XVII Epilogue

In this document I have explored some of the ways in which direct numerical simulation (DNS) of solid-liquid flow can be interrogated for useful results. The value added by DNS is that initial value problems for particulate flows can be solved as exactly as numerical methods will allow. The signal feature of DNS is that the particles are moved by forces computed from the fluid motion, as they should be; the modeling of forces needed by other approaches to particulate flow is not needed or done by DNS. In our work the calculation of forces is implicit because the mutual forces disappear in the variational formulation for the total solid-liquid momentum. In this we avoid the explicit computation of forces, on the one hand, and the modeling of forces on the other.

We developed two types of finite element packages: an ALE particle mover in which particles move on a body-fitted unstructured grid and a DLM particle mover in which particles move over a fixed triangular grid. The DLM calculation can be said to be over a fluid which is partitioned into particle and particle-free parts; the field of multipliers is defined on particles and is chosen so that the fluid there moves as a rigid body. The multiplier field is coupled with the rigid motion constraint in a manner analogous to the way in which the pressure is associated with the constraint of incompressibility.

The DLM method is very efficient; it runs matrix free, uses fast solvers and runs in parallel using multilevel preconditioners. With this method we can track thousands of particles in 3D. The number 1204 in the DLM simulation of the fluidization of 1204 spheres was chosen to simulate the motion of 1204 real spheres which we had previously used in experiments. This number is not near the limiting and unknown number for which such simulations may fail. It takes days to compute seconds of bed expansion, but at least we can compute and the computing will only get faster and better. It is probable that motions of tens of thousands of particles in 3D is an achievable goal short term.

Unstructured grids are convenient for complex geometries and unlike fixed grid methods they can be programmed for local mesh adaptivity in regions of close approach of particles. The ALE method carries the overhead of remeshing from time to time due to mesh distortion. Parallel algorithms based on domain decomposition are presently under development for the ALE methods.

There are many ways in which direct simulations may be interrogated for useful results. It has to be understood that DNS does not replace theory even though it gives rise to exact numerical solutions of the initial value problem for particulate flow. It is more appropriate to think of DNS as a surrogate for experiments. The simulations have some great advantages; you can suppress physical effects one at a time in simulations which is something that cannot be done in experiments. Virtual experiments also have the potential to replace real experiments in generating data which form the basis for correlations of the type used in engineering practice; the generation of Richardson-Zaki correlations in our study of fluidization of 1204 spheres is an example. Quantities needed for theory, like slip velocities are ever so much easier to determine in simulations than in experiments.

Direct simulations lead to better understanding of flow fundamentals in situations otherwise opaque. The fluidization by lift of slurries in horizontal conduits is a concept generated by direct simulations. Liquid-solid flows are a nonlinear dynamical system which give rise to typical bifurcations like that discussed in Chapter X, to periodic and even chaotic solutions. It is not possible to study such bifurcation by analytical methods or two-fluid models. DNS may be the only method to study bifurcations of particulate flow.

There are many technologies which depend critically on solid-liquid flows. Industries which utilize such technologies typically control operations with simplified models of particulate flow which can be run on PCs. It is widely believed and presently true that DNS is too slow and expensive to guide field operations. Such beliefs should always be revisited because the rapid expansion of software and hardware has a proven capacity for upward revision.

We have been trying to find the structure of data arising from DNS which can be used to form useful models. There are different kinds of models; effective media and models which require the modeling of forces on particles. Modeling forces is a big problem; for example, there are no good models of lift forces in slurries. At the risk of being tiresome I want again to call attention to the huge difference between the modeling of forces as is done in modeling and the computing of forces as is done by DNS.

There are two kinds of models which require the modeling forces; models in which the fluid motions are resolved by direct methods and the particles are moved by Newton’s laws using modeled forces and two-fluid models. Two-fluid models may be regarded as arising from averaging as was done in Chapter VI.

