Statistical and Visual Probing of Evolving Granular Assemblies

Laurence M. Smith

Chemical and Process Engineering
School of Engineering
University of Surrey

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Abstract

The majority of processes in the chemical and allied industries involve the storage and conveyancing of granular material, the physics of which is still not particularly well understood. Whilst some non-invasive techniques have been developed, much experimental work unfortunately interferes with the fields being investigated. For this reason and in conjunction with increasing computing power, there has been an increase in simulation based studies. Granular dynamics simulations, being based upon inter-particle interaction laws, give the potential to investigate assemblies at the “micro-level” and have been successful in modelling process conditions in a number of granular flow situations. To date, most analyses of these simulations are essentially static in nature involving “time snapshots”. However, in a granular dynamics simulation there is a wealth of data available on a time referenced basis which has the potential to allow a quantitative analysis of the dynamics of assembly evolution.

This dissertation describes the development and application of a toolkit for post-simulation analysis. However, the utilities within the toolkit would be equally applicable to large experimental data sets should such data sets exist. The application of the toolset focuses largely on the dynamics of heap evolution in both 2D and 3D with some supportive 3D work on hopper discharge. A major part of the work involves the application of time series techniques (including the wavelet transform) in the context of variable coupling during avalanching. Segregation by self-diffusion receives particular attention and a new mechanism is proposed by which segregation by particle size takes place in the boundary layer of a low impact feed heap displaying a clear velocity gradient during discrete avalanching. Periodic lateral surging is shown to enforce mixing for a high impact feed, a phenomenon which appears to switch off below a certain feed impact. Segregation by self-diffusion is also shown to take place with the conical section of a 3D discharging hopper (in the presence of a velocity gradient) which is in agreement with experimental studies. In the context of the discrete defining events which characterise the evolution of a granular assembly, the discrete wavelet transform is shown to be capable of identifying “time constants” in the absence of real periodicity. A flexible colour coded display capability (for both 2D and 3D) is shown to be helpful in investigating the dynamics in conjunction with the time series methods developed.
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CHAPTER 1. INTRODUCTION

1.1 Industrial perspective

The storage, flow and conveyancing of granular materials is of importance across a wide range of process industries and ranges from small scale applications such as tabletting in the pharmaceutical industry (Tüzün et al, 2002) through to large scale applications such as the bulk handling of coal, for example in power stations (Abou-Chakra & Tüzün, 2000). Problems experienced in bulk solids handling include flow control, flow measurement and blockage. A particular example is provided in power generation from coal where the rate of heat output is clearly a function of input mass flowrate (though other factors such as moisture content, feed air temperature etc. do have a significant impact). The measured input flowrate could be in terms of the rotational speed of the motor driving the screw (or other) feeder. However, because of problems such as blockage and variable particle size distribution, the actual flowrate of feed coal may not be being accurately measured with a consequent loss of efficiency and excessive costs. Another example concerns the design of storage silos where design methods involve assumptions about the stress distributions at the wall. Changes in wall stress distributions during hopper discharge have in extreme cases led to silo collapse. Fluctuations in bulk density have implications for product quality and composition control. Further, in relation to tabletting, where the clear aim is to maintain a constant dosage of active ingredients (Baxter et al, 2001), phenomena such as segregation and stratification and will clearly affect the homogeneity of a product mix. Problems of product degradation are also important due to the degree of agitation to which particles are exposed. This is of particular importance with regard to the storage and transportation of grain.

Design criteria for the storage and handling of bulk solids have largely been determined as a result of empirical methods such as the Beverloo correlation and subsequent modifications (as discussed in Nedderman, 1992) for the flow of granular material through orifices. However, whilst these methods can be successful in
predicting global phenomena such as flow rates, they do not address the nature of the assembly at the level of individual particles where, within the bulk, phenomena such as segregation and variations in voidage distribution may be important. In illustration of the potential for overlooking such problems, there is considerable evidence that the simple pouring of a homogeneous mixture with a size distribution can result in segregation or stratification for a variety of reasons including geometrical effects, density differences or variation in engineering design parameters such as feed rate (Baxter et al, 1998, Makse et al, 1998).

1.2 The nature of granular flow

Within the process industries, a wide variety of flow regimes are encountered including hopper discharge, heap formation, rotating drums, screw feeders and fluidised beds. Some of these are characterised by precisely defined constraining geometries (e.g. hopper discharge). However, others are characterised by evolving boundaries (e.g. heap formation). As opposed to fluid flow which is reasonably well understood and for which we have equations to model flow (e.g. the Navier-Stokes equation) and provide a suitable framework for design methods, granular flow is much less well understood. In particular, granular flow is characterised by discrete defining events such as failure under shear (for example avalanches) by which the granular assembly evolves. By comparison with fluids, for which the natural state of the constituent molecules is that of motion, the natural state of a granular material is that of rest. Furthermore, whilst one can realistically model the molecules in many fluids by spheres which interact (and for a dilute gas, infrequently), the vast majority of granular material consists of particles of irregular shape which are nearly always in contact with other neighbouring particles. Apart from the extreme case of smooth spheres, the interactions between particles will involve a frictional element due to small scale surface asperities. However, asperities on a larger scale can give rise to interactions of a much more complex nature as surface features of neighbouring particles “lock” with one another. Such interactions will give rise to “long range connectivity”, whereby a particle’s movements can have an impact on particles some
distance away. Granular materials are also known to adopt alternative packing arrangements. Even for spheres, there are alternative loose and close packing arrangements (see German, 1989) and the precise arrangement ultimately adopted by an assembly will be a function of the evolutionary process, for example slow feed to a heap, fast feed, feed with agitation of the base.

1.3 Theoretical and experimental approaches

Clearly, much experimental work has been done with regard to granular flow. However with regard to the underlying physics of the evolution of granular assemblies, it is very difficult experimentally to see or obtain measurements of what is going on inside the assembly. Invasive experimental methods tend to disturb the flow field and are therefore of only limited applicability. Some sophisticated non-invasive techniques have been developed for limited applications (e.g. Nikitidis et al, 1998). A basic requirement of any model is to predict stress and velocity fields in flowing granular materials. Theoretical methods such as Janssen's differential slice force balance method (as described by Nedderman, 1992) have been developed. However, these methods make assumptions concerning the uniformity of bulk properties. For example, Janssen's method which involves a force balance over an incremental slice of material assumes that stress is constant in a horizontal plane. Continuum methods ignore the effects of microstructure and do not consider particle properties such as size and shape distributions. The kinetic theory has been successfully applied to predict the flow of low density fluids where the distances travelled by particles between collisions are large relative to the sizes of the particles. By definition, the kinetic theory provides a model based upon interactions at the particle level and as such is a complement to continuum and other methods. Attempts have been made (Savage & Dai, 1993, Oger et al, 1996) with some success to apply the kinetic theory to lean phase granular flows, but also to dense slow shearing granular flows. Reasonable agreement has been found with the results of experimentation.
1.4 Simulation and granular dynamics

It is against the background of difficulties highlighted in previous sections that simulation methods have the potential to assist in our understanding of granular flows. Granular dynamics (GD) techniques, also referred to as discrete element (DE) techniques derive from molecular dynamics where statistical mechanics techniques are applied to the output from such simulation to determine thermodynamic and transport properties (Haile, 1992). Essentially, the GD technique involves the applications of the laws of classical mechanics to model interactions at the inter-particle level. For granular dynamics, interaction models involve a normal force law and can include a frictional force law (not applicable in the molecular dynamics domain). The simulation proceeds by evaluating the accumulation of forces at a time step on each particle to determine the components of translational and rotational velocity of each particle in the assembly which are assumed constant up to the next time step. The time steps are small enough to realistically model continuous flow. Alternative models for the normal interaction of particles include a Hooke’s law spring model, a contact mechanical Hertzian interaction and various Continuous Interaction (CI) potential models along the lines of the Lennard Jones potential for inter-molecular attraction and repulsion. Langston (1995) compared these interaction models and the results of such simulations for the filling and discharge of hoppers with direct experimentation and established knowledge of granular flows in silos.

A significant strength of GD techniques lies in the ability to investigate changes in particle parameters such as size, density and roughness as well as engineering parameters such as feed rate and impact velocity for stockpile formation. Most work to date has concerned 2D disks or 3D spheres. Some real processes are essentially 2D in nature, for example conveying cigarettes and in certain types of bottling where motion is one co-ordinate direction is disallowed. 2D simulations do to some extent represent equivalent cross-sections extracted from genuinely 3D processes (e.g. flow in an axially symmetric hopper). However, the inability of the particles (in 2D) to flow in and out of the 2D plane (which will happen in real 3D) must be taken into
consideration. Because of this limitation in the capacity to dissipate energy, there is the potential for phenomena to manifest themselves much more strongly in 2D than would be the case in 3D. However, much larger arrangements can be modelled by 2D simulations due to the limitations of processing power. For example a 10,000 particle 2D simulation of heap formation may give rise to a heap of (base) width greater than 200 particle diameters. However, the same number of particles in 3D might give rise to a base diameter of the order of 40 particle diameters which sets restrictions on the analyses that can be applied to the output data.

Of course, the majority of granular material consists of non-spherical particles, usually of different shapes and sizes. The modelling of micromechanical contacts for particles with disperse shapes presents a considerable problem. One possibility that has been applied with some success involves modelling "odd shaped" particles by bonding spheres together in rigid structures to create these shapes. This technique is known as constrained dynamics and is the subject of on-going work at the University of Surrey.

Granular dynamics is only one of a number of alternative simulation methods, but has the advantage that is based upon inter-particle interactions and so has the potential to allow investigation of an assembly from the mesoscopic scale upwards.

1.5 Broad aims of the thesis

The sections above have outlined bulk solids handling problems and briefly described alternative strategies to model and gain greater understanding of granular flows. Granular dynamics simulations are identified as one way of producing data sets at the particle level for the evolution of granular assemblies with a view to gaining a greater understanding of the physics governing granular flow. Granular dynamics simulations produce a vast amount of data, in fact time sampled multivariate observations based upon each particle. To date, GD simulations have been successful in providing supporting evidence for phenomena that are observed experimentally. However, it has
usually been done on the basis of observed snapshots (e.g. of stress or velocity distributions) at fixed (and often arbitrary) points in time. The dynamic evolution of the assembly has often been largely ignored. However, the dynamics of evolving assemblies in terms of periodicity, time constants and defining events is what really must be better understood in order to be able to solve process problems such as those described in earlier sections.

The aims of this thesis are to investigate suitable methods that can be applied to probe and investigate time dependent multivariate data such as that resulting from granular dynamics simulations, though applicable to any suitable data sets. In particular, one aim is to develop techniques to enable coupling of process variables in the context of the defining events in the evolution of granular assemblies. Whilst one aspect of the work is essentially mathematical, it is important always to be able to provide a visual representation as the human eye has a hugely greater capacity to detect patterning than machine implemented algorithms and so the second aspect of the work involves the implementation of a flexible visual display capability for both 2D and 3D data. An implicit aim of this thesis is to further justify the use of granular dynamics simulations in realistically modelling observed phenomena in granular flows. In this context, there will be some focus on the known mechanisms of heap evolution such as avalanching.

A number of issues present themselves both in 2D and 3D which require alternative approaches in order to bring focus on important phenomena. An example is an evolving heap where an Eulerian approach (for example focussing on a fixed cell and observing flow though it) suffers from the shortcoming that the cell probably only experiences a short period of significant activity as the heap boundary sweeps through it. However, a different perspective (the Lagrangian approach) is obtained when an individual particle is followed which may experience a prolonged period of activity if it remains in the dynamic boundary region and is propelled by a number of avalanches. Both approaches will be brought to bear where possible using the tools developed.
1.6 Structure of the thesis

Following this introduction, chapter 2 is intended to place GD techniques amongst other methods of investigation and to review the important work done in the area, in particular with regard to the work done at Surrey University by previous workers in developing the GD models that have been adapted and used for the work described in this thesis. The chapter concludes by pointing to the potential for the development of a toolset to derive more from the simulations.

Chapter 3 reviews methods (some from very different areas) that have potential to be applied to the output from GD simulations including any essential mathematics. Not all methods reviewed are actually applied in the work undertaken. Chapter 4 describes the components of the toolset actually developed and particular algorithms employed. Chapter 5 reviews significant results and findings from the application of the 2D toolset. Chapter 6 does the same for the 3D toolset. Brief conclusions will be summarised after substantial sections in chapters 5 and 6 before chapter 7 brings together an overall summary of the conclusions of the work with suggested directions in which it could be further developed.
CHAPTER 2. REVIEW OF GRANULAR DYNAMICS AND THE REQUIREMENT FOR POST PROCESSING ANALYSIS

2.1 Methods applied to granular flows

Before proceeding to describe granular dynamics simulations and to justify the requirement for sophisticated post processing tools, it is important to place the technique against a background of theoretical and other methods.

2.1.1 Theoretical continuum methods

Theoretical continuum techniques are relatively successful in modelling fluid flow. For example, undergraduate courses in fluid mechanics will develop the Navier-Stokes equation. With regard to the modelling of solids handling, some theoretical techniques have been developed for stress analysis and prediction of the flow field. Nedderman (1992) presents a good review of these methods. To take one example, the “differential slice stress analysis” method has been developed in various stages based upon the method originally introduced by Janssen in 1895. However, in this method, most bulk properties are assumed constant and independent of particle properties. For example, Janssen’s original analysis is based upon the assumptions that stresses are uniform across any horizontal section of the material and that the vertical and horizontal stresses are principal stresses. Whilst relaxation of assumptions such as these as described by Nedderman result in a more realistic modelling, these continuum techniques ignore the effects of microstructure (interactions at the inter-particle level) which determine the evolutionary path of granular assemblies. Nedderman also describes the application of plasticity theory to predict the velocity distribution in a granular material. Because these methods assume that stress and velocity profiles are linked by a flow rule, they are seen as potentially more useful than kinematic models for which velocity profiles will depend upon geometric factors and be independent of the stress distribution. However, development has been restricted to a limited range of flow geometries, for example hopper flow.
2.1.2 Empirical methods

Perhaps due to the importance for many years of the oil industry, fluid mechanics has been an important part of chemical engineering education, at the expense of a consideration of the theory of granular flow. As a consequence, design methods for bulk solids handling (for example silo design) have traditionally been purely empirical. In the previous section a very brief mention was made of theoretical continuum methods. However, currently, most design is based upon empirical methods. For example in predicting mass flow from orifices various correlations (e.g. due to Beverloo, discussed in Nedderman, 1992) have been established to predict mass flow as a function of bulk density, orifice diameter, coefficient of friction and the acceleration due to gravity. Empirical methods will clearly remain important for process design. However, there remains the requirement to better understand why phenomena such as segregation by particle size and flow blockage due to arching manifest themselves – answers to which will certainly allow the development of improved design methods.

