Leal (1984) using this method. Several two-dimensional and axisymmetric computations of both the steady and the unsteady motion of one- or two fluid particles or free surfaces can be found in the literature. This method is best suited for relatively simple geometries, and applications to complex fully three-dimensional problems

with unsteady deforming phase boundaries are very rare. The simulation of a single unsteady three-dimensional bubble by Takagi et al. (1997) is, perhaps, the most impressive example.

The third class is Lagrangian methods where the grid follows the fluid. Examples of this approach include the simulations of the unsteady two-dimensional motion of several particles by Feng et al. (1995) and Hu (1996); and axisymmetric computations of the collision of a single drop with a wall by Fukai et al. (1995). While this appears to be a fairly complex approach, Johnson and Tezduyar (1997) and Hu et al. (2001) have recently produced very impressive results for the three-dimensional unsteady motion of many spherical particles.

The fourth category is front tracking where a separate front marks the interface but a fixed grid, only modified near the front to make a grid line follow the interface, is used for the fluid within each phase. This main developer of this approach have been Glimm and collaborators (see, Glimm et al., 2001).

In addition to front tracking methods that are, in principle, applicable to the full Navier–Stokes equations, specialized boundary integral methods have been used for both inviscid and Stokes flows. For a review of Stokes flow computations, see Pozrikidis (2001) and for a review of computations of inviscid flows see Hou et al. (2001). The most recent addition to the collection of methods capable of simulating multiphase flows is the lattice Boltzmann method (LBM) reviewed, for example, in Chen and Doolen (1998) and Sankaranarayanan et al. (2002).

Because many of these methods have been developed relatively recently, no clear "winner" has yet emerged. Indeed, it is likely that, for each method, there is a set of problems where it exhibits advantages over others. Furthermore, it is equally likely that often the "best" method is the one that the investigator is most proficient with.

While numerical methods can be made more efficient, more accurate, and more robust, the most pressing need in the next decade is perhaps not in the development of new methods but in the use of the available methods to advance our understanding—to formulate a THEORY of such flows.

3. Complexity

Multiphase flows are inherently complex. Even limiting oneself to the relatively 'simple' case of disperse flows, as soon as realistic numbers of particles and turbulence are involved, the possibility of carrying out DNS quickly dissolves. Just as in single-phase flow, large-eddy simulation appears to be a natural way to attack this situation. This is an important topic that so far has been scarcely studied, but which needs to be pursued. It seems likely that there should be a unifying formulation that allows one to start with the full equations (DNS) and naturally progress toward averaged equations with point particles and extended particles in between. Some highly non-trivial flows could be modeled if large-eddy simulation of disperse flows were developed. For example, in annular flow, one may envisage an LES model to describe the flow of the core gas with suspended droplets, and a fully resolved simulation of the interface between the gas core and the liquid film.

More generally, the complexity of multiphase flow requires a reduced description which is—and most likely will remain—embodied in a set of averaged equations which, in order to be realistic and reliable, must be greatly improved with respect to the models currently in existence. The efforts of the past several decades have shown that it is futile to hope to attain this goal solely

on the basis of experiment and 'simple' fluid dynamics (e.g., single particles in idealized situations). For example, the issues of ill-posedness of these equations and implications about their basic physical content continue to linger. The new and critical capability which now can be brought to bear on the essential task of improving these models is the recently developed ability to conduct non-trivial numerical simulations of relatively complex flows. It must be stressed, however, that while this point is obvious, the details of how to use simulations as a guide for the formulation of realistic and robust averaged-equations models are still very unclear. It is necessary and urgent that the passage from computational results to theory development be addressed as a specific problem in its own right.

While in some cases, such as the disperse flows mentioned above, complexity of scales can hopefully be dealt with by means of reduced descriptions, there are others where such descriptions are not—or, at any rate, not yet—possible. The pinch-off of a liquid thread, the coalescence of bubbles or drops, the motion of a contact line are superficially simple examples the full simulation of which requires the ability to simultaneously account for spatial scales ranging over some seven orders of magnitude. Another example, enhanced oil recovery, depends on phenomena ranging from the level of single pores (micron scale) to reservoir scale (kilometers). Dealing with such problems requires the development of new theoretical tools and computational procedures.