Effective media, two-fluid models do not require the modeling of forces. Our study of the Rayleigh-Taylor instability arising in the direct numerical simulation of 6400 circular particles in Chapter VIII is a good example of an effective media two-fluid model. In that study we regarded the sedimenting suspension and the entrained fluid as another effective fluid. To realize the model it was necessary to come up with an effective density and viscosity; modeling forces was not required. It seems likely to me that the fluidization of 300 particles by lift studied in Chapter X can be modeled as an effective fluid, with an effective viscosity, density and zero surface tension. The waves which propagate on the top of the fluidized suspension look like waves which develop in two-fluid situations.

Maybe effective media two-fluid models in which model assumptions can be tested by DNS ought to be restricted to special situations like those mentioned in the prior paragraph. One two-fluid model of particulate flow which covers all situations is not likely to be an achievable goal since closures which work for some situations will not work for others.

In the literature one finds formulas for single particle lift which apply in special circumstances mainly for low Reynolds numbers. Rigorously derived mathematical formulas for the lift and drag on particles moving at finite Reynolds numbers do not exist and such formulas are put forward only as empirical results following out of experimental data, from real experiments and now from numerical experiments.

It can be said that two-fluid models and perturbations of Stokes flow have not worked all that well. An alternative to these methods is the method of correlations used in this book. This method leads *from data to formulas*. Data from experiments and numerical experiments are processed in the same way. This method makes maximum use of computers and storage tapping opportunities provided by new technology. I think that curve fitting plus computers and storage gives rise to new and great opportunities for particulate flow and multiphase science. The secrets are in the data and with digital technology we can interrogate this data.

Generating correlations from experiments is an old method on which many industrial applications are based but it has come to have a bad name, viewed as empirical and not fundamental. The great example is the Richardson-Zaki correlation which is the cornerstone of fluidized bed practice. My enthusiasm for correlations has to do with the surprising emergence of correlations from the simplest kind of post-processing of our numerical experiments. We have done lift correlations for single particles and for the bed expansion of many particles in slurries. The procedure we follow is to plot the results of our simulations in log-log plots of the relevant variables. The surprise for us is that these plots frequently come up as straight lines giving rise to power laws. For example, a single particle will lift-off in a Poiseuille flow at a certain Reynolds number $R = Ud/v$ for a given settling Reynolds number $R_G = \rho_f(\rho_p - \rho_c)gd^3/\eta^2$. When we plotted the lift off criterion from about 20 points we found that $R = aR_G^n$ with an intercept a and slope n in the log-log plot. The straight lines are impressively straight and we generated such correlations for lift to equilibrium, for the bed expansion of many particles and in non-Newtonian fluids. The existence of such power laws is an expression of self-similarity, which has not been predicted from analysis or physics. The flow of dispersed matter appears to obey those self-similar rules to a large degree.

We can get power laws when only two variables are at play; when there are three variables or more, it would appear that we get different power laws separated by transition regions. This is certainly the case for the Richardson-Zaki correlation; it has one power law relating the fluidization velocity to the solids fraction at low Reynolds number, and another at high Reynolds with a Reynolds number-dependent transition between. We got such correlations between three variables for slurries, and from experiments (see Chapter XV).

The direction of our work is to develop simulations to get efficient computation leading to 3D correlations. This will happen. Then we will get real engineering correlations from numerical experiments. I like this approach since it uses numerical simulations in a natural way evolving from their intrinsic properties rather than trying to fit them into a more familiar frame using models. I think that processing of data for correlations, from experiments, field data or simulations is a great new opportunity of the computer age and ought to be vigorously pursued.

The problem faced by models is how to get the various interaction terms right. Much of the time the guesses made for these interaction terms are poor and the predictive power of the model is not there. Better models must also make use of correlations for the interaction terms. For example, the Richardson-Zaki correlation gives an excellent correlation for bed expansion, but leaves the modeling of the drag force needed for a mechanist's model to imagination.

Let it be said that the active pursuit of correlations is an excellent direction for future research using computers in a new way with direct applications to both engineering practice and model construction.

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