Mathematical Modelling of Particles in Fluid Flow

Bruce R. Sutherland (University of Alberta),
Stuart Dalziel (University of Cambridge),
Eckart Meiburg (University of California, Santa Barbara)

August 18 - 22, 2014

This report presents a review of the material covered at the workshop “Mathematical Modelling of Particles in Fluid Flow”. The scope of the workshop was very broad both in terms of the range of problems covered (e.g. aerosol drug inhalation, cementing in oil and gas wells, avalanches, volcanic eruptions, sand dune evolution, etc) and the tools employed to understand the phenomena (e.g. theory guided by in situ observations and laboratory experiments, and various numerical modelling techniques including “level-set methods” and “smoothed particle hydrodynamics”). As well as lectures, group and individual discussions were actively encouraged. In particular, participants were asked to write perhaps more provocative questions on pieces of paper, which were then read and posed to the participants by a moderator on Monday and Wednesday afternoon. At the end of the meeting, the participants were asked to answer several questions on a Google poll. The content of the talks, the discussions, direct feedback and poll results are used to compose the details of this report.

1 Overview of the Field

Although the resuspension, transport and sedimentation of particles in a fluid is important in wide-ranging disciplines, a mathematical understanding of these processes remains elusive in all but the simplest circumstances.

Consider, for example, the process of sedimentation in which particles fall under gravity and accumulate at the ground. In the mid-nineteenth century, Stokes formulated the settling rate of a single sphere in relatively high-viscosity fluid. The model proved accurate in predicting the settling of highly dilute solutions (less than 1% by volume), but it under-predicted the settling rate of more dense solutions because the return flow of fluid around a particle hindered the settling of its neighbour. The effect of the return flow could be heuristically accounted for. But this still yielded incorrect predictions for the settling rate observed in experiments of moderately dilute suspensions.

Only 40 years ago was this relatively simple problem resolved [1]. Most issues, however, remain under active investigation. What is the influence of the domain size and geometry upon settling? What is the correct mathematical treatment of the thickening sediment layer at the bottom of the domain? At what point should this sediment layer be treated as particles in a fluid and at what point as fluid in a porous material? Under what circumstances can the particle-fluid matrix be described as a continuous, though non-Newtonian, fluid? How should one treat the behaviour of non-spherical and non-electrically neutral particles such as clay? How is sedimentation, coagulation and dispersal affected by turbulence? How is turbulence affected by the presence of particles (particularly colloidal molecules which have recently been used as drag reduction agents in pipelines)?

An indication of the active research in mathematically modelling settling particles in fluids flow is evident through several review articles in the well-cited Annual Review of Fluid Mechanics [2, 4, 5, 3].

More challenging still is the problem of sediment resuspension by a fluid moving over a bed of particles. In the simplest scenario, due to A. Shields (1936), particles are transported along the bed and possibly resuspended into the body of the fluid if the stress of the fluid acting on the bottom is sufficiently large to overcome the reduced weight of the immersed particle. In ongoing research, this criterion has been modified through various empirical formulae to account for turbulent flow and multiple particle sizes. But such approaches do not account for transient effects, such as wave-breaking on beaches, nor do they consider the possibility of resuspension from stagnation points in the flow where the stress is zero but the strain is large. The boundary conditions on the flow itself are modified by the presence of the particle layer (even if it is not yet moving) in ways that are not yet properly understood.

Understanding particle sedimentation, resuspension and transport has important consequences in environmental, industrial and medical sectors. Specifically, industrial applications include the management of waste water, dredging in river deltas, settling in tailing ponds and the determination of offshore oil drilling sites. Fisheries are concerned with nutrient transport in the benthic boundary layer. Aerosols such as dust and ash not only affect air quality, but dust raised by storms over the African desert act as a seed for the formation of hurricanes in the Atlantic Ocean. In medicine there is a need to understand drug transport through inhalation.

Historically, research into particle settling has been dominated by chemical engineers and environmental scientists. Their training gives them a valuable intuition for the dynamics of particles in fluids. But they do not bring to bear upon the problem the range of tools available to a mathematician.