But complexity does not arise only from the interaction of different scales: the physics governing important phenomena can itself be complex. Even limiting oneself to the restricted class of the flow of two immiscible fluids, it is quite easy to develop a long list of situations much more complex than those considered in the previous section. If one looks beyond disperse flows, the complexity of the problems vastly increases, and so does the potential of computational physics in attacking them. For example, no attempt has been made to carry out simulations of flow regime transitions. Churn-turbulent flow is a completely virgin territory. Phase distribution, the formation, evolution, stability, and break-up of slugs, and similar problems have only very recently begun to be addressed.

In a large number of engineering applications that involve multiphase flow, it is necessary to account for phase change, between liquid and solid as well as liquid and vapor. Most materials used for man-made artifacts are processed as liquids at some stage, for example, and the way solidification takes place generally has a major impact on the properties of the final product. The formation of microstructures, where some parts of the melt solidify faster than others, or solidify with different composition as in the case of binary alloys, is particularly important since the size and composition of the microstructure impact hardness and ductility. Boiling is one of the most efficient ways of removing heat from a solid surface and it is therefore commonly used in energy generation and refrigeration, for example. The large volume change and high temperatures involved can make the consequences of design or operational errors catastrophical and accurate predictions are highly desirable. The change of phase from liquid to vapor and vice versa usually takes place in a highly unsteady manner, within thin diffusion layers and in the presence of very convoluted phase boundaries. Only a few examples of direct numerical simulations of both the effect of flow on the formation of microstructures during solidification and boiling have been published in the last few years (Beckermann et al., 1999; Tonhardt and Amberg, 1998; Juric and Tryggvason, 1998; Son and Dhir, 1998; Esmaeeli and Tryggvason, 2003), and this is likely to become a very active area in the next few years.

Other systems include more complex physics such as rheological effects (non-Newtonian fluids, polymer solutions), chemical reactions (e.g., combustion), three-phase systems (contact lines, liquid–gas–solid suspensions), thin films (boiling crisis, coalescence, break-up), electric and magnetic fields, and others. The potential for complexity is virtually unlimited and even relatively simple systems will put considerable demand on computational resources and solution methodologies. Thus, for example, the effect of electric fields on the boiling of binary mixtures requires the solution of the fluid flow, species conservation, energy equation with phase change, as well as an equation for the electric field. While pioneering work has been done on some of these problems, for the most part the field is wide open.

4. Conclusions

Computation serves many essential roles:

- As a tool to develop our understanding of the basic physics: asking "what if" questions, clarifying the importance of physical effects (e.g., gravity, surface tension) by adding or removing them at will, and others.
- As an aid in closing the averaged equations: just as the effectiveness and physical realism of different single-phase LES formulations can be judged by comparison with DNS results, closure relations can be developed and tested against numerical simulations.
- As a means of solving actual problems: some relatively small-scale problems (e.g., in microfluidics) can be attacked by DNS; bigger problems can be treated by means of reduced formulations, such as averaged equations.
- As a device to *learn to compute better*: it was argued before that it is necessary to develop new ways to deal with the large amount of data made available by the simulations. It is also necessary to learn how to ask more penetrating questions, how to develop more powerful algorithms, how to deal with problems having a multiplicity of scales.

As always, what is feasible is not necessarily interesting, and what is important is not necessarily feasible. While it is a trivial statement that it is at the intersection of the feasible and the important that real progress will be made, it is not always obvious where this intersection lies. In particular, computational research is often accused of generating vast amounts of trivial or unnecessary information. It is evident that the multiphase flow community must resist the temptation of using existing codes to generate yet another unnecessary paper, and focus instead on what is truly important and innovative.