2.1.3 Review of experimental research

Obviously with regard to the statics and dynamics of granular material the literature contains a wealth of experimental work. A restricted number of pieces of research are briefly reviewed below because they provide a background against which the granular dynamics post-processing work of this thesis is set. The articles are selected for consideration because they relate to the phenomena that have been investigated by the post simulation toolset as the substantial work of this thesis.

Grasselli & Herrmann (1997) performed careful experiments in a turntable cell to investigate the angle of repose and other important angles with regard to granular heaps. Further they investigated the dependence of these on the presence of walls and on the fabric (texture) of the granular material and on the “memory” capacity of the
heap in terms of an initial fill structure. An important consideration discussed by the authors relates to the fill regime. It was found that without particular attention being paid to the fill procedure, experimental reproducibility was poor. A slow fill procedure was found to give good reproducibility. It is well known that granular materials can arrange themselves into different packing arrangements (for instance with widely varying voidage values) and that the granular heap will evolve by way of changes to the packing arrangement. Clearly the authors were experiencing this important phenomenon at the outset of their experimentation. The experimental set up was essentially two dimensional (the heap was retained between parallel walls. However, the authors describe the use of a cubic cell (with retaining walls separated far enough to remove wall effects) and make comparisons with genuine 3D heaps with only a 0.3 degree difference between the two. The essential experimental procedure involved tilting the heap to a maximum angle until an avalanche occurred and then repeating the procedure. The memory effect was evidence by the number of "tilts" until a constant angle of repose was obtained (and different from the "fill" angle of repose). These results that were observed with sand and glass splinters were not observed with glass spheres. A large part of the work in this thesis involves detailed investigations into the dynamics of free forming heaps evolving by a process of avalanching.

In a later article, Grasselli et al (1999) describe experiments involving the shape and evolution of a granular heap and its dependence upon the impact energy. They experimented with the impact height of lead beads onto the heap and observed heap evolution by a number of mechanisms. For most of the time, the new bead bounced down the heap until it was trapped, thus giving rise to a local change in the slope of the heap. However, rolling, ejection of other particles and occasional large avalanches were observed. The evolution of the heap was found to be a very complex phenomenon due to the way momentum is transferred during collisions, frictional properties and other forms of energy dissipation. However, the authors note that the growth of the heap displays a remarkably stationary state for which they construct a simplified model.
2.2 Segregation and feed-rate

Currently, one of the most studied aspects of granular material is flow against an essentially immobile surface. This can occur in boundary driven shear flow (Hirshfeld et al, 1997), avalanching during heap formation (Baxter et al, 1997), and de-mixing or radial segregation occurring in a rotating drum (Choo et al, 1998). Some of the more interesting phenomena observed during heap build-up include segregation and/or stratification, which can occur when a mixture of grain types is used in the pouring process (Koeppe and Kakalios, 1998). The phenomenon of particle segregation is widespread and occurs when particle mixtures are mixed and sheared (Hirshfeld and Rapaport, 1997), (Khosropour et al, 1997).

Segregation is often an unwanted phenomenon in bulk solids handling and over recent years, a debate has been taking place in the granular community concerning segregation and stratification by grain size. Makse and co-workers develop arguments supporting their theories concerning segregation in a number of articles. For example, Makse et al (1997) describe a number of quasi 2D experiments of poured granular flow of a mixture of two grain sizes against a retaining wall. One principal conclusion of the work is that stratification (into layers) can only occur when the angle of repose of the larger grain material is larger than that for the smaller grain material. The angle of repose will be dependent upon geometrical considerations such as the angularity of the material. A second conclusion was that segregation (where large and small particle species accumulate in different regions of the stockpile) is an inevitable (and unavoidable) consequence of the pouring process. However, Baxter et al (1998) in a series of quasi 2D experiments of heap formation for a mixture of borax pentahydrate granules showed clearly that stratification can occur when the angles of repose of the two granular species is the same. In addition, because granules were of the same material, particle density was identical. Stratification was found to occur for a slowly poured heap, but not for a high impact feed stream. The controlling mechanism was postulated as one of “capture” where for a high impact feed, entrant particles can become embedded on first contact with the heap. For a low impact feed, large particles
were thought to be less likely to become embedded and so could roll over fine grains and so cause stratification into the observed layers. The main implication of the work is that if the feed rate is sufficiently slow, then stratification can occur.

The mechanisms of segregation by particle size are clearly far from being well understood and there are currently conflicting schools of thought. The ability of granular dynamics simulations to provide data at the level of the individual particles provides the potential to better understand these mechanisms.

2.3 Simulation

This thesis essentially presents the results of the application of a post-processing toolset to data generated from granular dynamics (GD) simulations. This section is intended to justify the use of simulation methods in general and GD simulations in particular.

2.3.1 Simulation and experimentation

Of course, the conventional approach when developing a theoretical model is to perform suitable experiments in order to validate the model. However, in a wide range of applications, experimentation can be prohibitively expensive, dangerous or indeed impossible. It is particularly in these circumstances that computer simulations can help to validate a model or to throw more light onto a problem than can be achieved by other means. With regard to the investigation of granular flows, a significant factor is the inability to “see inside” a granular assembly. Furthermore, invasive probing has the potential to disturb the fields being investigated. Experimental work on granular flows is therefore limited in terms of its capacity to investigate microstructure and necessarily involves implicit assumptions. For example, to investigate velocity profiles during discharge from hoppers Cleaver & Nedderman (1993) describe the use of “tracer particles” which are introduced at known points in the assembly prior to discharge. The tracer particles are larger than the bulk particles and are retrieved by
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Sieving. Velocity is then derived from residence time before collection in the sieve. Such techniques are clearly capable of demonstrating important results, but involve implicit assumptions, in this case of a radial particle trajectory. Of course, such assumptions can be further investigated, but of perhaps more significance is the effect on the flow field of a particle of a different size from the remainder. Cleaver and Nedderman also describe disturbance of the flow field by the presence of the tube used to position the tracer particle within the bulk. Similar problems have been described with regard to the introduction of stress measuring transducers into an assembly, where difficulty was experienced in determining the orientation of the probe and also of the interference of the probe of the flow field.

2.3.2 Review of simulation models

A range of simulation methods have been developed and adapted to investigate granular media. The alternative methods are each capable of representing different aspects of real granular systems to a greater or lesser degree than each other. It depends upon what the simulator is trying to achieve as to which method is most suitable. A significant factor to be considered is the size of the simulation (in terms of number of particles) and the computing power available. A brief review of the three main methods is given below along with argument in support of the granular dynamics method used to produce the data investigated in preparation for this dissertation.

2.3.2.1 Cellular automata methods

Cellular automata methods pioneered by Bak et al (1988) led to the development of the theory of self organised criticality. A cellular automaton model involves a lattice of discrete cellular variables where the local stability is governed by simple rules. The application is not restricted to the sandpiles of Bak et al. However, for such a sandpile, a local site (containing grains) that is supercritical according to the rules will relax to a state of local stability by the transfer of grains to local sites. Of course this may make these neighbouring sites supercritical in turn requiring further transfer of grains. Thus the consequent chain reaction can give rise to avalanching phenomena which are
characteristic of a real evolving sandpile. The CA lattice could in a simple instance be just the height above a point on the base of the highest particle positioned above that point. However, the mapping of direction of motion and rotational orientation of particles were mapped to onto a CA lattice by Baxter & Behringer (1990, 1991) in modelling hopper flow. CA simulations have been shown to produce agreement with experimentation at the macro-scale; for example, Makse et al (1997) reproduced stratification in a study of poured binary heaps. However, CA simulations suffer from the disadvantages that they do not account for explicit inter-particle interactions and realistic time and length scales of avalanches. However, they are computationally relatively inexpensive and potentially offer the facility to simulate larger granular assemblies than, for example, granular dynamics.

2.3.2.2 Monte-Carlo methods

Monte-Carlo methods (so called because of the implications of randomness for casino gambling) have been widely used in statistical physics. MC methods involve the evolution of an assembly through a sequence of randomly generated configurations. Each configuration is based upon the previous one and must pass an acceptance test based upon statistical thermodynamics. Reasonable representations of thermalised molecular systems have been shown to result. However, an acceptance test in the case of granular material is probably less realistic because the natural position is one of rest. Rosato et al (1986) studied size segregation in a vibrating bed by MC simulation. However, the slow shearing flows that are studied in this dissertation are unlikely to be well modelled by the MC method because it lacks the capability to incorporate the collective behaviour of particles for which connectivity can span a number of particles.

2.3.2.3 Granular dynamics

Granular dynamics (discrete element) techniques derive from molecular dynamics where statistical mechanics techniques are applied to the output from such simulations to determine thermodynamic and transport properties (Haile, 1992). Essentially, the simulation technique involves the applications of the laws of classical mechanics to
model interactions at the inter-particle level. For granular dynamics, interaction models must involve a normal force law and a frictional force law (not applicable in the molecular dynamics domain). The simulation proceeds by evaluating the accumulation of forces from interactions between neighbouring particles at a time step on each particle to determine the new components of translational and rotational velocity of each particle in the assembly which are assumed constant up to the next time step. The time steps are small enough to effectively model continuous flow. GD simulations are therefore completely deterministic as opposed to the randomness associated with Monte Carlo methods.

Granular dynamics simulation work has been undertaken at the University of Surrey for some time with the pioneering work done by Langston whose work is briefly reviewed in section 2.4. Alternative models for the normal interaction of particles include a Hooke’s law spring model, a contact mechanical Hertzian interaction and various Continuous Interaction (CI) potential models which can include both attraction and repulsion terms in the same way as the Lennard-Jones potential used to model inter-molecular attractions. A comparative review of the inter-particle interaction laws used in granular dynamics is presented by Langston et al (1995a).

For the CI model, typically the potential energy between a particle pair is given by the short-range repulsive (SRP) analytic form,

$$
\phi(r) = \varepsilon \left( \frac{\sigma}{r} \right)^n
$$

(2.1)

where \( r \) is the centre-to-centre separation of the pair and \( \sigma \) (small particle diameter) and \( \varepsilon \) (potential energy at \( r=\sigma \)) respectively set the distance and energy scales of the interaction. The parameter, \( n \) is the characteristic particle index which describes the ‘hardness’ of the interaction. A little more detail of the simulation model is given in appendix A1 with a description of “reduced units” in appendix A2.
2.4 The work of Langston

From the results of simulations for the filling and discharge of hoppers, Langston (1995a, 1995b, 1995c, 1996) compared the interaction models described in the previous section with direct experimentation and established knowledge of granular flows in silos. With regard to the CI model, an initial aim of the work was to investigate the effect of normal and tangential (inter-particle) interactions on hopper flow. An important aspect of the work involved the combination of the normal CI force with the Mindlin equation to model tangential friction and to establish the credibility of the method to model processes realistically. The simulation output was compared with theory and experimentation with regard to stress distributions, velocity and voidage profiles and discharge rates.

For the static case, normal stresses were found to be near the active limit and thus in agreement with continuum theory and with recent experimentation. For hopper discharge, normal stresses near the orifice were found to tend towards the passive state which is also observed experimentally. 3D normal stresses were found to reflect the same trends as in 2D although there was some reduction in fluctuations of stresses across the hopper. Flowing shear stresses in 3D showed a minimum towards the centre of the hopper and are thus in agreement with continuum theory which predicts zero shear at the centre. Wall stress calculations for both the static and dynamic case resulting from the simulations also showed some agreement with established criteria. Good agreement with theory and experimentation was obtained with regard to velocity profiles, voidage profiles, rupture zones and discharge rates.

With regard to validation of the CI model at the meso scale, i.e. in terms of the motion of individual particles, Langston ran some small scale 2D simulations (of a few hundred particles) and made direct comparisons with 2D experiments. The experimental procedure involved photographing the flow of wooden “draughts” and comparing with simulation graphic output. Good agreement was found in terms of particle movement (e.g. rotation) but importantly, phenomena such as “arching” (when
the orifice is too small) and “layering” during the initiation of flow were found to be equivalent in the experiments and the simulations. For both experiment and simulation, the radial flow field was demonstrated for a mass flow hopper.

Validation of the 3D model employed by Langston could obviously not be done in a similar way to the 2D case. However, the non-invasive technique of “Gamma Ray Tomography” was applied to investigate solids fraction (voidage) patterning in the static case and during flow of a bed of Canadian maple peas. Good agreement was found between experiment and a soft sphere simulation model. The soft sphere model, where the particle interactions scale with the particle diameter rather than the microcontact asperities, was shown to realistically represent the structure of the bed. Langston et al (1996) extended their hopper flow simulations to include air-impeded discharge from a conical hopper by imposing a radial flow field of counter-current air applied through the use of an Eulerian grid.

2.5 The work of Baxter

As a logical consequence of the success of the work of Langston, Baxter’s work (Baxter, 1998, Baxter et al, 1997, 1998) has focussed attention upon heap formation and stability. The three main themes of the work are an evaluation of the usefulness of the angle of repose as an indicator of particle properties, an investigation of the microstructural properties of granular heaps, and an investigation of size segregation behaviour of poured granular mixtures.

