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Report on a symposium on "Computational approaches to disperse multiphase flow"

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Abstract

Some themes and developments emerged in the course of an IUTAM Symposium on "Computational Approaches to Disperse Multiphase Flow" held at Argonne National Laboratory on October 4–7 2004 are briefly summarized.

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1. Introduction

A symposium on "Computational Approaches to Disperse Multiphase Flow", sponsored by the International Union of Theoretical and Applied Mechanics and generously supported by the Office of Basic Energy Sciences of the US Department of Energy was held at Argonne National Laboratory on October 4–7, 2004. The symposium attracted about 90 participants from 15 different countries. There were 48 oral presentations and an additional 17 poster papers. The proceedings will be published by Kluwer in the near future (Balachandar and Prosperetti, in press).

Although many fluid mechanics and multiphase flow conferences usually feature several sessions devoted to computation in multiphase flow, this was one of the few symposia exclusively devoted to this activity. It was an opportunity to review a considerable amount of high-quality recent work on computational multiphase flow. It afforded an excellent picture of the contemporary activities in this field and prompted a series of reflections.

The symposium was punctuated by three special lectures. The opening lecture was given by Hinch, who discussed of the scaling of velocity fluctuations induced by sedimenting particles. The closing lecture was given by Joseph, who summarized the picture of the current status of high-end scientific computations in multiphase flow research as it emerged from the talks presented at the symposium. It was his opinion that the current width and depth of research bodes well for the future of computational multiphase flow. On Wednesday

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(October 6th) the lunch was followed by "Some reflections on multiphase flow" by Hetsroni. His presentation ranged from some historical notes on boiling, dating back to the Bible and Homer, to reflections on scientific progress in boiling research, to recent statistics on papers published in the "International Journal of Multiphase Flow".

In this paper we do not intend to summarize the various contributions to the symposium but, rather, to use some of them as examples for more general considerations.

2. Physical understanding

Together with experiment and theory, computation has already been for a long time an integral component of multiphase flow research. A striking feature common to most papers presented at the symposium was the power, maturity and sophistication reached by this approach.

A few papers conclusively demonstrated that, for some problems, computing is the only means by which key physical phenomena can be elucidated. A prime example was Magnaudet's analysis of Leonardo's paradox, i.e. the instability of the rectilinear path of an ascending bubble. The modern history of this problem goes back several decades and is well known. For a long time it was believed that the zig-zag or helical path of an ascending bubble was due to vortex shedding. The association with an instability of the laminar wake was first found experimentally by de Vries et al. (2002). The crucial contribution of Magnaudet was to show that this instability only occurs when the deformation of the bubble is sufficient large. This result was obtained by constraining the bubble shape to remain spheroidal, and by varying its eccentricity. It would be exceedingly difficult (though perhaps not impossible if the Morton number is varied by using different liquids) to achieve this result experimentally and furthermore, in an experiment, the purity of the liquid and the absence of surface contamination are always an issue.

Another case in point was Matsumoto's presentation on the detailed action of surfactants at the surface of a rising bubble. While the general physical mechanism at work has been known for a long time, this was the first example of the microphysical processes acting at the bubble surface and their impact on the local flow field.

As a third example, one may cite the work of Tryggvason and Elghobashi on the mechanism of drag reduction by bubbles injected in a turbulent flow. The two simulations studied very different situations in terms of bubble sizes and flow type (channel versus boundary-layer, respectively), but both elucidated subtle phenomena which would be accessible by experiment only with great difficulty. Tryggvason showed the great impact of bubble deformability on the rearrangement of vortical structures in the channel contributing to drag reduction, while Elghobashi pointed out the key role of effective compressibility introduced by a space-varying gas volume fraction.

3. Complex physics

Over the last few years the computational capabilities of several groups have reached such a level of sophistication that we are now able to take a first-principles look at complex microphysics that arises in a variety of problems. A striking example of the insight that computation can deliver in these situations was offered by the work of Dinh, Nourgaliev, and Theofanous, who studied the sudden exposure of a liquid drop to an incident Mach-3 flow. Their computations exhibited a sequence of phenomena as beautiful as they are bewildering, and in front of which intuition is all but powerless. This group described extremely sophisticated numerical methods by which it is possible to make sense of what one sees on the very high speed video recordings of actual experiments. Free-surface simulations in this parameter range are a problem of daunting complexity which, however, is amenable to computation by use of the recently developed "AUSM+" algorithm, which couples the level-set technique with the method of characteristics.