The coming of age of powerful computational capabilities must be ranked as one of the most important turning points in the history of multiphase flow research. The last decade has seen the development of several extremely effective algorithms which, coupled with hardware of unprecedented power, make the computation of complex flows now possible. Although our ability to directly simulate more and more complex multiphase systems will certainly increase dramatically in the next few years, it is important to realize that our desire to compute will always outstrip it. Even if we could fully compute the behavior of a system, we may easily imagine, for example, that we might want to be able to incorporate simulations into a real-time control system that dynamically explored the consequences of several possible control actions. Thus, the

condensation of knowledge obtained by direct numerical simulations into reduced or averaged models that allow faster predictions will remain at the core multiphase flow research for a long time to come.

Computing is linked to Mathematics, on one side, and to Computer Science, on the other. The first link has always played an important role in multiphase flow simulation, but the same cannot be said of the second. Fields where major progress is likely include visualization, data mining, programming philosophy and techniques, and others.

Before concluding, it is important to mention problems of a different nature, which have begun to emerge in all their seriousness in the last few years, namely the EDUCATION of students and new researchers in the field of computation and how "computational knowledge" and even software is shared.

No experimentalist would build his/her tools completely from scratch: any experimental setup contains vital components, such as cameras and lasers, that are purchased from commercial vendors. With a few important exceptions, in this respect, the computational researcher is still operating in the dark ages. Although commercial codes are available for solving engineering problems, these codes are generally unsuitable for state-of-the-art research. Their limitations—such as robustness in favor of accuracy and limited access to the "guts" of the codes—are understandable, but the result is that most research codes must be written by the group that intends to use it. In many cases, a sophisticated piece of software does not survive the graduation of the student who wrote it. While many research groups make their codes available, and advanced codes have been turned into generally available packages, it is clear that a major cultural change is called for.

The complexity 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 by dynamically adapted, are putting such simulations beyond the domain of what a typical Ph.D. student, or even a small research team, can accomplish over the span of a few years. To make the learning and development process faster it is essential to find ways to provide adaptable, well-documented, software components to new users. A related problem, which plagues the developers of new codes, is their validation: the complexity of these codes is such that in many cases the only tools for validation are other, independently developed, codes. In this situation, the ability to validate a code often depends on the circle of acquaintances of the developer—obviously an unacceptable situation. And, finally, integration: one can envisage a future in which, in some cases, complex computational research tools will be assembled from components developed by different research teams. How is this going to happen? How will this affect the perceived "productivity" of the individual teams? How do we move from a "cottage industry" to a "big science" mentality? The major onus in establishing a climate in which these questions will find a good answer rests on the funding agencies.

5. Overview of the individual contributions

In addition to the authors of this Summary, the task group on Computational Physics consisted of S. Balachandar (University of Illinois at Urbana), Shiyi Chen (Johns Hopkins University), Lance Collins (Cornell University), Martin Maxey (Brown University), Olivier Simonin (University of Toulouse), and Theo Theofanous, T.N. Dinh, and R.R. Nourgaliev (University of

California at Santa Barbara). The documents they prepared will be found in a special issue of *Multiphase Science and Technology* and in the *Transactions of the Workshop on Scientific Issues in Multiphase Flow*.

Rather than focusing on these individual contributions, in the previous pages we have tried to outline the broad issues emerging from them as well as the discussions held at the Workshop. Here we present a brief synopsis of each participant's input to the task group.