The work focuses particularly on investigating the effect of design criteria such as feed rate and impact velocity of the feed stream on the heap and the implications of model parameters which determine inter-particle interactions. With regard to particle properties, for example, Baxter investigated the dependence of the angle of repose on contact stiffness for both 2D and 3D simulations. For the 2D case, contact stiffness was found to be significant in determining the angle of repose. However, for the 3D case the relation was shown to be considerably less significant. The suitability of the
GD simulation technique to investigate microstructural imaging (in terms of stress, velocity and voidage distributions) was clearly demonstrated where, for example, dips in stress distribution at the base of the heap were shown to be restricted to rather specific and idealised conditions. In general, the distribution of forces at the base was found to be sensitive to simulation conditions such as contact stiffness.

With regard to mixing and segregation phenomena, some recent research (Makse et al, 1998) has suggested that particle properties (as measured by the angle of repose) are the sole determining factor in determining the extent of segregation. However, Baxter’s work has suggested that design parameters such as those influencing the feed stream are more important and that careful design considerations can help to prevent or limit unwanted segregation; see for example Baxter et al (1998).

2.6 The CI model used in this thesis

Appendix A gives a little more detail on the CI model and the “reduced units” used in the simulations that are analysed in this thesis. The CI model has been demonstrated by both Langston and Baxter to be successful in producing realistic representations of bulk deformation. Soft sphere (disk in 2D) interaction models like CI allow particle overlap and involve explicit interactive forces between particles that in a real assembly would not actually be in contact. However, the success of such models is because locally, due to the packing arrangements, particles are having an effect on those nearby despite not being in actual contact. Clearly, particle overlap is not a true physical interpretation of the inter-particle interaction. However, the incorporation of frictional engagements gives rise to particle displacements that themselves are realistic. Evidence of “long range connectivity” from Baxter’s work resulting from the implementation of the CI model is evidence of its potential to model phenomena such as rupture zones.
A significant strength of DE techniques lies in the ability to investigate changes in particle parameters such as size, density and roughness as well as engineering parameters such as feed rate and impact velocity for stockpile formation. Future work in the area is likely to include the modelling of cohesion which is of much greater significance in the handling of fine powders such as cement and the influence of particle shape. Most work to date has concerned 2D disks or 3D spheres. The modelling of micromechanical contacts for particles with disperse shapes presents a considerable problem. One possibility is to model “odd shaped” particles by bonding spheres together in rigid structures to create these shapes. This technique is known as constrained dynamics and work on this is underway at Surrey University (Schettino, 2003).

2.7 The potential for post-processing of simulation data

The term granular dynamics clearly implies that the dynamics of an assembly are being addressed, which of course they are from the point of view of the model. However, many of the published results from granular dynamics simulations are essentially static in nature, for example, “snapshots” of stress distributions and velocity profiles (e.g. Langston et al, 1995). Whilst workers in the area produce time plots, in general the evolutionary nature of granular assemblies is not addressed. The granular dynamics continuous interaction (CI) method described above involves a model of the interactions between particles in an assembly. Normal and tangential forces on a particle are accumulated from interactions with neighbouring particles. These normal and tangential forces give rise to translational and rotational accelerations and hence to particle movements. The output from a simulation is therefore on a particle basis and are essentially components of position vector, components of velocity vector, components of normal forces between individual particles and components of frictional forces between particles. Since output can be sampled with a frequency governed only by the size of the update algorithm timestep, the basic output data is a multivariate time series of particle related variables – i.e. one multivariate time series for each particle. Thus there is a natural progression to a
Lagrangian approach to the investigation of evolutionary phenomena, i.e. following
the experience of individual particles. However, with regard to the assembly as a
whole, other variables such as components of stress, voidage, local velocity gradients
etc. must be derived from the particle related variable values and suitably averaged on
a regionalised grid system. We can therefore apply a complementary Eulerian
approach to the investigation of evolutionary phenomena.

Certainly there is value in inspecting time referenced “snapshots” – for example to
investigate wall stresses in a dispensing hopper. However, there should be some
rational basis for selecting appropriate times for snapshots which implies some kind of
time series approach. However, over and above considerations of snapshot selection is
a requirement to investigate the evolutionary dynamics of assemblies and the coupling
of variables.

Some important work concerning the evolution of the microstructure of granular
materials has been done by Koenders and co-workers (Koenders, 1997, 1998,
Koenders et al, 2001). The work concerned the strain dependent evolution of a
heterogenous material. An assembly subjected to incremental straining developed
“structures” with regard to local stiffness. Spectral analysis was applied spatially
which pointed to length scales related to the observed structures. The work of

Time series can display a variety of patterning phenomena including trending
(increase or decrease), periodicity (cycles) and discrete catastrophic changes
superimposed on random noise. With regard to regular periodicity, the concept of a
time constant (equal to the period) is obvious. However, the determination of time
constants in the context of discrete events that do not occur regularly is rather more
difficult. The coupling of variables in terms of correlation is clearly routine. However,
the coupling of discrete changes within two time series is not so straightforward,
although it has the potential to be revealing.
Review of granular dynamics and the requirement for post processing analysis

Time series analysis is largely concerned with pattern recognition in a particular sense. However there is potential for the application of more conventional pattern recognition techniques to the spatial nature of GD simulation data, for example with regard to the identification of regions of interest, for example avalanching regions in a cross-section through a 3D heap.

Within the multivariate time series and time referenced spatial arrays that can be output data from GD simulations there should be a great deal of evidence to help gain an understanding of the physics governing the evolution of granular assemblies. It is the entrapment of this evidence particularly concerning the evolutionary dynamics of granular flows that is novel and is the aim of this thesis.
CHAPTER 3. A REVIEW OF ANALYSIS TECHNIQUES POTENTIALLY APPLICABLE TO LARGE SIMULATION DATA SETS

3.1 Introduction

The previous chapter essentially supports the granular dynamics simulation approach in the context of gaining a greater understanding of granular flows. The chapter concluded with a justification for the implementation of techniques in addition to the “snapshot” approach that has usually been applied. This chapter reviews approaches that have been born out very different fields of study, but may find application to the results of granular dynamics simulations. Not all of these techniques have been applied, as this chapter is a review. For those techniques such as the wavelet transform that have been further developed and applied in this thesis, sample applications will be briefly mentioned in this chapter along with the basic theory, leaving a thorough discussion of the method of application until the next chapter.

Implicit in the work of this thesis is the notion of patterning and pattern recognition and whilst the main thrust is in relation to patterning in the temporal sense, there is certainly scope for pattern recognition as applied to spatial images. For example, for a plan (surface) view of an avalanching heap we might need answers to questions such as “what defines the boundary of an avalanching region?” In this context, tree structured pattern recognition methods could be applicable and are reviewed. However, the thesis is not about pattern recognition interpreted as image recognition as would be understood, for example, in the case of robot control of production lines. This chapter will therefore not review neural network and fuzzy logic methods which are currently fashionable in “conventional” pattern recognition. The chapter starts with a brief overview of conventional multivariate methods.
3.2 Multivariate analysis

The particle attribute data that is naturally output at sampled time points from granular dynamics (GD) simulations is clearly multivariate in nature. There is certainly the potential to apply multivariate analysis. However, it is difficult to place these techniques outside the context of a static analysis as opposed to addressing the dynamics which is the main thrust of this thesis. However, in a review chapter such as this it would be hard to justify their complete exclusion and so a very brief review of the most important techniques follows. Applications are across the range of physical and social sciences where model building, discrimination, classification or dimensional reduction are involved. For a thorough review of multivariate techniques, see Johnson & Wichern (1998).

3.2.1 Discriminant analysis

This technique involves placing a vector of characteristics into one of a number of pre-defined alternative classes. An example would be allocating an individual a credit rating as either good average or poor based upon a financial record. A process example would be placing a vector of process observations into one of a number of known states (e.g. within control, requiring corrective action etc.).

3.2.2 Cluster analysis

This involves grouping subsets of entities into mutually exclusive groups (clusters) based upon the similarities between the entities. Unlike discriminant analysis, groups are not pre-defined. However, discriminant analysis can follow naturally from Cluster analysis. Of course, any clustering may not be meaningful in terms of identifiable characteristics. However, with regard to data resulting from granular dynamics simulations, it might be that a cluster of particles, if located in close proximity, could define a region of physical interest.
A review of analysis techniques potentially applicable to large simulated data sets

3.2.3 Principal components analysis

This technique involves reducing the dimensionality of the vector of observations by transformation. The underlying principle is that initial variables in the vector may be highly correlated among themselves. Principal components analysis transforms to a reduced set of uncorrelated variables. The presumption is that one proceeds to work with only the first few (significant) components.

3.2.4 Factor analysis

This involves identifying a more fundamental set of variables from which the observation (vector) is derived. For example, in process control, Factor Analysis could provide the transformation from a more fundamental set of variables (which might not be immediately measurable) to the control variables themselves. For GD simulations, it is possible that Factor Analysis could reveal a fundamental dependency that would increase understanding of the underlying physics. There is a Principal Components solution to Factor Analysis.

3.2.5 Multiple regression

Multiple regression as an extension to simple two variable least squares regression is concerned with model building. In particular it involves methods of determining the “best” functional relationship between a single dependent variable and a subset of potential independent variables. Forwards selection and backwards elimination strategies exist to determine which variables are included or excluded from the model. The notion of a linear model (transformation) underpins much of multivariate analysis.
3.3 Pattern identification/location techniques

This thesis is concerned with extracting useful information from large data sets with particular emphasis on evolutionary dynamics. Techniques specifically related to dynamics such as Fourier analysis of periodicity will be dealt with later. However, within the large 2D and 3D data sets that result from GD simulations, there are likely to be "regions of interest" which need to be identified and defined and hopefully tracked. Examples of such regions of interest might include avalanching regions in a stockpile, regions of high stress in a feed hopper etc. In this context, some of the methods that have been applied in other areas of study are worthy of consideration.

Much of the published literature concerning pattern techniques is associated with recognition of 3D objects based upon results from some kind of scanning such as grey scale levels for a black and white picture (e.g. Terauchi et al, 1991). Range image matrices where the scanning results in a matrix of depths is another important form of image scanning and has considerable similarity with derived local average arrays (such as voidage or stress) from the results of GD simulations (see for example Hoffman & Jain, 1987). Since the basic requirement is to identify and locate real objects, most of the published material concerns algorithms for detecting boundaries, edges etc. For example, in a black and white aerial picture of a pitched roof, detection of the ridge line might be a requirement. Whilst much of the literature in this area only has application to "real world" object recognition, with regard to the large data sets considered in this thesis, there is the potential to fruitfully apply some of the techniques. Certainly, in the context of phenomena such as rupture zones, edges and boundaries are likely to be of particular interest.

3.3.1 Hierarchical tree structured methods

For binary patterns (arrays containing only zeros and ones), tree structured methods (quadtrees, octrees) are described in the literature (e.g. Samet, 1982, 1991 and Shaffer & Samet, 1988) and essentially reduce the requirement to record repeated values
A review of analysis techniques potentially applicable to large simulated data sets

(redundancy). The requirement to record each of a number of identical adjacent observations conforming to a "binary" breakdown (e.g. fours, fours of fours etc) is avoided. In the process, the early emergence of nodes in the tree (for the 2D case) signify large square regions of uniformity. Appendix C illustrates the construction of a quadtree from a sample binary image.

Importantly, tree traversal algorithms have been around for some time and might provide the framework for region identification and tracking. For the purpose of identifying regions in GD simulation data, conversion to a binary representation by some form of thresholding would be an initial requirement. These tree structured methods provide a way of introducing proximity grouping. Although in principle initially only "square" proximity regions would be initially identified, small squares adjacent to large squares can be linked. Extension to 3D and 4D are programmatically more complex, but do afford the potential to locate phenomena in space. With regard to large simulation data sets, the potential drawbacks concern the storage of large data structures in RAM and CPU cycles in traversing extremely large trees.

Tree methods also exist to define contours (strip trees, polyhedral approximation, e.g. Bell & Pau, 1990). Thus, if the boundary of a region could be identified (e.g. by gradient analysis, then it could be represented in tree form. In addition to these tree methods, the concept of pointer systems in general (e.g. to trap gradients, near neighbour relations) has application potential.

3.3.2 Region Growing Techniques

With regard to image analysis, data driven/region growing techniques are described in the pattern recognition (e.g. Besl, 1988) where, for example, gradients can group array elements into surface primitives, for example, planar surface primitives, ridge-top surface primitives. These surface primitives are grouped at a higher level to obtain a re-construction of surfaces. For example, a number of adjacent planar surface primitives with the same gradient could be merged into one larger plane surface. The
work relates specifically to range image data (derived from photo image data), where the range image is a matrix of “depths”. The published methods are designed to ultimately recognise 3D object from 2D images where in addition, edge detection, fold detection etc. are involved. Whilst the full application of the techniques described are not immediately applicable to the large data sets involved in this thesis, techniques associated with the initial stages of surface primitive identification could prove useful in locating pattern regions that may or may not have been pre-defined. The development of these techniques has progressed from fitting planes to measures of curvature (e.g. Hoffman & Jain, 1987).

3.3.3 Pattern Thinning and Contour identification

Pattern thinning techniques (e.g. Arcelli, 1981) relate to the extraction of the skeleton of a shape with protrusions such as a starfish shape. Clearly, one of the primary intentions is data compression, but in the process, shape features are revealed. Attacking the problem from an alternative direction, there is much published material relating to contour thinning, the reduction to a minimum number of adjacently linked points to define a contour between a region and the background. The use of chain codes to define a contour is also described. Chain codes are basically pointer linked lists structures that relate contour elements, for example the perimeter of a hill. There is considerable published material concerning efficient algorithms for deriving the chain codes. In common with the tree structured and region growing techniques, there is potential here for application in terms of region definition.

3.3.4 Pilot testing of quadtree routines

In the early stages of the work of this thesis, it was thought that region identification might be a significant part of the work with potential to locate and track regions of interest. Some pilot test routines were implemented in Borland Delphi © and found to be capable of pinpointing regions within binary arrays (i.e. arrays where the numbers are either 0 or 1). However, as the work progressed, the focus of attention moved to temporal issues and in particular discrete events and so no further development took
place. However, there is still scope in the application of these tree structured methods where conversion to binary format is appropriate.