Calculations of a similar nature, but in the more familiar incompressible limit, were described by Zaleski, whose enhancements of the volume-of-fluid method mark a considerable improvement over the level of accuracy and sophistication of this approach only a few years back. Concerning the old issue of sharp versus diffuse interface, Udaykumar went as far as arguing that maintaining the interface sharp is not more expensive than having it diffuse. He demonstrated this point with simulations of droplet impacting, spreading, and falling off a cylinder. This is clearly a big step forward over various front capturing and front tracking methods of the past decade. Dhir demonstrated the power of combining the level-set approach with conventional Navier–Stokes codes by describing simulations of time-evolving and merging vapor–liquid interfaces during nucleate boiling. Numerical predictions of how a single vapor bubble detaches or a collection of bubbles interact as they nucleate are in excellent agreement with the companion experiments.

4. Molecular dynamic simulations

Another significant advancement that was clear from the symposium was the use of molecular dynamics as a computational tool to access multiphase phenomenon that can only be addressed at the molecular scale. Bridging the length scales has been and continues to be a holy grail in computational physics. A significant advancement toward this end was presented by Chen. He outlined an approach whereby the continuum Navier–Stokes simulation at the macroscale can be coupled to the concurrent molecular simulation at the atomistic scale. The coupling between these two approaches is achieved through constrained dynamics in an overlap region. He validated this novel approach with a simulation of sudden-start Couette flow over a rough wall at the nanoscale. Another significant contribution in this area was described by Takagi, who elucidated the microscale energy structure of nanobubbles in metastable water through molecular dynamics simulations.

The potential for molecular dynamic simulations to uncover the complex physics of contact-line problems makes this application a very attractive one. McLaughlin described investigations of the frictional resistance to contact-line motion, the causes of contact-line pinning, and the origin and extent of slip near the contact-line. Among other results, he found that, at small driving forces, there is evidence for a stick-slip behavior and the possibility of contact-line pinning even on molecularly smooth surfaces.

5. Lattice-Boltzmann methods

A good share of presentations dealing with solid particles was taken up by Lattice-Boltzmann methods (LBM). It was clear that LBM has made significant advances over the last decade and offers an attractive approach to simulating complex multiphase flow problems. This was demonstrated by Sommerfeld, who used LBM to obtain resistance coefficients of particles of several nonspherical shapes such as cubical, spheroidal and cylindrical, in laminar and turbulent flows. Aidun used the Lattice-Boltzmann method to address the difficult problem of handling particles near contact. His simulations illustrated the importance of accurately resolving the normal stresses arising from lubrication forces to prevent large errors in the representation of such close range interactions. He presented a particular variant of LBM which removes prior limitations in dealing with such close contact and thereby improves the accuracy substantially.

The real power of LBM shows up in its ability to easily handle a suspension of particles. The symposium saw two presentations of this kind, one by Koch and the other by Sundaresan. Koch and co-workers considered simulations of a suspension of spherical particles in a plane Couette flow. In addition to LBM for the carrier phase they also used a tracer algorithm to simulate the convective and diffusive motion of a chemical species. From these simulations at moderate Reynolds and Stokes numbers, they measured momentum, heat, and mass transport in sheared suspensions.

Prediction of mesoscale phenomena, without empirical modeling at the microscale, is a nontrivial problem of fundamental interest. The need to simultaneously resolve from the mesoscale down to the microscale poses a great computational challenge. Recent simulations by Derksen and Sundaresan have demonstrated the ability of LBM to span the wide spectrum of length scale ranging from flow features smaller than a particle to mesoscale wave structures, an order of magnitude or more larger than the particles. They were able to obtain quantitative information on the transition from homogeneous fluidization to an inhomogeneous state with traveling one-dimensional waves.

6. Novel computational approaches

The symposium showcased several innovative numerical approaches which offer great promise for addressing a variety of dispersed multiphase flow problems. Banerjee presented impressive simulations that capture the coarsening phenomenon of dispersed phase in a phase-separating binary fluid subjected to shear. An efficient approach for direct numerical simulation of Brownian motion of particles was discussed by Patankar. In his approach, the random component of the force on a particle is calculated from the hydrodynamic force obtained by solving the fluctuating hydrodynamic equations.