- Balachandar addresses the hydrodynamic forces exerted on a single rigid particle. He points out the difficulty in unambiguously prescribing the fluid force when the particle is immersed in a complex, unsteady, and spatially dependent flow. The conclusion that the reader draws from this survey is that point-particle Lagrangian models, in which the motion of each point particle is dependent on the specification of the fluid force in terms of local flow parameters, are perhaps near the end of their useful life. It is necessary to go beyond these models and develop more realistic extended-particle models and computational techniques. This point is also made in several other contributions (Collins, Maxey, Tryggvason).
- Chen gives an overview of Lattice Boltzmann Methods. He points out the great computational advantages (efficiency, flexibility, ease of parallelization, applicability to high-Knudsen number regimes, and others), but also some drawbacks (e.g., the inability to easily handle large density ratios between the phases). The achievements of Lattice Boltzmann Methods are impressive and it is useful to continue work in this area.
- Collins focuses on the turbulent transport of aerosol particles, turbulent modulation by a suspended phase, collision, coalescence, and break-up of drops and bubbles, and the effect of polymers on turbulence. While cautious on the wisdom of continuing work on point-particle models, in the systems he considers (aerosol transport, cloud physics, inhalation drug therapy, polymer solutions, and others) particles are indeed very small and dilute and these models are still useful. They must be supplemented, however, by progress on basic issues such as collision and coalescence modeling. Like Balachandar, he touches upon the difficulties associated with an understanding of turbulence modulation in this context. He stresses the need to tackle problems in a concerted way by theory, computation and experiment, all addressing the same parameter range, so as to leave as few "loose ends" as possible.
- Hu presents an exhaustive review of the finite-element methods available for the description of fluid-particle flows: arbitrary Eulerian–Lagrangian scheme, stabilized space-time method, distributed Lagrange multiplier. A common problem is the description of particle collisions, which are numerous and frequent in dense systems: a first-principles description seems impractical, due to computational time and to the need to include features such as particle roughness. Hence approximate methods to deal with collisions are necessary, but not yet adequately developed. Hu also presents several computational examples of particles suspended in Newtonian and visco-elastic fluids.
- Maxey's contribution recognizes the progress made with point-particle models, but stresses the importance of moving beyond them for further progress. He describes in detail the force coupling method for the Lagrangian tracking of finite-size particles suspended in a fluid and considers it as a "bridge" between point and extended-particle models. While one should not lose sight of the many challenges which exist at the level of computational techniques and their efficient implementation, he stresses that it is equally important to put the computational

results to good use for an understanding of the physics and the development of approximate models of engineering value. This is a crucial point also stressed by Tryggvason and Prosperetti.

- Prosperetti treats several issues related to the averaged description of multiphase flow: averaging, stability, hyperbolicity, and the essential role of direct numerical simulation in guiding the formulation of more satisfactory averaged equations. He makes the point that averaged equations must necessarily be the workhorse of theoretical and design work involving multiphase flows in engineering, and discusses some basic limitations of the available equations. In this perspective, the development of reliable equation models can be seen as the over-arching goal of theoretical multiphase flow research. In his view, the direct numerical simulations newly made possible by progress in algorithms, software and hardware are the key ingredients in developing a better generation of averaged equations.
- While Simonin feels that point-particle Lagrangian models need to be improved, he is optimistic for their life in the near future: (1) Dynamic effects in particle-laden turbulent flows have been studied extensively for the last 15 years, but many open questions of great interest remain concerning, for example, heat and mass transfer in reactive turbulent flows or particle–turbulence, particle–particle and particle–wall interactions for non-ideal hard-sphere particles; (2) In a short-term perspective, LES is the only approach which allows one to represent realistic turbulent Reynolds number and to account for complex geometries. LES combined with a Lagrangian approach is well suited for intermediate-scale numerical simulations provided it is based on accurate DNS for the computation or modeling of the subgrid effects. Furthermore, he argues that an LES methodology should be developed for the two fluid equation models.
- Theofanous, Dinh, and Nourgaliev make a strong case that the multiscale treatment of multifluid flow holds the key to progress. They describe an approach that decomposes the simulation of a topologically complex multiphase flow into simulation of large-scale discontinuities and solution of disperse flow problems in domains dynamically encapsulated by such discontinuities. They consider these multiscales approaches as the first step toward uncovering the principles that govern pattern formation in multiphase flow. In the face of the huge variety of multiphase flow phenomena, they advocate a strategy in which certain prototypical problems should be worked on first, so that the lessons learned in this process can fruitfully be applied to other cases. Their list of these "higher priority" problems includes slug flow in horizontal and inclined pipes, churn-turbulent flow in large-diameter pipes, and critical heat flux in pool and flow boiling.
- Tryggvason describes techniques and issues related to the numerical simulation of free-surface flows. He points out that many tools exist which are adequate for dealing with the simpler cases in which the phases (be they fluid or solid) are coupled only through the exchange of momentum (see Hu et al., 2001; Bunner and Tryggvason, 2002, for example). The next step must be the development of techniques that can describe more complex physics: heat transfer, phase change, electric and magnetic fields, and others.

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