3.4 Applicable kinetic theory and statistical mechanics

Classical thermodynamics provides a framework of relationships between properties of macroscopic systems, for example heat capacities at constant heat and constant volume. However, classical thermodynamics does not provide information concerning the value of any particular property, nor does it attempt to relate to any particular molecular model. Statistical thermodynamics which is applied to equilibrium systems starts from the basis of a molecular model and allows the calculation of particular macroscopic properties. In particular, ensemble averaging is shown to equate to time averaging allowing the derivation of thermodynamic properties such as entropy and Gibbs free energy in terms of distributions of molecular positions and momenta. Statistical mechanics is essentially the extension of the ideas of statistical thermodynamics to systems where particles are strongly interacting and for non-equilibrium systems. In the non-equilibrium case, transport coefficients (self-diffusion coefficients, shear and bulk viscosity, thermal conductivity) are derived as integrals over time of appropriate autocorrelation functions. Molecular dynamics simulation methods which are based upon an inter-molecular interaction model therefore provide data which is ideally suited to statistical mechanical treatment to allow the calculation of thermodynamic and transport properties of fluids. Granular dynamics as a derivative of molecular dynamics clearly provides data suitable for statistical mechanical treatment. However, it must be remembered that the nature of granular flow is very different from that of a fluid. Certainly, the natural state for the particles in a granular material is that of rest while the natural state for molecules in a fluid is that of motion. Thus concepts such as temperature do not truly apply to a granular material, though granular temperature as a concept can apply to the degree of agitation over and above the rest state. The kinetic theory of gases is well established, applies well to ideal gases and has been adapted for other fluids, for example the Enskog
theory (See McQuarrie, 1976). Some workers (Savage & Dai, 1993, Oger et al, 1996) have applied the such adaptations of kinetic theory to granular flows. However, for the granular flows considered in this thesis, distances travelled between particle collisions are much less than this and so care should exercised in the application of the kinetic theory for such flows.

Mixing and segregation are phenomena that receive particular attention in this thesis. Statistical mechanics provides techniques for the quantification of these phenomena where, for example, microturbulence gives a measure of local activity and self-diffusion coefficients give a measure of the degree to which particle species tend to separate. It is not appropriate in this thesis to attempt to integrate a substantial amount of statistical-mechanical theory. However, the equations that have been applied in respect of self-diffusion in multi-component mixtures are developed below.

3.4.1 Statistical mechanics of self-diffusion in thermalised flow systems

Einstein first showed that the one dimensional diffusion coefficient is related to mean square displacement by the relation:

$$D = \frac{\langle [x(t) - x(0)]^2 \rangle}{2t}$$  \hspace{1cm} (3.1)

where $x$ is displacement and $t$ is large compared to the average time between collisions.

The 3D equivalent is

$$D = \lim_{t \to \infty} \frac{\langle [r(t) - r(0)]^2 \rangle}{6t}$$  \hspace{1cm} (3.2)

Where in this case $r$ is the displacement vector.

The Green-Kubo relations for any property $A(t)$ express the mean square displacement of that property as an integral over a time correlation function (McQuarrie, 1976):
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\[
\lim_{t \to \infty} \frac{\langle A(t) - A(0) \rangle^2}{6t} = \int_0^\infty \langle A(\tau) \dot{A}(0) \rangle d\tau
\]  

(3.3)

So, if \(x(t)\) is the property and \(v(t)\) is velocity, then we have:

\[
D = \int_0^\infty \langle v(\tau) v(0) \rangle d\tau
\]  

(3.4)

Thus the diffusion coefficient \(D\) is an integral over all time lags, \(\tau\), from 0 to infinity of the average (over all time origins) of the velocity autocorrelation function. The traditional approach to the determination of this integral (e.g. Oger et al, 1996 and Savage & Dai, 1993) has been to assume a functional form (usually exponential) for the decay of the velocity autocorrelation function (VACF) as outlined below, and calling upon results from the kinetic theory.

Let \(a_v(t) = \frac{\langle v(t)v(0) \rangle}{\langle v(0)v(0) \rangle}\) be the normalised VACF

whence \(D = \langle v(0)v(0) \rangle \int_0^\infty a_v(t) d\tau\)

Assume \(a_v(t) = \exp(-\beta t)\), i.e. an exponential decay with time. So

\[
\frac{d}{dt} a_v(t) = -\beta \exp(-\beta t) \quad \text{and} \quad \beta = -a_v(0)
\]

Numerically differentiating to obtain \(a_v(t)\) at \(t = 0\)

\[
a_v(0) = \lim_{\Delta t \to 0} \frac{\langle v(\Delta t)v(0) - v(0)v(0) \rangle}{\langle v(0)v(0) \rangle \Delta t}
\]

\[
= \lim_{\Delta t \to 0} \frac{\langle v(0)(v(\Delta t) - v(0)) \rangle}{\langle v(0)v(0) \rangle \Delta t}
\]

\[
= \lim_{\Delta t \to 0} \frac{\langle \Delta v v(0) \rangle}{\langle v(0)v(0) \rangle \Delta t}
\]

But the VACF is independent of the time origin, so

\[
\beta = -\lim_{\Delta t \to 0} \frac{\langle v \Delta v \rangle}{\langle v^2 \rangle \Delta t}
\]  

(3.5)
In the literature, expressions for the relaxation constant $\beta$ derived from the kinetic theory are developed, resulting in an expression for the self-diffusion coefficient (e.g. Oger et al, 1996).

With regard to diffusion in granular systems, clearly the natural state is the stationary rest position. So, compared to a gas, for example, where diffusion takes place due to the random thermalised motion, diffusion can only take place in flow situations where velocity, $v$, in the above equations must be a peculiar or fluctuating velocity relative to the mean flow. So, if we define a fluctuating velocity:

$$C = v - u$$  (3.6)

where

$u$ = mean stream velocity  
$v$ = velocity of particle  
$C$ = fluctuating velocity

Referring back to equation (3.5),

$$\beta = - \lim_{\Delta t \to 0} \frac{\langle C \Delta C \rangle}{\langle C^2 \rangle \Delta t}$$  (3.7)

The limiting expression defines local microturbulence, being a measure of the degree of local agitation over and above the stream velocity. Further, $\frac{\langle C^2 \rangle}{2}$ defines a local granular temperature; see Natarajan et al (1995), Nikitidis et al (1998).

Schaink & Hoheisel (1992) conducted a fairly early molecular dynamics study of velocity autocorrelation functions and self-diffusion in multicomponent mixtures and in particular investigated the assumptions of the Enskog kinetic theory as applied to self-diffusion coefficients. The authors initially discuss work by Alder & Wainwright (1967, 1970), where the significant findings were of a slowly decaying non-exponential tail of the velocity auto-correlation function and discrepancies between the theoretical and MD simulation values for self-diffusion coefficients. The comprehensive study indicates that at moderate densities, vortex processes are
responsible for the long-time tails of the VACF. Results for higher densities explain a negative deviation from the Enskog values for the self diffusion coefficients. However, these studies were of molecular systems (not granular) and discretion should be taken when considering the application to granular flows.

A number of workers have applied statistical mechanical techniques to granular flows and simulation data. Savage & Dai (1993) investigated self-diffusion for granular flow between close rough walls by a theory based upon the classical kinetic theory and by granular dynamics simulations. Close agreement was found between the two results and so in this case, the assumption of an exponential decay of the autocorrelation function would appear to be reasonable. However, the GD simulations involved constrained flow to be within a “well defined” shearing domain (by maintaining shear velocities at the edges of the simulation box). Part of the simulation work used a hard sphere model assuming instantaneous collisions. Kinetic theory as applied to granular flows is derived from classical kinetic theory which further assumes distances travelled between collisions to be large compared to molecular diameter. A soft sphere model with finite contact time was also used to allow for collisions of more than two particles. However, for this work, the results would appear to be restricted to a highly thermalised flow regime (with similarities to ideal gas flow) and with the shear flow domain artificially and ideally maintained by the simulation procedure. In a similar piece of work, Oger et al (1996) showed that measurements of self-diffusion and granular temperature on a two dimensional air table are in good agreement with predictions from kinetic theory and from the results of simulations that were of a similar nature to those of Savage and Dai. In particular, the process was stationary and allowed long times for the determination of velocity fluctuations. The granular dynamics simulations investigated in this thesis are for realistic flows found in real processes (e.g. hopper discharge and stockpile formation). The interaction model also involves a frictional component and the flows are slow with enduring particle contacts. In this context one must question whether the assumptions based upon the kinetic theory to derive self-diffusion coefficients are entirely appropriate.
3.5 Wavelet analysis

The wavelet transform has been around for a little over a decade after pioneering work by a number of mathematicians including Grossmann and Morlet (1984), Daubechies (1988) and Mallatt (1989). Essentially, the major breakthrough in terms of a practical implementation was the convergence of the two academic areas of mathematics and signal processing. Signal processing engineers had long been familiar with iterated filter banks which are the practical means by which a wavelet transform is effected. Strang and Nguyen (1997) bring together the fundamentals in a standard text. Wavelet transforms have been applied in many diverse areas of study largely because they provide a description of a data set in terms of location (in time or space) and scale (frequency). The two-dimensional wavelet transform has particular application to digital image processing and pattern recognition.

3.5.1 The one-dimensional wavelet transform

Spectral analysis (see section 4.6.1) as performed by the Fourier transform will reveal frequency components within a signal, but will not reveal their location in time. If periodicity exists for the duration of the whole series, then Fourier methods provide the required decomposition. However, many signals of interest (and particularly the output from GD simulations) have important signal disturbances that may be periodic over a short part of the series or may involve frequency changes or may even be simply transient. To detect short-lived periodicity, it is possible to calculate spectra for sections of the series (the Windowed Fourier Transform). However, to do this it is required to have some prior knowledge of the duration of periodicity that is being investigated. The wavelet transform can perform an analysis on the basis of time and frequency (called scale) in one go and can detect transient disturbances.

As compared to Fourier analysis where a series (signal) is decomposed into a weighted sum of sinusoids where the Fourier coefficients are the weights, the wavelet transform decomposes a signal into a weighted sum of orthogonal wavelet functions. These
wavelet functions are of short duration and are localised in time and so are well placed to detect and quantify local (in time) disturbances. Appendix H gives the defining equations for a wavelet transform. The reconstruction formula of a function $f(t)$ decomposed by the discrete wavelet transform is given by equation (3.8).

$$f(t) = \sum_{j,k} \gamma(j,k) \Psi_{j,k}(t)$$

(3.8)

In equation (3.8), $\gamma(j,k)$ are the wavelet weighting coefficients and $\Psi_{j,k}(t)$ are the orthogonal wavelet functions, $j$ is a dilation index and $k$ is a translation index. All wavelets are the same shape and are derived by scaling (dilation) and translating (shifting along the time axis) a mother wavelet. Wavelets occur in families, normally named after the discoverer. In this thesis, all wavelet transforms are dyadic, which means that the scaling of the mother wavelet is only by factors of 2. Thus a wavelet at any scale is half as wide as one at the next scale up. This is defined by equation (3.9) below (also appendix H3) where again, $j$ is a dilation index and $k$ is a translation index.

$$\Psi_{j,k}(t) = 2^{-j/2} \Psi(2^{-j} t - k)$$

(3.9)

Equation (3.9) shows that given a (large) mother wavelet, two wavelets at the next smallest scale can be created both with $j=1$ and either $k=0$ or 1. The significant point is that at each subsequent smaller scale, there are twice as many wavelets which are half as wide. Any wavelet coefficient $\gamma(j,k)$ gives the weight of that wavelet (at scale $j$ and translated by $k$) within the decomposition of the signal. The difference from the Fourier transform is that the decomposition now has positioning (by translation) of localised disturbances at different scales.

The discrete wavelet transform is implemented by a procedure called the iterated filter bank (see Strang & Nguyen, 1997 or Young, 1993). Each iteration of the filter produces half as many wavelet coefficients as the one before at a scale of scrutiny twice as coarse. The first filter iteration on a series of length $n$ gives $n/2$ wavelet coefficients at the smallest scale of scrutiny. The package Matlab © provides a limited
A review of analysis techniques potentially applicable to large simulated data sets

number of wavelet transforms in the Wavelet Toolbox. In addition, others provide libraries of routines for other transforms (e.g. The Katholieke Universiteit of Leuven, Belgium has produced the WAILI toolbox). Whilst for display purposes, it is useful to implement the transform within Matlab (which has a programming capability), with regard to this study there is a requirement to implement routines in a more flexible manner and so the discrete wavelet transform has been implemented from scratch in a set of C++ classes. Details of the C++ classes are given in appendix E. The implementation of the discrete wavelet transform as an iterated filter bank is discussed more fully in the next chapter (section 4.7.2). Here, some selected applications of wavelets are briefly reviewed.

Roy et al (2001) describe a de-noising algorithm for series associated with flow models. The method involves the wavelet transform of first differences of the series and on artificially “noised” samples was shown to give a clean separation of noise. De-noising is a standard application of wavelet analysis.

Gençay et al (2001a) describe the use of the discrete wavelet transform in filtering out “seasonalities” in foreign exchange volatility models where such periodicities are the source of miss-specification of the models. Essentially, the wavelet transform is again being used as a “de-noising” tool due to its ability to perform a resolution at many different scales (frequencies).

Salvetti & Lombardi (1999) describe the application of a wavelet cross-correlation technique to the analysis of mixing in the context of two coaxial jet streams. In what they refer to as Wavelet Cross-Spectral Analysis, the cross scalogram between the wavelet transforms \( W_f \) and \( W_g \) of two time signals \( f(t) \) and \( g(t) \) is defined as \( W_f^* W_g \). Here, the wavelet transforms \( W_f \) and \( W_g \) were continuous and functions of scale and translation and * means complex conjugate. The results of the cross-spectral analysis gives rise to a function in the two variables of scale and translation which can be suitably represented as a grey scale diagram where the times and scales corresponding to a correlation (correspondence) of the two wavelet transforms are
clearly highlighted as bright regions on the diagram. A visual comparison between scalograms was shown to reveal qualitatively similar patterns, in this case the different scalograms were derived from time series sampled at different locations (that were significant with regard to the dynamics of vorticity and mixing).

Gençay et al (2001b), describe the use of the discrete wavelet transform in the analysis of foreign exchange rate volatilities where volatilities follow different scaling laws at different time horizons. They also describe the application of a wavelet cross-correlation analysis also in the context of foreign exchange volatilities at different frequencies.