Perhaps the greatest fundamental advances in the understanding of particle transport by fluid flows has been accomplished through the development of numerical simulations. Historically the first numerical approaches were based on averaged forms of the Navier-Stokes equations complemented with closure relations that mimicked the classical approaches for turbulence modelling [6]. However, these closure relations were derived from heuristic arguments, and suffer the same limitations as the numerous turbulence models available at present. Their major drawback is the lack of universality: the models contain a set of parameters that can be flow-dependent or hard to determine experimentally. Therefore the performance of the averaged models is unreliable and the results can be flow-dependent. In addition, the well-posedness and stability of the various averaged models are not intensively studied. To our knowledge, there are no successful attempts for the development of a homogenization theory similar to the one developed for porous media flows.

To help overcome these difficulties, more than a decade ago methods were developed to solve efficiently the full Navier-Stokes and particle equations for problems with a large number of particles [7], [8]. Unlike direct simulations of turbulence, the simulation of particulate flows requires additional relations to account for particle interactions. The spatial scale of such interactions can vary from zero (elastic collisions) to the lubrication scale (interactions in very viscous fluids). These cannot be realistically resolved by any numerical discretization. Approximations, such as the penalty method, fictitious domain method and immersed boundary method, necessarily sacrifice accuracy for efficiency in order to reduce the complexity of the overall problem and make it solvable. With the advance of powerful parallel computer clusters, the direct simulation approach has the potential to become a tool for modelling certain particulate flows of practical interest.

All this said, the most realistic prospect for a breakthrough in the description of particulate flows will likely involve a combination of mathematics guided by experiments, observations and and simulations that combine the direct approach with the solution of the averaged equations, similarly to the numerical upscaling developed for porous media flows [9].

The workshop brought together applied mathematicians with researchers actively engaged in numerical modelling and laboratory experiments of particle resuspension, transport and sedimentation. The common objective was to advance mathematical and computational models used in industry, the environment and in medical science.

Interdisciplinary interactions were established through the cross-pollination of ideas between mathematicians and practitioners as well as the exchange of ideas between researchers with medical, engineering and geophysics backgrounds.

2 Recent Developments and Open Problems

The exponential growth in speed and memory of computers has greatly advanced the study of particles in fluid flow. But much more progress needs to be made to understanding how to mathematical model the physics governing interactions between individual particles and complex fluid flows.

Our workshop identified the following as some of the most significant open problems:

1. When particles have a diameter comparable to the dissipative (Kolmogorov) scale in a turbulent flow, no one knows what are the expression of forces acting on those particles. The interplay of particles with turbulence is poorly understood: does the presence of particles enhance or damp turbulence?

2. If a particle is deformable (eg a bubble, a water droplet, a fiber, a capsule), how does the surrounding fluid affect the particle and how does the particle deformation affect the fluid? Does the deformation act as an additional reservoir of energy?

3. The growth of water droplets in a cloud provides a particular challenge. The microscopic ($\sim 1\mu$m) growth phase is understood from thermodynamics. The rapid growth of large droplets ($\sim 250\mu$m) has been modelled through the engulfment of smaller drops as the large droplet falls through them. But it is not well understood how the combined physics and chemistry of condensation, surface tension, etc affect the growth of moderately large droplets.

A far greater challenge involves understanding systems having a high concentration of particles. In addition to the problems above, particle-particle interactions with a fluid greatly complicates the problem. Our workshop identified the following open questions:

1. It remains a challenge to capture erosion of a bed of particles by an overlying fluid flow. Though heuristics exist to model erosion by steady flows, the understanding of particle resuspension and transport by transient bursts in turbulent flows and about points of flow separation (as at the top of sand dunes) remains poorly understood. When erosion does begin to take place, large particles can eject small particles from the particle bed through the process of "saltation", adding to the complexity of modelling such flows.

2. The settling of a dilute suspension of spherical particles is well-understood, and progress has been made in understanding the settling of anisotropic particles and moderately dense suspensions. Poorly understood are the complex dynamics of flocculation, which occurs when the particles (such as clay) are attracted to one another through electostatic forces. Individual flocs are fractal-like structures whose settling rates in fluid are poorly understood as is the effect of hydrodynamics forces upon the structure of the settling particles.