There were several presentations which exhibited the capability to simulate the dynamics of thousands of interacting spheres. Michaelides presented his new code "Proteus" which brings together elements of the immersed boundary, lattice-Boltzmann, and direct-forcing methods. He showed results for the settling of 1232 interacting three-dimensional rigid particles. Kajishima presented an immersed boundary technique for the simulations of particle laden turbulence in a suspension of over 2000 particles. Based on the simulation results, he suggested that particle rotation may play an important role modifying the carrier–phase turbulence.

Several direct-forcing options were discussed and compared by Uhlmann and Pinelli. A new method in which the fluid is treated as compressible and the particle Reynolds number is finite was described by Hu, who illustrated his approach with a simulation in which 100 particles fall inside a closed box. Pianet and Muradoglu described improved methods based on fixed grids for the computation of solid–fluid and fluid–fluid disperse flows, respectively. In his presentation, Maxey advanced the force-coupling method, which uses a set of finite force multipoles to represent each particle, as a cost-effective alternative for simulating a large distribution of interacting particles.

Thus, for the large-scale simulation of complex dispersed multiphase flows a range of numerical schemes show great potential. The simulation of thousands of particles could hardly have been imagined just five years ago, and is another clear manifestation of the coming of age of computational multiphase flow.

7. Turbulence

The difficulties inherent in the fields of turbulence and multiphase flow in themselves make turbulent multiphase flow a truly grand-challenge problem. The importance of which was quite evident from the number of presentations that addressed this topic either directly or indirectly.

So far, point–particle models have been the most widely used approach to turbulent disperse flow computation. The limitations of these models were discussed by Eaton, who presented results from a detailed model-free simulation of decaying isotropic turbulent flow around a sphere. Despite its limitations, the point–force approach remains quite popular, as at present there is no alternative for investigating these systems. Several groups have made elegant application of this model to elucidate the complex physics of turbulent disperse flows. The effect of carrier–phase turbulence on the preferential accumulation, segregation and deposition of particles was addressed in the presentations by Soldati and Collins. The modeling of fluid–particle and particle–particle interactions in a turbulent flow was considered by Squires. Bec showed that heavy particles in a random flow form multifractal structures.

The action of turbulence on point-like particles can also be modelled by introducing stochastic terms in the particle equation of motion. Mito described an application of this type to droplet dispersion and deposition in an annular flow, while Loth modified the Langevin equation for the particle motion to mimic the anisotropy of near-wall turbulence and compared the results with those found by allowing the particles to interact with "real" turbulence obtained from DNS.

Large-eddy simulations have become a powerful computational tool in the study of single-phase turbulence and its extension to multiphase turbulence would be desirable. Lakehal described an adaptation of the method to breaking surface waves on a beach. For applications to disperse systems, however, the large-eddy simulation approach encounters the difficulty that small particles respond to the sub-grid scales, and that there is far less universality at the smaller scales than in single-phase turbulence. A possible approach, described by Mashayek in the context of a point–particle model, is to augment the particle equation of motion by a random force mimicking the effect of the unresolved eddies.

In addition to turbulence as usually understood, disperse flows also exhibit pseudo-turbulence. In this case the fluid velocity fluctuations are not caused by the flow as in normal turbulence, but are primarily due to the action of particles or bubbly transiting randomly in the neighborhood of the observation point.

8. Conclusions

Two points were made abundantly clear at the IUTAM Symposium. In the first place, computational multiphase flow suscitates a strong interest in the fluid mechanics community—a heartening corollary being that the quality of much of the work in this field is quite high. Secondly, for people like us who have been following developments in this discipline for many years, it was extremely gratifying—and perhaps even somewhat surprising—to gain such a palpable appreciation of the maturity of the field, its impressive development, and the level of complexity and detail that progress in hardware and algorithms currently permit. It is hard to imagine that an external observer coming to the meeting with misgivings about the usefulness of computing in multiphase flow would have left nurturing the same doubts.

Together with the enhanced appreciation of the role of computing, it is wise to always keep firmly in mind the other two legs of progress in science—theory and experiment. This is all the more true in multiphase flow in which we are still faced by problems of such magnitude and complexity that it would be unrealistic to imagine solving by computing alone.

Yadigaroglu (2003) has proposed the "brand name" Computational Multi-Fluid Dynamics, or CMFD. It is too early to tell whether the community will adopt the acronym but, as Juliet puts it, "What's in a name? that which we call a rose by any other name would smell as sweet" (Shakespeare, 1623). Judging from this symposium, this seems to be spirit in which the computational fluid dynamics community has embraced the challenge posed by the numerical simulation of multiphase flows.

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