Because of the capability of the wavelet transform to reveal fractal structures, the transform has been applied to investigate turbulent fluid flow. Zhou et al (2000) applied a one-dimensional wavelet transform to the analysis of particle velocity fluctuation in a circulating fluidised bed. The transform was shown to discriminate between the different scales of fluctuating velocity component within the vertical and horizontal components of fluctuating velocity. In particular there were greater contributions in the vertical fluctuating component at higher scale (lower frequency) than for horizontal fluctuating velocity components. Dyadic grids with vivid “forking” revealed a fractal structure (self-similarity) for both horizontal and vertical fluctuating velocity components, particularly in the horizontal case.

Mudde & Van Den Akker (1999) describe the application of the Haar wavelet transform to fluid velocity components in a bubble column at different gas fractions. Investigation of the standard deviation at successive levels of decomposition revealed a tendency towards a constant value as a function of gas fraction with the decrease being strongest for the higher gas fractions revealing that the flow is more turbulent for higher gas fractions.

Marone et al describe the application of two alternative wavelet transforms (Haar and Third Derivative Gaussian, TDG) to systolic blood pressure in an attempt to
discriminate between sick and healthy patients. They plot the standard deviations of wavelet coefficients at the different levels of decomposition and found that at the 5th level, the Harr wavelet gives a clear discrimination, though the TDG does not.

Alsberg (1999) describes the application of the wavelet transform to traditional cluster analysis. Multiscale cluster analysis is compared with conventional cluster analysis which has excellent resolution in time, but no resolution in frequency and Fourier cluster analysis for which the reverse is true. Multiscale cluster analysis is seen to sit between the two because information in both the time and frequency domains are incorporated. The method described involves clustering when fine level detail (to a particular level) has been removed. However, clearly, clustering could equally be on the basis of fine detail at a particular level. In fact the principle of applying multivariate techniques to wavelet transformed data is implicit in the later discussion of discriminant analysis.

3.5.2 The two dimensional separable wavelet transform

In a similar way to which the one-dimensional wavelet transform performs a decomposition of a time series into localised wavelets at different scales, so the two dimensional separable transform performs a similar task on a two dimension data set (array). However, the separable transform results in a decomposition in terms of horizontal disturbances, vertical disturbances and diagonal disturbances. These decompositions are separate and in terms of the obvious application to grey scale visual images provide the potential for edge and boundary detection. There is a wide variety of applications published in the literature mainly in the areas of data compression and pattern recognition/identification. Particular application areas include encoding of medical images, transmission of video images and fingerprint classification and identification. A few examples are now listed. Mishra et al (2001) describe the application of wavelet analysis to sequential cardiac images. Przelaskowski (2001) examines alternative tools for the archival and transmission of medical image data. Lee & Kim (2001) describe an image retrieval system based upon

The above applications are rather general but demonstrate the diversity of applications of 2D transforms. Applications closer to the subject material of this dissertation include the following. J. Ko et al (1998) describe the application of a two dimensional wavelet transform correlation technique in the context of Particle Image Velocimetry. Essentially PIV involves the analysis of planar images (of velocity vector components). They cite the presence of non-periodic and quasi-periodic phenomena and also the occurrence of error values as the reason to apply wavelet techniques. They also maintain that for fast varying flows with fine spatial structure, traditional PIV (autocorrelation) approaches fails to capture the small time and length scales of the flow field evolution. In principle, the ability of the wavelet transform to filter in time and frequency allows cross correlation of features at different lengthscales at different physical locations in the flow. There are many applications of two dimensional wavelet transforms to turbulent fluid flow. An early paper by Farge (1992) describes wavelet transforms and examples of their use in the analysis of turbulence. Farge et al (1999) describe an algorithm based upon transform coefficient thresholding for vortex extraction.

With regard to the data analysed in this thesis the potential for the application of a 2D transform is mainly with regard to surface and cross-sectional data from 3D simulations where activity of interest takes place. There is of course potential to use the transform for the output from 2D simulations although, taking the case of heap formation, probably only small regions would display disturbances of interest (as compared to the surface of a 3D avalanching heap). The capacity of the 2D transform in terms of edge detection has potential since it is likely that precise (fine-grid) spatial location of defining events will be at edges (of avalanches, for example).
CHAPTER 4. DEVELOPMENT OF THE ANALYSIS TOOLSET

4.1 The scope of the work

The data sets that are the focus of the toolset developed in this thesis result from GD simulation code developed at Surrey University. The initial simulation development work was undertaken by Langston (1995a, Langston et al, 1994, 1995a, 1995b, 1995c, 1996) who developed 2D code (written in Fortran 77) including polydispersity for the investigation of flow in hoppers. Langston also developed 3D code for the monodispersed case, again in order to investigate hopper flow. The capability was increased by Baxter (Baxter, 1998, Baxter et al, 1997, 1998) who developed his own 2D code (also written in Fortran 77) and applied it particularly to stockpile formation. Baxter also took Langston’s 3D code and developed it further (moving into Fortran 95) to incorporate the polydisperse case, again particularly with regard to stockpile formation but also implicitly with regard to hopper discharge. For the investigations in this thesis, Baxter’s 2D and 3D codes have been adapted internally where necessary and have provided data sets for subsequent post-processing on a personal computer. Baxter’s code runs on the (CPE) departmental supercomputer at the University of Surrey.

Within the context of this work there was a requirement to strike a balance between “internal processing” (i.e. particular code added to the existing Fortran code) and “post-processing” where the output was analysed after the simulation run. There are obvious advantages in internal processing including the power of the supercomputer, the ability to sample down to the time steps of the update algorithm and the availability of all process variables. However, there is often an iterative procedure with regard to getting internal processing correct (for example with regard to sampling rate) where some post processing allows corrective action to be taken internally. However, the advantages of post processing are the availability of a variety of PC software. In particular this includes a relational database capability (in this case visual dBase) and platforms that support PC databases, provide a colour graphics capability (Borland ©
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Visual C++ and Borland Delphi) and link well with Microsoft products. Routines added internally to the Fortran simulation code have included algorithms to calculate locally averaged variables such as components of the stress tensor and voidage, rotation of co-ordinate axes and monitoring of the evolving stockpile with regard to positioning of the feed hopper to regulate feed stream impact.

In this chapter, applicable background mathematics and algorithms of methods actually implemented are included in addition to any mathematics presented in chapter 3.

4.1.1 The basic intentions

Granular flows, especially heaps, evolve displaying characteristics which may involve regular periodicity over short or long scales of both time and space, but also on the basis of discrete events which are localised in time and space. In an experimental environment, these periodic and discrete events may be visible or partially visible from the outside. However, obtaining appropriate measurements (such as stresses and velocities) at the right place and time is very difficult experimentally. However, such values are available as output from GD simulations, but again the difficulty is in determining where and at what time to perform further investigations. Temporally, there is considerable scope limited only by the size of the time step of the simulation update routine.

It is the basis intention within this work to investigate the appropriateness and applicability of a range of methods. A primary intention is to attempt to couple variables (correlation). However, as mentioned previously, the time and place of sampling along with the sampling rate are of critical importance. From this perspective, much of the work is associated with time series analysis and signal processing.
Development of the analysis toolset

In addition to specialised time series and correlation techniques, since the output from GD simulations is simply arrays of numbers, there is a requirement to “view” the process being simulated (e.g. a heap). To this end, toolsets have been developed for both 2D and 3D simulations to enable a detailed inspection of views (e.g. cross sections) of the assembly at particular points in time. These toolsets incorporate colour coding of particles and regions on the basis of output variable values (e.g. components of velocity vector) and are used in conjunction with the time series methods to gain a greater understanding of assembly evolution.

4.2 Overview of applied methodology

The analyses will be restricted mainly to stockpile formation (heap evolution) but also to hopper discharge. Hopper discharge involves a constrained geometry which in some senses is simpler. The unconstrained geometry and moving boundaries of an evolving heap present more opportunities but also present considerable computational difficulties. With regard to heap evolution the prime intention is to investigate the nature of the boundary layer and the events taking place therein for different flow regimes. Whilst one is setting out to gain a greater understanding of the physics of granular flows, a principal intention must remain to relate analyses to process parameters to give applicability to significant results. In particular the process parameters involved will be the feed rate and feed mix.

Both two dimensional simulations (of disks) and three dimensional simulations (of spheres) will be investigated. The two dimensional case is both simpler computationally and allows larger geometries to be studied. However, whilst some real industrial processes are “quasi-2D”, most are obviously 3D and so whilst it is expected that two dimensional simulations have the potential to extend our understanding of granular flows, comparisons should be made to results from three dimensional simulations. Even with ten thousand particles, the geometrical dimensions of a three dimensional simulation are quite small as compared to those obtained in two
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dimensions. With this constraint born in mind, the intention is to extend the analyses performed in 2D with supportive 3D analyses.

It has been mentioned that the novel aspects of this work involve analyses to investigate dynamics. However, there must essentially be some static analyses and indeed "freeze-frame" supportive display analyses. For example, whilst perhaps most interest might be within a heap boundary layer, clearly the regions below the dynamic boundary layer need consideration and are likely to be static. Much of the work naturally involves time series. However, there is no reason to restrict a series subscript to time and indeed the work will involve some elements of spatial analysis.

Two fundamental approaches will be taken in this work in terms of dynamic analyses. The output from the simulations is essentially time referenced variables which are individual particle attributes (e.g. components of velocity). The natural analysis is therefore Lagrangian, i.e. following a particle's experience over time as is moves through the assembly. However, this will be complemented by an Eulerian approach where the experience of a fixed region in space is investigated over time as particles flow though. The Eulerian approach naturally involves calculating regional (e.g. cell) averages derived from particle attribute values. For an evolving heap, this will be closely associated with investigations of the boundary layer and will require care when deciding upon cell sizes.

4.3 Specific techniques and routines

4.3.1 Rotation of co-ordinate axes

For the 2D case, the simulation code was written with the $x$ co-ordinate direction horizontal and the $y$ co-ordinate direction vertical. However, the evolution of a heap is by avalanching down the free surface. The slope obviously fluctuates slightly over time, but a representative angle can be chosen by calculating surface gradients at sample times to allow transformation to a new set of axes with the $x$ direction down
the right hand slope and the new $y$ direction perpendicular to this. The transformation with a clockwise axis rotation of $\theta$ is performed by the transformation equations below.

\[
x_{\text{new}} = x \cos \theta - y \sin \theta \tag{4.1}
\]
\[
y_{\text{new}} = x \sin \theta + y \cos \theta \tag{4.2}
\]

These equations implement a transformation matrix:

\[
\begin{bmatrix}
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{bmatrix}
\]

Working in the transformed co-ordinate system, the transformed $x$ velocity is now an avalanche velocity (for the right hand side of the heap) and one can more readily calculate meaningful velocity gradients and appropriate components of normal and shear stresses for the investigation of coupling (see figure 5.24).

For inspection of planar vertical cross sections in the 3D case, rotation of axes was implemented by a transformation matrix:

\[
\begin{bmatrix}
\cos \varphi \cos \theta & \cos \varphi \sin \theta & \sin \varphi \\
-\sin \theta & \cos \theta & 0 \\
-\sin \varphi \cos \theta & -\sin \varphi \sin \theta & \cos \varphi
\end{bmatrix}
\]

Here, $\theta$ is an anti-clockwise rotation of the $x$ and $y$ axes about the vertical $z$ axis, followed by an anti-clockwise rotation by an angle $\varphi$ of the $x$ and $z$ axes about the new $y$ axis.
4.3.2 Lagrangian and Eulerian approaches/ determination of derived local average values

Because granular dynamics simulations are based upon interactions at the particle level, the variables that are immediately available as output are particle attributes (components of position vector, velocity, forces, accelerations etc.). Thus a Lagrangian approach is perhaps natural – i.e. following the experience of particles as they flow through the assembly. However, the interest of a process engineer is in terms of bulk properties (local stresses, voidages, average velocities etc.). These will be derived over local regions as averages, thus implying an Eulerian approach. However, we face problems when combining variables derived from the two sources (particle attributes and locally defined averages) when investigating the dynamics of the system. Considering the example of a Lagrangian approach, following a particle in order to try to couple velocity and stress, velocity presents no problem because it is a direct particle attribute. However, because stress is derived on a local average basis and probably over a grid cell system, the particle as it moves from one cell to another will record a step change in local stress. Thus the time series trace for stress will show discontinuities which will interfere with any analyses to investigate periodicity or other disturbances. This problem is not just a factor associated with a fixed grid cell averaging system. Even if we allow the co-ordinate system to follow the particle (for example averaging over a sphere centred on the particle) we will still see step changes in the trace because other particles will be entering and leaving the cell surrounding the particle.

4.3.3 Voidage and local density

Within an evolving granular assembly, re-arrangements that contribute to its evolution will necessarily be facilitated by changes in the local packing density. In fact it has been shown (Tuzun et al, 1988) that dilation of a packed assembly is necessary before flow can occur. The degree of association between a measure of packing (or its opposite, voidage) and other simulation variables (e.g. particle rotation, stress) is certainly something that needs investigating to gain a greater understanding of how...
granular systems evolve. However, if we take local bulk density, the grid size over which we attempt to measure it is a determining factor of its value. In the extreme, density measured over the whole assembly is obviously just the bulk density whereas at a very small scale (much smaller than the individual particles, local density is either 0 or 1 dependent upon whether the sample point is covered by a particle or not.