3. Although avalanches and turbidity currents (submarine avalanches) have been investigated for many decades, the dynamics of a mobile suspension of particles and their eventually run-out remains poorly understood. The modelling of each phenomenon is fundamentally different because particles provide most of the momentum in snow and rock avalanches, whereas the momentum of the interstitial fluid plays an important role in avalanches of rock, sand and clay down the continental shelves of the ocean. In systems with a wide range of particle sizes, the run-out is much larger than predicted by present mathematical models. This is because small particles can gain substantial momentum through collisions with larger particles and the effective rheology of the fluid as 'seen' by the large particles is altered by the presence of small particles.

4. In very dense particle suspensions (pastes, slurries, cements), the macroscopic properties of the flow are non-Newtonian, meaning that the strain on the medium is not proportional to the applied stress. It remains poorly understood how the rheology of such media (which characterize the stress-strain relationship) depends upon the range of particle shapes and sizes, their concentration in the fluid medium, and possibly other factors. (For example, in foam, deformability and surface tension also play a role.)

As well as these challenges in mathematical and physical modelling of fluid-particle systems there remain outstanding problems in experimental and numerical modelling:

1. Despite advances in multigrid methods, mesh refinement and parallel computing, numerical models that resolve individual particles in fluids at this time can capture on the order of 10^4 particles interacting over time scales of seconds. It remains a challenge to bridge the gap between such simulations and physical systems with billions of particles in time scales of hours or longer. To do so requires the determination of appropriate scaling laws that allow us to upscale our findings from small-scale DNS simulations and laboratory experiments to larger-scale phenomena.

2. Likewise there remains a gap between numerical models of industrial processes in the energy and chemical industries in which the flows are confined within complex containment systems involving mixers and sieves.

3. On a more fundamental level, in some circumstances there is a disconnect between laboratory experiments and numerical simulations. In order to provide validation of numerical models, experiments should be performed of very simple configurations to collect data that can be used for direct comparison with simulations.

Finally, an ongoing challenge is the recruitment and training of next generation of graduate students. The study of particles in fluid flow requires solid foundation in mathematics and physics. And so it is unfortunate that most physics departments have shifted their focus away from fluid dynamics research. Numerical modelling thrives in mathematics and engineering departments. But there remains a need for more laboratory experimentalists researching fundamental, rather than focused industrial, processes.

3 Presentation Highlights

Talks were given by seven plenary speakers whose research spanned the range of physical, industrial and environmental problems as well as experimental, observational and numerical investigation methods. Collectively they summarized the advances and outstanding research problems facing the community of scientists examining particles in fluid flow. Synopses of these talks are given below.

1. Stuart Dalziel: *The impact of a droplet on a bed of particles*

   This talk focused on dropping things. Dr Dalziel discussed experiments and their physical interpretation for a number of novel configurations with work spanning nearly twenty years. He began with a brief discussion of the role of the hydrodynamic wake behind a rigid body falling onto a bed of particles and how this vortex-ring-like wake could be more important for resuspending particles than the classical ballistic mechanism. From this he moved on to looking at how a vortex ring by itself could resuspend material in an otherwise quiescent flow. This work, which can be viewed as a prototype for resuspension due to turbulence, demonstrated the role of deposition of secondary vorticity, through viscosity, leading to boundary lager separation as a resuspension mechanism. He demonstrated the approximate self-similarity of the craters produced by the vortex rings and the energetic relationships in the system.

   Dr Dalziel then returned to a variant of his initial problem to consider a falling droplet rather than a rigid sphere. Looking from afar, the droplet produces a ‘splash’ that is superficially similar to that of a solid particle, but that raises somewhat more material than might have been expected. Dr Dalziel also talked briefly about the additional dynamics if the droplet if the fluid is enclosed in a membrane that ruptures on impact, instantaneously removing the restoring force for waves in the system and resulting in a previously unseen Richtmyer-Meshkov growth mechanism.

   The final configuration considered was Richtmyer-Meshkov instability of a granular layer subject to an impulsive vertical acceleration. As with the classical instability, surface features are inverted and amplified by an acceleration directed towards the lighter phase (air). Elements while the overall mechanism can be identified as Richtmyer-Meshkov, there are features that can be understood as the triggering of avalanches.

