

## EPSRC CCP5 Workshop on Particle Simulation Techniques for Colloids, Pastes and Powders.

Cavendish Laboratory,  
Mandingley Road,  
University of Cambridge  
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CCP5 held a workshop on mesoscale particle modelling of colloidal liquids, pastes and granular systems at the Cavendish Laboratory, Cambridge on the 1st of April 1999. The meeting, which was the first of its kind for CCP5, was well-attended with in excess of 40 participants. The purpose of the workshop was to bring together theoreticians and simulators involved in modelling these materials at the microstructural particulate level. The focus was on calculating properties of practical/materials science relevance such as rheology.

There are still many technical challenges associated with the particle modelling of these systems. These are primarily ones of establishing the most relevant length and timescales to include in the computer model. Modelling these systems from the atomistic level (a sort of 'bottom up' approach) is not feasible and moreover, even if it were, would not be effective procedure for identifying the key physical and dynamical processes that are responsible for the material's behaviour. (There is not much you can easily do with the co-ordinates and positions of millions of atoms!) The important dynamical processes and interactions that govern the physical behaviour (mechanical, rheological and structural) take place on the mesoscale. The atomistic approaches, Molecular Dynamics and Monte Carlo would completely miss these because of the quantity of information they would provide. To make progress and minimise the number of particles that need to be followed in a simulation, it is necessary to identify the key distance and lengthscales operating in the material that determine its physical properties. To a certain extent, the starting point for this is physical intuition, but this has to be justified by the success of model in reproducing a range of experimentally verifiable phenomena. Inevitably, a series of iterations and refinements to the model will then be required.

With this prologue in mind, this workshop was concerned with particle modelling of (a) colloidal liquids, in which solid particles are suspended in a liquid 'host' medium (b) dry powders, in which a gas fills the interstices between the granules, and (c) pastes, which are like very high concentration colloidal liquids that are so viscous that they have solid-like characteristics on 'short' timescales. The scientific and technical issues, which are actually to a large extent the same, were discussed for all of these systems. The morning session commenced with Tony Ladd (Chemical Engineering, University of Florida at Gainesville) who gave a talk outlining the technical challenges associated with Lattice Boltzmann simulations of colloidal liquids. In this technique the solvent is represented by a distribution of 'particles' on a lattice. The boundaries of the colloidal particles have to map on to this fluid lattice, the methodology for achieving this most realistically is still an active area of debate.

Eric Dickinson (Department of Food Science, University of Leeds) talked about particle modelling of particle gels such as are found in foods. In these systems the interactions between the particles

are quite strong and ‘sticky’ at short range, so the particles can form irreversible ‘bonds’ between them when they approach and which then have a significant orientational dependency. These strong interactions dominate the physical properties, and consequently a relatively simple model for the solvent was considered to be sufficient to a first approximation (the Brownian Dynamics method). A full treatment of the solvent hydrodynamics was not deemed so important for this class of systems.

I gave a talk on algorithms at the Brownian Dynamics level. The Brownian Dynamics, BD, simulation technique invented by Ermak in 1975 was the first to provide a numerical scheme for integrating the Smoluchowski (position Langevin) equation. This is a basic model for colloidal liquids that ignores many-body hydrodynamic effects. Each colloidal particle is assumed to be ‘hydrodynamically’ isolated and subject only to a Stokes drag and uncorrelated Brownian Forces. The original Ermak BD algorithm is still widely used. I showed the results of BD simulations carried out with alternative algorithms which offer significant improvements in numerical efficiency. These were developed in collaboration with A.C. Branka (Polish Academy of Sciences, Poznan, Poland). These were based on, for example, Runge-Kutta and Smart Monte Carlo. These modifications are quite simple to implement and can lead to factors of two or three at least increase in timestep while at the same time giving more accurate thermodynamic and static properties.

The morning session was concluded with a lively open discussion, led by John Melrose (Cavendish Laboratory, Cambridge). One of the main discussion topics in this part of the first session was: what elements of the hydrodynamics in the system is it necessary to incorporate in the model? For concentrated dispersions, and especially at high shear rates, so-called lubrication forces between the colloidal particles are probably the most important terms. These are essentially pair-wise additive and therefore can be incorporated in a particle simulation code relatively efficiently. The physical origin of this term is when two colloidal particles approach closely the liquid between them gets ‘squeezed out’ but with great reluctance, so there is an effective repulsive force between the particles, which is proportional to their relative velocity of approach. This interaction diverges at sphere contact (assuming them to be hard spheres) which means that, in this continuum level description, the two spheres can never touch! When the particles attempt to move apart, there is an effective attraction force.

The afternoon session was commenced with Ugur Tüzün (Chemical Engineering, University of Surrey) who talked about Granular Dynamics simulations and tomographic imaging of granular beds. One of the problems holding back theoretical developments of granular materials has been, until recently, that there were no effective non-intrusive probes that could investigate the state of the inside of a bed of granular material as it is conveyed or simply standing in a heap, for example. Our understanding of granular materials was confined to their behaviour at the surface (e.g., wall pressures on silos) and macroscopic properties such as flow rates. This has made particle simulation techniques particularly valuable. Granular Dynamics, an extension of Molecular Dynamics has proved effective in its relatively short history. One of the recurrent themes of discussion was again the appropriate lengthscale and timescale for the interparticle interactions to include in the model. Granular particles can be said to be in ‘contact’ over a wide range of distance scales. Two typical granules are rough and therefore are in ‘contact’ at the asperity micron level at numerous points where the two mountainous surface profiles touch. It was argued that this, however, was not the appropriate scale upon which to base the computer model. Rather, the particle scale was the appropriate scale

to describe the assembly. The particle 'contact' is assumed to occur over a reasonable fraction of the particle's surface. It is assembly dynamics and statics that are most appropriately followed, rather than asperity micromechanics which are on a much finer and therefore more poorly defined surface topography. John Baxter (Chemical Engineering, University of Surrey) gave a presentation showing a movie of particles discharging from a model silo, work carried out in collaboration with Ugur Tüzün. Various engineering conditions were changed and the discharge characteristics were shown to depend on these variables. Paul Langston (Chemical Engineering, University of Nottingham) discussed the simulation procedures for modelling pastes, using a continuum finite element level description of the interstitial fluid.

This was a very successful workshop in my opinion. There was much lively and informed discussion from the participants and the attendees. The local arrangements were admirably organised by John Melrose and Meg Staff of the Cavendish Laboratory.