Co-ordination number is a potential measure of local density. With regard to granular dynamics simulations, the co-ordination number is the number of neighbouring particles for whom distance between the centres minus the sum of the radii is less than some arbitrary critical value. Co-ordination number is essentially computationally inexpensive to calculate; see for example Baxter (1998). In fact the update routine of the simulation makes use of a local neighbourhood list (of particles adjacent to each particular particle) which essentially provides the necessary information. As a measure of local density co-ordination number is to some extent usable for an assembly of equal sized particles. However, unfortunately, a plot of co-ordination number for any particle is a step function as during local rearrangements, even a small change in inter-particle separation can move a neighbouring particle from being “co-ordinated” to “un-coordinated” or vice versa. This over-sensitivity is a problem when attempting to couple local voidage (as measured by co-ordination number) with other measures such as rotational velocity which are genuinely continuous. The “step function” nature of co-ordination number changes over grid cell averages can be somewhat smoothed by local (moving) average filtering of grid cell values. However, ultimately it will still move in discrete steps. Moving average filtering means that instead of using the co-ordination number within a cubic cell, the value taken for that cell would be the average calculated over itself and neighbouring cells, being thus an extension of the simple one-dimensional notion of moving average technique for time series. For an assembly of different sized particles, co-ordination number for any particle is more a function of the particle size than the local density that it is experiencing, though changes in co-ordination number are potentially more usable.
Perhaps the ideal measure of local density would involve taking grid cells of an appropriate size (perhaps of the order of the size of 2-3 particles) and calculating the percentage of that volume which is occupied by particles. In principle, an array of a large number of points within each cell could be checked for “cover” by particles. However, computationally this involves a very large number of calculations and extremely large arrays. A less computationally expensive method of achieving the same result is to set up a square array (in 2D) for each particle size where array elements (corresponding to a grid mesh) are calculated as 1 if within the particle or zero outside. Each particle therefore carries with it an array of 0’s and ones that can be allocated to cells covering the whole assembly with a totalling over cells (followed by division by the number of grid points within a cell) to obtain the packing fraction. By this method, the number of points tested for coverage is a very small fraction of that otherwise required.

Packing (or voidage) as calculated in the previous paragraph is only applicable on a local average basis. Obviously a particle within a region can be attributed the local voidage for that region. However, because in this work we follow particles (the Lagrangian approach) as well as following what happens within fixed regions (the Eulerian approach) it would perhaps be useful to have a voidage measure specific to particles. This is particularly important when attempting to couple variables where misleading conclusions could be reached because of spurious step changes in local voidage as a particle moves from one cell to an adjoining one. The freedom to move experience by any particle will be measured by the number and closeness of immediate contacts. Taking the two dimensional case, if we take a circumference around a particle (at a radius slightly larger than the particle radius) and sample equally spaced points around this circumference and count the percentage of such points which are “covered” by a neighbouring particle then this can act as a packing measure. Subtraction from 100 obviously gives a voidage measure which is referred to as the “annular voidage measure”. Figure 5.23 in section 5.3.2 shows how points within a particle are allocated to a grid cell. The annular voidage measure will be relatively continuous (dependent upon the frequency of point sampling around the
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particle) and could also be averaged over grid cell regions. The method can be extended to the 3D case with a distribution of test points spread around the spherical surface at a suitable distance from the particle.

4.3.4 Components of the stress tensor

There are obviously 9 components of the stress tensor. However, if we constrain ourselves to plane strain, there are four components to calculate. For the continuous interaction model used in the simulations there are only two types of inter-particle forces that can make contributions to the components of the stress tensor – the normal interaction force and the tangential (frictional) interaction force. The two dimensional (plane strain) components of stress are derived using equations (4.3) to (4.6) below.

The usual convention of stress subscripts is adhered to where, in two dimensions, the first subscript refers to a plane normal to the axis referred to by the subscript. The second subscript refers to the direction of the stress. So, for example, \( \sigma_{yy} \) refers to stress in a plane normal to the \( y \) direction but acting in the \( x \) direction – i.e. a shear stress. The contributions to the stress in a cell due to the interaction between two particles is deemed to apply at the mid point between particle centres. The contributions from particle pairs with a mid-point within any cell are thus accumulated to give the total component for that cell. According to Seville et al (1997), the accumulation of contributions is by the equations below.

\[
V_{2D}\sigma_{xx} = \sum F_i x_m x_n + \sum F_i x_m x_n \tag{4.3}
\]
\[
V_{2D}\sigma_{yy} = \sum F_i y_m y_n + \sum F_i y_m y_n \tag{4.4}
\]
\[
V_{2D}\sigma_{yx} = \sum F_i x_m y_n + \sum F_i x_m y_n \tag{4.5}
\]
\[
V_{2D}\sigma_{xy} = \sum F_i y_m x_n + \sum F_i y_m x_n \tag{4.6}
\]

In equations (4.3) to (4.6), \( V_{2D} \) is the sample volume (in our case a planar cell area), \( F \) is the force vector \( x_n \) is the contact \( x \) component vector (from particle centre to particle centre).
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Subscript u indicates unit vector, n indicates normal vector and t indicates tangential vector. The system of equations can be suitably adapted to derive stress components in 3 dimensions.

4.3.5 Preliminary analysis and calculation of essential attributes

The output from GD simulations is traditionally a set of multivariate time series of attribute vectors (one set for each particle). Within constrained geometries, for example hopper flow, the system boundaries are defined and any particle can be specified by its co-ordinates with respect to the fixed system boundaries. Whilst this is clearly a benefit in strict computational terms, considerations are to a large extent limited to regional (Euleurian) analyses, i.e. analyses based upon regions (which particles move through). However, the system boundaries for an evolving heap move as the heap evolves and whilst there is the advantage of more easily being able to adopt a Lagrangian approach (i.e. follow the experience of particles), there is the computational difficulty of dynamically determining system boundaries. For example, to analyse boundary layer flow in an evolving heap, it is required to determine where particles are situated with regard to arbitrarily defined (calculated) moving boundaries.

4.3.6 Determination of system boundaries for the 2D heap

The output from the GD simulations is a set of sampled arrays of co-ordinate and velocity component data. Essentially there are two problems here. Firstly it is required to define which particles are in the heap. This is particularly important because local averages such as components of velocity vector can become very unrepresentative if particles which are not actually in the heap are included in the averaging procedure. For a hopper feed situation where there is a significant height of the feed point above the heap, the method used was to define the current height of the heap according to some rule. Those particles below this height are defined to be within the heap. Deceleration of particles (on impact into the heap) was tried as the defining criteria; i.e. the position of the highest particle experiencing a deceleration defined the top of the heap. However, the situation is not trivially simple as particles may decelerate on
impact with other particles only a short distance from leaving the hopper and so
deceleration on its own can give rise to a false definition of the top of the heap.
Ultimately, the algorithm used involved counting at each sampling time of data output,
the numbers of particles in layers of thickness 1 particle diameter, parallel to the base
and working down from the feed point until a layer was found with a particle count
above a limiting threshold. The top of the heap was defined as the highest layer which
contained a minimum number of particles (for example 15 with a hopper orifice of
width 10 particle diameters), this being extremely unlikely to occur in the free fall
region between the heap and the hopper.

The second problem is to determine the lateral boundaries of the heap. This is
necessary in order to perform stratum analyses, for example to investigate velocity
profiles at different distances from the heap surface. This process is necessarily
arbitrary, but an algorithm was developed to process the coordinate data against strata
(layers) of a suitable depth (e.g. 1 particle diameter). The extreme leftmost and
rightmost particles in each layer were assumed to define the boundary positions. Of
course, it is always possible that a "rogue" (e.g. avalanching) particle can find itself
somewhat detached from the bulk giving an unrealistic definition of boundary. This
and a few other associated problems can be resolved by using a moving average
definition of the boundary, i.e. the boundary at a layer is defined as the average of
those found in the layer and in those layers immediately above and below. The method
of moving averages is a simple filtering technique applied in time series and signal
processing.

4.3.7 Determination of system boundaries for the 3D heap

Determination of the top of the evolving heap was on a similar basis to the 2D case.
The top of the heap was defined as that height above the base where a layer parallel to
the base contained a suitable number of particles (as compared to the number of
particles that would fit within the feed orifice. Again, the algorithm progressed down
from the feed point until a suitable layer was found.
Finding the heap boundaries in the 3D case was done by allocating particles to cubic regions of suitable size (e.g. 2 particle diameters). In plan view, the algorithm worked down each column of such cubic cells until a non-empty cell was found (which was also below the defined top of the heap. Again as in the 2D case there is the potential for “rogue” particles to give a false boundary or for local small troughs to do the same. A two dimensional moving average technique (over a plan view 3 by 3 set of cells) was found to resolve the problem.

4.4 Kinetic theory and statistical mechanics

Section 3.4.1 of the previous chapter discusses kinetic theory and statistical mechanics in a little more detail. However, with regard to the analyses implemented, the following section is included.

4.4.1 Quantification of diffusion

In this thesis, evidence is later presented for the mechanisms by which segregation by particle size takes place. Hard evidence of diffusion really requires the calculation of self-diffusion velocities and/or coefficients of self-diffusion. For an individual particle, the fluctuating velocity, \( C \) is defined in equation (4.7) below as the vector difference between the velocity, \( c \), of that particle and the mean local velocity \( u \).

\[
C = c - u
\]  
(4.7)

Nikitidis et al (1998) describe the calculation of self-diffusion velocities in hopper flow. McQuarrie (1976) has shown that the self diffusion coefficient (in two dimensions) can be expressed as an integral over time of the fluctuating velocity autocorrelation function (equation 4.8)

\[
D = \frac{1}{2} \int_0^\infty \langle C(0), C(\tau) \rangle d\tau
\]  
(4.8)
In equation (4.8), $D$ is the self-diffusion coefficient, $\tau$ is the time lag between fluctuating velocities $C$ and the angle brackets indicate averaging over different time origins. The integral in equation (4.8) is from 0 to infinity. In practice, the integral would be calculated numerically over a suitably long interval.

4.5 Rationale for applied structures

Carefully selected data structures can dramatically simplify available analyses and make more sophisticated analyses available. Brief mention has been made (section 3.3.1 and appendix C) to the use of tree structures in region analysis of binary arrays. Tree structures are essentially a particular form of “linked list” whereby pointers link data items in a flexible way. Some pilot routines were successfully implemented to analyse binary arrays using quadtrees where square regions (of ones) are defined by nodes on the tree. However, this was not developed any further as the main thrust of the work concerned evolutionary dynamics.

The codes for the granular dynamics simulations (and in-situ routines added for the purposes of this study) were all written in Fortran (77 and 95). The output from these codes is of simple text files. With regard to ensemble particle attributes, this naturally gives rise to a file (of particle attributes – components of position vector, components of velocity etc.) for each sampling time. However, in addition to the data at each time point being regarded as an “individual” static data set to be investigated, the data is essentially multivariate time series which requires probing in a number of different ways. If we take the example of output for particle data, one would want to follow particular individual particles through time. On the other hand, one would want also to be able to take a particular point in time and investigate all particles. In a similar manner, if we take the example of the application of attribute averaging (e.g. stress or voidage) over a gridded cell system, we would want to be able to follow what happens to a cell over time, but also to take a point in time and move from cell to cell. Whilst contrived and convoluted code in Fortran or any other language can ultimately meet
these requirements, it would mean the opening and closing of a very large number of files. A convenient solution is to hold the output data in a relational database. One important powerful facility of relational databases is the construction and use of composite indices which facilitate programmed access to the data in a number of ways. By the use of pointers, database indexes provide the effect of a composite sort on the data, but also rapid (indexed) access to particular records. Filtered “views” on the data making use of indexes are useful in refined probing. Since the work involved in this thesis is largely post processing analysis, there is a requirement to flexibly manipulate the data and this can be conveniently done using a relational database.

4.5.1 Database structures

A number of different database tables were implemented in the completion of this thesis, but for illustrative purposes, the structures of the tables designed from the output from some 2D simulations is shown in figures 4.1 and 4.2. There are two main tables employed here. The table “Particle” contains one record for each particle at each sampled time. Fields 1 and 2 (time and particle number as strings) form the composite (key) indices. The other fields are obvious particle attributes such as components of position vector and velocity vector.
**Development of the analysis toolset**

<table>
<thead>
<tr>
<th>Field</th>
<th>Field Name</th>
<th>Type</th>
<th>Length</th>
<th>Dec</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
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<td></td>
</tr>
<tr>
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</tr>
<tr>
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<td>NUMERIC</td>
<td>7</td>
<td>3</td>
</tr>
<tr>
<td>6</td>
<td>R</td>
<td>NUMERIC</td>
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<td>3</td>
</tr>
<tr>
<td>7</td>
<td>XVEL</td>
<td>NUMERIC</td>
<td>7</td>
<td>3</td>
</tr>
<tr>
<td>8</td>
<td>YVEL</td>
<td>NUMERIC</td>
<td>7</td>
<td>3</td>
</tr>
<tr>
<td>9</td>
<td>RVEL</td>
<td>NUMERIC</td>
<td>7</td>
<td>3</td>
</tr>
<tr>
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</tr>
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<td>NUMERIC</td>
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<td></td>
</tr>
<tr>
<td>12</td>
<td>DIST_SURF</td>
<td>NUMERIC</td>
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<td>3</td>
</tr>
<tr>
<td>13</td>
<td>XVELGRAD</td>
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<td>THETA</td>
<td>NUMERIC</td>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td>15</td>
<td>ANN_VOID</td>
<td>NUMERIC</td>
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<td></td>
</tr>
<tr>
<td>16</td>
<td>SI</td>
<td>CHARACTER</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>SJ</td>
<td>CHARACTER</td>
<td>2</td>
<td></td>
</tr>
</tbody>
</table>

*Figure 4.1, Structure for table PARTICLE.DBF. SI and SJ are string equivalents of the co-ordinates of the grid cell in which the particle finds itself.*

The table “Particle” has two composite indices as detailed below.

**Index 1, TIME+PART_NO_ST.** This composite index, where + means concatenation, facilitates searching of the table by particle number within time – i.e. one can follow all particles at a time.

**Index 2, PART_NO_ST+ TIME.** This composite index facilitates searching of the table by time within particle number – i.e. one can follow a particle through time.

Fields 1, 2 and 3 (TIME, SI and SJ) in the second table “Regions” in figure 4.2 are also used in composite indices. SI and SJ are string equivalents of grid cell references I,J; so, for example, I = 7 means SI = “07”. The other fields in the table are regionally derived averages such as components of the stress tensor.
Table “Regions” has two indices as indicated below

**Index 1, TIME+SI+SJ.** This composite index allows traversal of the table by cells within time.

**Index 2, SI+SJ+TIME.** This composite index allows a cell attribute to be followed over time.

### 4.5.2 Tables linked as a relational database.

A relational pointer can be set up between the two tables (from Particle to Regions) to allow access to the local average attributes appropriate for any particle at any time. Thus as any piece of code follows a particle, the appropriate local average attributes are available as if they were fields in the table “Particle”. Figure 4.3 illustrates the many to one mapping of table Particle to table Regions.