2. Rama Govindarajan: *Droplets: sinking/rising under gravity; clustering; imparting buoyancy*

Dr. Govindarajan's talk was in two parts. The first part was about three-dimensional simulations of an initially spherical single drop of fluid rising under gravity through another fluid. A comprehensive phase diagram of symmetry-breaking and bubble-breaking were discussed and the connection made to dynamics. She also asked how a rising bubble is fundamentally different from a sinking drop. The second part was about dynamics of droplets in the vicinity of vortices, when the droplets were allowed to grow and shrink. Inertia and thermodynamics are important in the resulting clustering and dynamics. She showed that particles can cluster in unexpected regions, and that buoyancy due to phase change can modify the dynamics a lot. The relevance of this work to clouds were discussed.

3. Andrew Hogg: *The flow of fluidised particles*

   The 2010 eruption of Eyjafjallajokull, Iceland posed many problems for the operational forecasting of the atmospheric dispersion of volcanic ash and the assessment of the risk for air travel; European airspace was closed for several weeks . Mathematical models of the ash dispersion encompassed advection by the atmospheric winds, diffusion by atmospheric turbulence and settling under gravity. But The models neglected the sustained perturbation to the atmospheric stratification caused by the intrusion of the ash plume.

   In this study we investigate how ash intrusions may be driven by buoyancy processes associated with the disruption of the atmospheric stratification and we show that these effects may be dominant within the first few hundred to thousand kilometers from the volcano. This suggests that current operational models of such motions are flawed due to their omission of these effects and that the risk to aircraft due to airborne ash may not be fully assessed.

4. Jim McElwaine: *Particle sedimentation and resuspension in geophysical flows*

   Avalanches, turbidity currents, debris flows and pyroclastic flows are all gravity currents driven by the weight of solid particles. How these particles move vertically within the flow, including their entrainment and deposition, critically effects the flow dynamics. For example a debris flow where the solid particles are fully suspended is much more mobile than one where granular friction is dominant. In other flows a two layer structure often occurs with a dilute particle cloud above a shallow dense layer. Dr. McElwaine formulated a simple model that can reproduce this behaviour and showed the results of direct numerical simulations. He gave a comparison with lab experiments and field data and showed how these effects can be incorporated in shallow water models.

5. Eckart Meiburg: *Double-diffusive sedimentation*

   When particles settle through thermal and/or compositional density gradients, double-diffusion may fundamentally alter their dynamics. The example of sedimentation from buoyant, freshwater river plumes into the saline ocean below serves to explain the fundamental physical principles. In typical estuaries the density contribution of the sediment is less than that of the salinity, so that the overall stratification is stable. Within this overall stable density profile, however, the sediment itself is unstably stratified. Its available potential energy can be released in the form of double-diffusive fingering, which drastically alters the effective settling velocity of the sediment. This effect has been demonstrated in laboratory flow visualization experiments. For the purpose of modeling the global sediment cycle, it is essential to have accurate estimates of the sediment flux from river plumes, as rivers represent the main vehicle responsible for the transport of sediment from land into the coastal oceans. In spite of its importance, however, a generally accepted comprehensive description of the double-diffusive sediment flux from river plumes is still elusive, and scaling laws and/or reliable quantitative measurements of this sediment flux as a function of the governing flow parameters are as of yet unavailable. Traditionally, this flux has been estimated based on the Stokes settling velocity of the individual sediment grains, without accounting for double-diffusive effects.

   Dr Meiburg explored the nonlinear regime of such processes by means of two- and three-dimensional direct numerical simulations (DNS). The initial instability growth in the DNS is seen to be consistent with the dominant modes predicted by linear stability analysis. The subsequent vigorous growth of individual fingers gives rise to a secondary instability, and eventually to the formation of intense plumes that become detached from the interfacial region. The simulations show that the presence of particles with a Stokes settling velocity modifies the traditional double-diffusive fingering by creating an unstable 'nose region' in the horizontally averaged profiles, located between the upward moving salinity and the downward moving sediment interface. The effective thickness l_s (l_c) of the salinity (sediment) interface grows diffusively, as does the height H of the nose region. The ratio H/l_s initially grows and then plateaus, at a value that is determined by the balance between the flux of sediment into the rose region from above, the double-diffusive/Rayleigh-Taylor flux out of the nose region below, and the rate of sediment accumulation within the nose region. For small values of $H/l_s \leq O(0.1)$, double-diffusive fingering dominates, while for larger values $H/l_s \geq O(0.1)$ the sediment and salinity interfaces become increasingly separated in space and the dominant instability mode becomes Rayleigh-Taylor-like. A scaling analysis based on the results of a parametric study indicates that H/l_s is a linear function of a single dimensionless grouping that can be interpreted as the ratio of in- and outflow of sediment into the nose region. The simulation results furthermore indicate that double-diffusive and Rayleigh-Taylor instability mechanisms cause the effective settling velocity of the sediment to scale with the overall buoyancy velocity of the system, which can be orders of magnitude larger than the Stokes settling velocity.

While the power spectra of double-diffusive and Rayleigh-Taylor dominated flows are qualitatively similar, the difference between flows dominated by fingering and leaking is clearly seen when analyzing the spectral phase shift. For leaking-dominated flows a phase-locking mechanism is observed, which intensifies with time. Hence the leaking mode can be interpreted as a fingering mode which has become phase-locked due to large scale overturning events in the nose region, as a result of a Rayleigh-Taylor instability.

6. Joseph Monaghan: *How to simulate several liquids and species of particles using SPH*

   SPH (smoothed particle hydrodynamics) is a particle method that replaces a fluid by a set of particles that interact according to the equations of fluid dynamics. In his talk Dr Monaghan described how SPH can be used for problems involving liquids containing particulate matter which he referred to as dust. The dust particles were considered sufficiently numerous to allow them to be treated collectively as a fluid which was represented by a set of SPH particles which interact with the fluid SPH particles by drag terms. He showed how solid bodies (stirrers) can also be handled by replacing them by SPH particles in a straightforward way.

7. Anne-Virginie Salsac: *Fluid structure interaction of a microcapsule in flow*

   A capsule consists of an internal medium enclosed by a semi-permeable membrane that controls exchanges between the environment and the internal contents and has a protection role. Natural capsules are cells, bacteria or eggs. Artificial capsules are widely used in industry (pharmaceutical, cosmetic, food industry, etc) for the protection of active substances, aromas or flavours and the control of their release. They are also used in bioengineering applications, such as drug targeting and artificial organ fabrication.

   In most situations, capsules are suspended into another liquid and are thus subjected to hydrodynamic forces when the suspension is flowing. The motion of the suspending and internal liquids creates viscous stresses on the membrane, which lead to its deformation and possible breakup. The three-dimensional fluid-structure interactions may be modelled coupling a boundary integral method (for the internal and external fluid motion) with a finite element method (for the membrane deformation). This Dr Salsac showed to be a stable and accurate coupling strategy. She concentrated on the case of ellipsoidal capsules and explored their motion and deformation when subjected to a simple shear flow.

   When designing artificial capsules, it is also necessary to control and tune the capsule deformation, so that it has the desired behaviour. Dr Salsac showed how the mechanical properties of microcapsules can be obtained from a microfluidic experiment.

4 Scientific Progress Made

As intended, the significant progress was made through the cross-fertilization of ideas stemming from different disciplines. Feedback provided by the Workshop participants after the meeting expressed great excitement at the breadth of topics covered. Many participants were inspired by seeing numerical and experimental techniques used in other disciplines.

Laboratory experimentalists were inspired by the new techniques (discussed by David Rival) to measure flow through porous media. Many researchers were excited to see the range of numerical methods used to model particulate flow.

As an example for cross-fertilization among different fields, double-diffusive particle dynamics (discussed by Eckart Meiburg) were understood to be important in a broad range of applications. Important examples can be found in the fields of environmental multiphase fluid dynamics (the global sediment cycle, sedimentation from buoyant freshwater river plumes, the formation of giant submarine fans with volumes of millions of km^3 such as the Bengal/Ganges fan off the coast of India), climate change (the dynamics of rain droplets in clouds, the removal of CO_2 from the surface of the ocean by marine snow, deep-sea CO_2 sequestration), energy (the formation of deep-sea oil and gas deposits by submarine turbidity currents), water supply and sustainable development (loss of storage in water reservoirs as a result of sedimentation).