---

**Figure 4.2, Structure for table REGIONS**

<table>
<thead>
<tr>
<th>Field</th>
<th>Field Name</th>
<th>Type</th>
<th>Length</th>
<th>Dec</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>TIME</td>
<td>CHARACTER</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>SI</td>
<td>CHARACTER</td>
<td>2</td>
<td></td>
</tr>
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<td>3</td>
<td>SJ</td>
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<td></td>
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<td>NUMERIC</td>
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<td></td>
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<td>NUMERIC</td>
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<td></td>
</tr>
<tr>
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<td>NUMERIC</td>
<td>9</td>
<td>4</td>
</tr>
<tr>
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<td>NUMERIC</td>
<td>9</td>
<td>4</td>
</tr>
<tr>
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<td>DVDX</td>
<td>NUMERIC</td>
<td>9</td>
<td>4</td>
</tr>
<tr>
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<td>NUMERIC</td>
<td>9</td>
<td>4</td>
</tr>
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<td>NUMERIC</td>
<td>9</td>
<td>4</td>
</tr>
<tr>
<td>11</td>
<td>S_YY</td>
<td>NUMERIC</td>
<td>9</td>
<td>4</td>
</tr>
<tr>
<td>12</td>
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<td>NUMERIC</td>
<td>9</td>
<td>4</td>
</tr>
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<td>S_YX</td>
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<td>9</td>
<td>4</td>
</tr>
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<td>NUMERIC</td>
<td>9</td>
<td>4</td>
</tr>
<tr>
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<td>VELY</td>
<td>NUMERIC</td>
<td>9</td>
<td>4</td>
</tr>
<tr>
<td>16</td>
<td>RVEL</td>
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<td>9</td>
<td>4</td>
</tr>
<tr>
<td>17</td>
<td>VOIDAGE</td>
<td>NUMERIC</td>
<td>7</td>
<td>2</td>
</tr>
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<td>18</td>
<td>SMALL</td>
<td>NUMERIC</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>LARGE</td>
<td>NUMERIC</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>ALL</td>
<td>NUMERIC</td>
<td>2</td>
<td></td>
</tr>
</tbody>
</table>
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Figure 4.3. Tables “particle and “Regions” as a relational database

A number of other database tables were created for specific purposes. For example, the table “Partlist” (figure 4.4) contains derived attributes of each particle for 3D simulations. This table was used to select suitable particles to generate series for further analysis, for example by the wavelet transform.

<table>
<thead>
<tr>
<th>Field</th>
<th>Field Name</th>
<th>Type</th>
<th>Length</th>
<th>Dec</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>PART_NO_ST</td>
<td>CHARACTER</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>TIME_ENT_S</td>
<td>CHARACTER</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>TIME_ENT</td>
<td>NUMERIC</td>
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<td></td>
</tr>
<tr>
<td>4</td>
<td>TOTALTIME</td>
<td>NUMERIC</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>BOUNDTIME</td>
<td>NUMERIC</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>DISTTRAV</td>
<td>NUMERIC</td>
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<td>2</td>
</tr>
<tr>
<td>7</td>
<td>XFIRST</td>
<td>NUMERIC</td>
<td>6</td>
<td>2</td>
</tr>
<tr>
<td>8</td>
<td>XLAST</td>
<td>NUMERIC</td>
<td>6</td>
<td>2</td>
</tr>
<tr>
<td>9</td>
<td>YFIRST</td>
<td>NUMERIC</td>
<td>6</td>
<td>2</td>
</tr>
<tr>
<td>10</td>
<td>YLAST</td>
<td>NUMERIC</td>
<td>6</td>
<td>2</td>
</tr>
<tr>
<td>11</td>
<td>ZFIRST</td>
<td>NUMERIC</td>
<td>6</td>
<td>2</td>
</tr>
<tr>
<td>12</td>
<td>ZLAST</td>
<td>NUMERIC</td>
<td>6</td>
<td>2</td>
</tr>
</tbody>
</table>

Figure 4.4, Structure for table PARTLIST.DBF

Table “partlist” was indexed on a number of fields. An example is BOUNDTIME (time spent in the boundary layer). This allows an effective search on this field to allow selection of particles spending a lot of time in the boundary layer.
4.6 Time series and signal processing

Time series analysis and signal processing are related disciplines. Time series analysis generally involves observed series such as unemployment figures and interest rates. Signal processing as applied by engineers concerns electronic signals. There is considerable overlap of the two, though sometimes conventions differ.

4.6.1 Spectral analysis

Any time series can be viewed or analysed with respect to either the time domain or the frequency domain. In the time domain (a normal time series graph with the appropriate variable plotted against time), we can observe fluctuations of the series in time and possibly locate times of significant activity, which are suitable for further, more detailed, investigation. However, apart from very simple cases, it is difficult in the time domain to identify precisely any components of periodicity. A graph in the frequency domain gives a spectral decomposition, with frequency on the horizontal axis and the strength of periodicity at each frequency on the vertical axis. The time series is transformed via the Fourier transform of the autocovariance function into the frequency domain as described below to establish the dominant characteristic frequencies in the signal (see, for example, Gottman, 1981).

Given a set of $N$ data points, $x_t$, where $t$ is a time reference, the series mean is defined by,

$$
\bar{x} = \frac{1}{N} \sum_{t=1}^{N} x_t
$$

(4.9)

The autocovariance function at lag $k$ is estimated from the sample of $N$ data points, $x_t$, by:

$$
C_k = \sum_{t=1}^{N-k} (x_t - \bar{x})(x_{t+k} - \bar{x})
$$

(4.10)
This function gives, for each value of the lag $k$, a measure of the degree to which the variable $x$ repeats itself with a period equal to $k$. The function in equation (4.10) can be normalised so that it is unity at zero lag by dividing by a variance term to give what in time series analysis is called the autocorrelation function $r_k$. However, it should be noted that some disciplines refer to $c_k$ as the autocorrelation function. The discrete Fourier transform (see Brigham, 1988) of the autocovariance function is the power spectrum, $I(f)$ as a function of frequency, $f$, given by equation (4.11).

$$I(f) = \frac{1}{2\pi} \left[ c_0 + 2 \sum_{k=1}^{N-1} c_k \cos(k2\pi f) \right] \quad (4.11)$$

Routines are in the public domain for calculation of the Fast Fourier Transform. However, for the purposes of flexibility (e.g. sampling rate), in this study, the codes for the autocovariance function and the discrete Fourier transform were implemented from scratch.

### 4.6.2 Cross correlations

The obvious starting point for an investigation of coupling is Pearson’s product moment correlation coefficient which can be extended into a cross correlation function by lagging one or other series. For paired observations $(x_i, y_i; \ i = 1, ..., n)$, the correlation coefficient for un-lagged observations is given by equation (4.12), where all summations are from 1 to $n$.

$$r = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum x_i^2 - n \bar{x}^2} \sqrt{\sum y_i^2 - n \bar{y}^2}} \quad (4.12)$$

For a correlation of $x$ with $y$ values at lag $t$ (i.e. $x$ values are paired with $y$ values $t$ time points previously), equation (4.13) below applies, where summation (and appropriate
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calculation of means) is from 1 to \( n - t \). Equation (4.13) defines the cross correlation
function as a function of \( t \).

\[
    r_t = \frac{\sum (x_{i+t} - \bar{x})(y_i - \bar{y})}{\sqrt{\sum x_{i+t}^2 - n\bar{x}^2} \sqrt{\sum y_i^2 - n\bar{y}^2}} \quad (4.13)
\]

The cross correlation function will be particularly applied to coupling of discrete
wavelet transforms.

4.7 Wavelets transform implementation

The basic concepts and fundamental equations concerning wavelet transforms are
given in section 3.5.1 in the previous chapter. Examples from a variety of disciplines
were also given in illustration of the diversity of applications of the transform. Here
the practical implementation of the iterated filter bank as used in the C++ classes
(appendix E) in this work is given.

4.7.1 Implementation of the one dimensional wavelet transform

Implementation of the one dimensional discrete wavelet transform is by a procedure
called the iterated filter bank (see Strang & Nguyen, 1997 or Young, 1993). The first
filter iteration on a series of length \( n \) gives \( n/2 \) wavelet coefficients at the smallest
scale of scrutiny. The next iteration produces \( n/4 \) wavelet coefficients and so on. The
wavelets at each subsequent iteration are twice as wide as those of the previous
iteration and thus represent a coarser scale of scrutiny. The reconstruction of the
original signal involves the sum of each wavelet scaled by its wavelet coefficient
(equation 3.8) plus what remains of the signal (after the implementation of the last
filter bank iteration) called the scaling function.
4.7.2 The iterated filter bank

The standard way of representing a filter in signal processing is by the $Z$ transform notation. Filtering involves convolving a signal (vector) with the filter signal (vector). A particular wavelet transform applied in this dissertation is the Deslauriers-Dubuc (2,2) transform. It will be used here as an illustration of the iterated filter bank technique. This particular transform has filters (in $Z$ Transform notation):

Low pass

$$h^-(z) = -0.125 z^{-2} + 0.25 z^{-1} + 0.75 z^0 + 0.25 z^1 - 0.125 z^{-2} \quad (4.14)$$

High pass

$$g^-(z) = 0.25 z^{-2} - 0.5 z^{-1} + 0.25 z^0 \quad (4.15)$$

A filter bank (showing also the signal reconstruction) is illustrated in figure 4.5 below. In figure 4.5, $X$ is the input signal, $g^-$ and $h^-$ are the high pass and low pass filters respectively, $g$ and $h$ are the low pass and high pass synthesis filters respectively and $Y$ is the reconstructed signal. $\gamma$ is the signal of wavelet coefficients and $\lambda$ is the signal of scaling factor coefficients.
The implementation of one filter iteration proceeds as follows. The signal, $X$, is convolved (separately) with each filter ($g_-$ and $h_-$) to produce two output signals. Each of these signals is downsampled (discarding the second and each subsequent alternate sample value). The resulting downsampled output from the high pass filter gives rise to a set of wavelet coefficients ($\gamma$). There is an equal number of scaling factor coefficients ($\lambda$) resulting from the downsampled output from the low pass filter.

An iterated filter bank as implemented involves filtering (with both filters) and subsequent downsampling. At each iteration, the $\gamma$ signal of wavelet coefficients is retained and the $\lambda$ signal of scaling factor coefficients (now half length) is input at the next stage of iteration. The process is repeated as far as required (i.e. until the coarseness of the detail is no longer required – or until the process runs out of sample values.

The implementation described is a true transform (of a vector with a transformation matrix) when it is noted that the wavelet coefficients are placed in the high order positions in an output vector. This is illustrated in figure 4.6 for an initial input signal of length 16 where $S$ stands for scaling factor coefficient and $W$ stands for wavelet coefficient. Arrows indicate iterations. After the fourth iteration, there is only one
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signal (scale factor) value left and so the process must stop. (W1 are the smallest detail wavelet coefficients).

<table>
<thead>
<tr>
<th>S0</th>
<th>S1</th>
<th>S2</th>
<th>S3</th>
<th>S4</th>
</tr>
</thead>
<tbody>
<tr>
<td>S0</td>
<td>S1</td>
<td>S2</td>
<td>S3</td>
<td>W4</td>
</tr>
<tr>
<td>S0</td>
<td>S1</td>
<td>S2</td>
<td>W3</td>
<td>W3</td>
</tr>
<tr>
<td>S0</td>
<td>S1</td>
<td>W2</td>
<td>W2</td>
<td>W2</td>
</tr>
<tr>
<td>S0</td>
<td>S1</td>
<td>W2</td>
<td>W2</td>
<td>W2</td>
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<tr>
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<td>W1</td>
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<tr>
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<td>W1</td>
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<td>S0</td>
<td>W1</td>
<td>W1</td>
<td>W1</td>
<td>W1</td>
</tr>
</tbody>
</table>

Figure 4.6. The full wavelet transform of a vector of size 16.

A one dimensional wavelet transform is often represented as a "dyadic grid". The resulting wavelet coefficients in the final column of figure 4.6 are positioned in figure 4.7 in dyadic grid form. Here, scale is the vertical axis and time (or location) is the horizontal axis.
4.7.3 Shapes of wavelets

Different wavelet shapes result from different pairs of wavelet transform filters. The Deslauriers-Dubuc\((2,2)\) wavelet produced by the low and high pass filters given by equations (4.14) and (4.15) has the shape illustrated in figure 4.8. This shape is particularly applicable to the peaked series that result from the GD simulations.
4.7.4 The one dimensional wavelet transform and coupling of discrete events

Granular flows are characterised by discrete events in time and space. Examples are failure under shear and avalanching. To gain a greater understanding of the physics of such phenomena, coupling of the key variables is a requirement. The output from granular dynamics simulations is essentially multivariate time series in terms of variables at the particle level (e.g. components of velocity vector) or local average variable values derived from variables at the particle level (e.g. voidage). It is these variables for which we need to investigate the coupling in the context of discrete defining events. The wavelet transform picks up local fluctuations at different scales within a time series. In fact after a wavelet transform, the original series can be reconstructed from each of the constituent wavelets scaled by their coefficients and added to the residual scaling function.