Some who had not heard of smooth-particle hydrodynamics (discussed by Joseph Monaghan), a technique championed in astrophysics, were inspired to learn and adapt this method to their own research. New interpolation methods in the context of immersed boundaries will be employed by the broader numerical community to enhance the accuracy of simulations of particle-particle and particle-boundary interactions.

The different numerical modelling approaches all have their strengths and weaknesses. The Workshop made progress in identifying schemes that can provide the most insight for a given problem at reasonable computational cost.

The multiphase problems in geophysical fluid dynamics have lots of similarities with processes occurring in chemical process industries. Generally, there is a need for tacking problems that occur in nature with all its coupling of multi-physics. Some researchers appreciated scaling techniques and empirical methods used to start with a "toy problem" and build it up to a complicated scenario. Conversely, some researcher benefited by seeing asymptotic techniques used to simplify complex scenarios.

Computational strategies for fully resolved particulate flows have moved on considerably - and perhaps now reliably reproduce physical flows and effects That said, many of the numerical models developed are looking for applications. And many of the laboratory experiments presented would benefit from accurate numerical models that could give more microscopic insight into the observed macroscopic dynamics. The dialogue afforded by the meeting has brought these groups together. Experimentalists have been given guidance to design and analyze their studies in a way that can be modelled numerically with direct comparison of results. The close collaboration between computational and experimental researchers is crucial, as both sides can contribute in areas that are not easily accessible to the other group.

5 Outcome of the Meeting

As evident from feedback following the meeting, immediate benefits of the Workshop include the wide-ranging new collaborations that have been created and past collaborations that have been reinvigorated by topic raised.

New links have been forged between numerical modellers who have been developed different simulation methods but see the potential for advancement through technology exchange. This includes application of particle-resolving simulations, smoothed-particle hydrodynamics and lattice-Boltzmann methods to the chemical process industry. Research into fibers in fluid flow have provided a new challenge for some of the numerical modellers that will now be pursued.

New experimental results into turbidity currents and avalanches have inspired some modellers to apply their codes to these circumstance. This research has also inspired an experimentalist working on fibers to advance his research to the study of particle-laden flows and it has given new insight to a sedimentologist to reinterpret his observations of submarine channels.

New test cases have been developed to combine different numerical technologies and laboratory experiments. The novel use of hydrogel to study flow through porous media will be adopted by several of the experimentalist participants. New research is planned to use this technique to examine pore-pressure-driven flows.

Finally, new interdisciplinary collaborative partnerships were formed between researchers focusing on fundamental fluid dynamics and applied mathematics on one hand, and researchers interested in bio-, aerodynamical and environmental applications on the other.

References

[1] G. K. Batchelor, Sedimentation in a dilute dispersion of spheres, *J. Fluid Mech.* **52** (1972), 245–268.

[2] R. H. Davis and A. Acrivos, Sedimentation of noncolloidal particles at low Reynolds numbers, *Annu. Rev. Fluid Mech.* **17** (1985), 91–118.

[3] E. Guazzelli and J. Hinch, Fluctuations and instability in sedimentation, *Annu. Rev. Fluid Mech.* **43** (2011), 97–116.

[4] A. Guha, Transport and deposition of particles in turbulent and laminar flow, *Annu. Rev. Fluid Mech.* **40** (2008), 311–341.

[5] C. Kleinstreuer and Z. Zhang, Airflow and particle transport in the human respiratory system, *Annu. Rev. Fluid Mech.* **42** (2010), 301–334.

[6] F. Toschi and E. Bodenschatz, Lagrangian properties of particles in turbulence, *Annu. Rev. Fluid Mech.* **41** (2009), 375–404.

[7] R. Glowinski, T. Pan, T. Hesla, D. Joseph, and J. Periaux, A fictitious domain approach to the direct numerical simulation of incompressible viscous flow past moving rigid bodies: application to particulate flow, *J. Comput. Phys.* **169** (2001), 363–385.

[8] N. Sharma and N. Patankar, A fast computation technique for the direct numerical simulation of rigid particulate flows, *J. Comp. Phys.* **205** (2005), 439–450.

[9] Y. Efendiev, T. Hou, and X.-H. Wu, Convergence of a nonconforming multi scale finite element method, *SIAM J. Numer. Anal.* **37** (2000), 888–910.