Pearson's product moment correlation coefficient measures the degree to which two variables are linearly related and can be extended into a cross correlation function by lagging one or other series. The formulae are given in equations (4.12) and (4.13). Such correlation studies on observed time series are fine if the data is not governed by time dependent defining events. In illustration, if over time we measure pressure and temperature for a fixed volume of gas, then a straight correlation calculation (using equation 4.12) should reveal a high coefficient because the variables pressure and temperature are related. However, as mentioned above, many of the variables that are derived from granular dynamics simulations are potentially coupled in a very different manner and are very much characterised by abrupt changes related to catastrophic events such as failure under shear. In principle, since wavelets detect discrete changes in series, then there is the potential to attempt to correlate wavelet coefficients. The wavelet correlation technique developed in this study essentially involves a kind of filtering, where we filter out all disturbances within the data other than those at a particular scale - picked up by the wavelet at that scale. We therefore focus in on the limited number of significant disturbances revealed at that scale by calculating a
correlation coefficient of transform coefficients from two series. One must be careful with the subsequent interpretation of any calculated correlation coefficient because a large number of points will be found near the origin of a scatter of wavelet coefficients (where little is coming through the filter) with a limited number of points away from the origin. With correlation studies it is always advisable to visually inspect the scatter in addition to considering the statistical significance of the coefficient itself as spurious correlations are possible.

In an attempt to couple variables in the context of discrete events, one can work with either the calculated values of the wavelet coefficients or the absolute values of those coefficients. By working with absolute values there is the potential to detect a wider range of variable couplings, not only because negative peaks are regarded as positive, but because of the way in which the wavelet transform decomposes a series is not simple.

4.7.5 Significance of correlations of wavelet coefficients

The discrete wavelet transform is derived by the application of filters. It is well known (the Slutsky effect, see Gottman, 1981) that the application of a suitable linear filter to a pure (random) noise signal can generate pronounced periodicity and in fact is the basis for moving average time series models. So, without evidence to the contrary, the values of any correlation coefficients calculated on wavelet transform coefficients might contain contributions that are artefacts of the filtering technique. In addition, to perform a wavelet transform on a series of a fixed length, the series needs to be extended at both ends to allow convolution with the filter vector. The transform routine developed for this thesis involved “periodising” the series prior to filtering. There is always the potential here that peaks in wavelet coefficients could be artefacts of this periodising.

The significance of a correlation coefficient (against a null hypothesis of zero correlation) is found by comparing with a critical value looked up from tables. The
critical value is dependent upon to the length of the series. In order to validate the wavelet correlation procedure in terms of significance, simulations were run producing wavelet coefficients for 5000 pairs of random series which were then correlated. The simulations were therefore with the null hypothesis set to true and any large values of correlations resulting are the result of random chance. An inspection of the sorted values of the correlation coefficients obtained allows the determination of a critical value. For example, the critical 5% value will be at the 95\textsuperscript{th} percentile of the sorted array of correlation coefficients. The results obtained are in very good agreement with those quoted in standard tables. Table 4.1 below shows the simulated critical values for correlation coefficients on scale 2 transform coefficients (64 of them) for series of length 256. Tabulated alongside are relevant standard book values.

<table>
<thead>
<tr>
<th>2 tailed significance</th>
<th>Critical value</th>
<th>Table value</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>0.248</td>
<td>0.242</td>
</tr>
<tr>
<td>0.025</td>
<td>0.278</td>
<td></td>
</tr>
<tr>
<td>0.01</td>
<td>0.320</td>
<td>0.316</td>
</tr>
<tr>
<td>0.005</td>
<td>0.347</td>
<td></td>
</tr>
</tbody>
</table>

*Table 4.1. Simulated critical values for correlation coefficients of scale 2 wavelet coefficients.*

There is clearly excellent agreement between the simulated critical values and the table values and so the conclusion is that the significance of correlation coefficients calculated from absolute values of wavelet coefficients can be determined in the usual way.

### 4.7.6 Lagged correlations and determination of time constants

In the presence of sustained periodicity, the Fourier transform is the technique used to determine frequencies of component oscillations within a time series. However, the Fourier transform is only capable of detecting regular periodicity and in fact is incapable of locating the position within the series of any short lived periodicity. The coupling of variables output from granular dynamics simulations may well be on the
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basis of a time lag between defining events in two series, i.e. a disturbance in one series comes before a later disturbance in another series. The wavelet correlation technique can be extended here in an attempt to investigate such time constants and in particular is capable of helping to find such time constants even when the discrete events are not positioned regularly in time. By simply lagging (shifting) one set of wavelet coefficients backwards or forwards before calculating the correlation coefficient (i.e. using equation 4.13), any significant correlation at that lag points to a time constant of length determined by the scale of the wavelet and the amount of lag. Table 4.2 below converts wavelet scale and lag into sampling time.

<table>
<thead>
<tr>
<th>Wavelet scale 1</th>
<th>Wavelet scale 2</th>
<th>Wavelet scale 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lag 1</td>
<td>2 sampling units</td>
<td>4 sampling units</td>
</tr>
<tr>
<td>Lag 2</td>
<td>4 sampling units</td>
<td>8 sampling units</td>
</tr>
<tr>
<td>Lag 3</td>
<td>6 sampling units</td>
<td>12 sampling units</td>
</tr>
</tbody>
</table>

Table 4.2. Sampling time equivalent to scaled wavelets at different lags.

In illustration, with a series of length 256, there will be 128 (smallest) wavelets at scale 1 of nominal width 2 sampling units. A shift (lag) of 1 wavelet is therefore a shift of 2 sampling units. A shift (lag) of 2 wavelets is therefore a shift of 4 sampling units. Taking the bottom right table entry, because a scale 3 wavelet has nominal width 8 sampling units, shifting 3 times will be equivalent to 24 sampling time units.

Salvetti & Lombardi (1999) describe the application of a wavelet cross-correlation technique that results in what they call a cross scalogram. Because this is essentially a (dyadic) 2D matrix in the form of figure 4.7 (representing scale and translation) of numbers, the best way to identify significant values is by grey scaling or by simple 3D block diagram. Here, essentially the matrix consists of components of an “inner product” where high values denote an association at that location and scale. However, the techniques will not help in determining time constants for which one set of wavelet coefficients must be lagged. There is the potential to extend the ideas of Salvetti &
Lombardi by lagging one set of wavelet coefficients before calculating the cross scalogram. A significant number of large values might point to a time constant equal to the lag employed.

With regard to the identification of time constants, the calculation of a correlation coefficient between lagged wavelet coefficients has been described. A suitable summary is in terms of a "wavelet cross correlation matrix" as illustrated in figure 4.9 where in illustration, a significant coefficient of 0.8 is indicated for scale 1 (smallest scale) wavelets at lag 1.

<table>
<thead>
<tr>
<th>Lag</th>
<th>Scale</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td></td>
<td>0.2</td>
<td>0.3</td>
<td>0.1</td>
<td>0.0</td>
<td>0.1</td>
</tr>
<tr>
<td>1</td>
<td>0.8</td>
<td>0.2</td>
<td>0.2</td>
<td>0.4</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.3</td>
<td>0.4</td>
<td>0.1</td>
<td>0.1</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.1</td>
<td>0.1</td>
<td>0.3</td>
<td>0.2</td>
<td>0.3</td>
<td></td>
</tr>
</tbody>
</table>

*Figure 4.9. Example of a wavelet correlation matrix.*

The above "wavelet coefficient cross-correlation matrix" can help in identifying time constants in the presence of events which are discrete in time, but not periodic in the true sense of the word. However, the technique will only couple events which are represented at the same wavelet scale — e.g., scale 1 coefficients for one series correlated with scale 1 coefficients for the other series. However, it is possible that events in two series might be coupled by wavelets at different scales and so, for example, there is the potential to cross-correlate scale 2 wavelet coefficients from one series with scale 1 coefficients from another. Unfortunately there are different numbers of coefficients in the different scales and so some form of rationalisation must be performed. For example, if we are cross correlating scales 1 and 2, because there are twice as many scale 1 wavelets as scale 2, a possible approach would be to
average successive pairs of scale 1 coefficients before cross-correlating with scale 2 coefficients. However, other possibilities exist – for example, select the larger from each successive pair of scale 1 coefficients to cross-correlate with scale 2 coefficients.

### 4.7.7 The one dimensional wavelet transform utility

Facilities associated with the one dimensional wavelet transform were incorporated into a windows screen interface. This is not intended to be of professional quality and is always in the process of refinement. A sample screen is shown in figure 4.10.

![Image of the screen interface for facilities associated with the one dimensional wavelet transform.](image-url)

**Figure 4.10. The screen interface for facilities associated with the one dimensional wavelet transform.**

The essentials of the utility are that a particle is selected from the listbox towards the left. The particles are ordered on the basis of a selected index. For example the button “Boundperc” switches the index to “percentage of time spent in the boundary layer). Two associated variables are selected from the listbox towards the right (currently set for illustrative purposes as $x$ velocity and $x$ component of angular velocity). The
wavelet transforms of the two selected variables are calculated based upon an initial sampling time and a sampling increment. The transforms can be displayed simultaneously at the different scales of decomposition on a second screen as illustrated in figure 4.11, where the traces on the top graph are the original series and the finest scale detail coefficients are plotted on the bottom graph.

![Figure 4.11. The graphical display utility for wavelet transforms](image-url)

The graphical facility of figure 4.11 was used in preparatory work and allows two decompositions to be simultaneously compared. However, for the purposes of published articles, the data was transferred to Microsoft Excel © for the preparation of more professional looking graphs.

The bottom right part of figure 4.10 allows the display of the wavelet cross-correlation matrix — i.e. is used to display lagged correlations between wavelet coefficients at different scales.
4.7.8 Implementation of the two dimensional separable wavelet transform

The signal to be transformed here is a $n \times n$ grid of numbers where the obvious application is in image processing where many of the significant developments have taken place (for example data compression). For a dyadic breakdown, the dimensions must be a power of two, for example 256 by 256. As with the one dimensional transform, facilities are provided in Matlab and in other libraries. However, in this study, there is the requirement to implement routines in a flexible way and to link with other routines, for example correlation functions. A pilot 2D wavelet transform has been implemented in C++ where the algorithms are described in more detail in appendix F. The particular implementation was of a separable wavelet transform. The algorithm uses the filters of the one dimensional transform and the signal is successively row transformed (both high and low pass filters) and sub-sampled to give columns which are then transformed (both high and low pass filters) and sub-sampled. What results from the transform is an array of coefficients that measure scale disturbances in the horizontal direction, the vertical direction and also along diagonals. As with the one dimensional transform, the complete multi-resolution need not be performed. The process can be stopped at any point where the remaining weighted scaling factors give what remains of the image after the detail captured by the wavelets has been removed.

For illustrative purposes, figure 4.12 shows how an 8 by 8 array is transformed into 4 sub-arrays after one stage of the transform.
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In figure 4.12, sub-array LL1 contains the scaling factor coefficients after detail has been removed. It would need to be up-sampled in both directions to recreate an 8 by 8 (blurred) image. Sub image HL1 contains vertically detail wavelet coefficients, LH1 contains horizontally detail wavelet coefficients and HH1 contains diagonal detail wavelet coefficients. The coefficients need to be scaled by the wavelets themselves to create the image detail components. It should be emphasised that the two dimensional wavelet transform allows the positioning within a two dimensional grid of disturbances at different scales of scrutiny, but in terms of horizontal, vertical and diagonal detail. A simple idealised illustration using a simple image constructed of horizontal, vertical and diagonal lines is given in figure 4.13 (a and b). As mentioned, the components of detail are derived by scaling wavelet coefficients by the wavelets themselves.
4.8 The graphics tools

Separate graphics tools involving flexible colour coding of particles on the basis of their attributes have been developed for 2D simulations and 3D simulations.

4.8.1 Simulation output filtering

The output from a granular dynamics simulation has been previously described as a set of discrete multivariate time series (one series of observations on an attribute vector for each particle), where the rate of sampling and the nature of the output vector are pre-definable. Typically, the elements of the output vector include components of the particle position vector, the velocity vector (including rotational velocity) and the components of force on each particle. However, other attribute values such as distance from the free surface are calculated after the simulation. In the context of this section, ‘filtering’ involves restricting the consideration to particles whose attribute vectors comply with a set of pre-defined threshold values. We have for each particle an attribute vector \( \mathbf{a} = (a_1, a_2, \ldots, a_n) \). We define a lower threshold vector \( \mathbf{l} = (l_1, l_2, \ldots, l_n) \) and an upper threshold vector \( \mathbf{u} = (u_1, u_2, \ldots, u_n) \). A vector \( \mathbf{h} = (h_1, h_2, \ldots, h_n) \) is defined with logical (true or false) components, \( h_i \), such that \( h_i = \text{true} \) if \( a_i > l_i \) and \( a_i < u_i \), otherwise \( h_i = \text{false} \). A particle will be included in the filter analysis if and only if all the \( h_i \) are \text{true}. The simple filtering described has been applied in two ways, firstly to refine time series for further analysis and secondly with regard to the colour coded...
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display capability of the two dimensional graphics toolset. So, for example, a simple time series might be used to identify the time of a discrete avalanche and then a colour coded display of particles could be developed on the basis of components of velocity, to establish a local velocity profile. The implication is that by further threshold filtering (for example by colour coding those particles that are rotating or in a region of high shear, for example) one can further identify the particle-level dynamic processes in the assembly in a sequentially refined manner. This might lead to further time series analysis to investigate suitable cross-correlations between variables or analyses of periodicity. The toolset consists of a number of components which are perpetually in a state of development. Figure 4.14 shows an early prototype screen interface for routines that produce a number of time series including filtered series for the heap boundary layer for the 2D case.

Figure 4.14: the time series analysis interface
A facility within the screen interface of figure 4.14 displays samples of particle trajectories based upon entry time into the heap. The example of figure 4.15 illustrates cratering for a high impact feed where particles (in this case on the left) are projected upwards and outwards before flowing outwards more uniformly.

![Figure 4.15: Individual particle trajectories for a high impact feed illustrating cratering](image)

### 4.8.2 Filtered colour coding

The interactive display tool developed has the capacity by standard windows controls (radiobuttons, checkboxes, command buttons) to colour code particles in a time snapshot on the basis (for example) of velocity or acceleration components, coordination number and residence time in the heap. In no way is the front end intended to be to a professional standard as it is perpetually in a state of development as the potential for detecting different phenomena requires adaptation of the screen objects. An example for 2D simulations is shown in figure 4.16 where particles are colour coded to reveal the profile of lateral component of velocity for a heap evolving in a low impact feed regime at a time of significant avalanching on the right hand side of a heap.
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4.8.3 The three dimensional graphics tools

Clearly, displays for 3D simulations are restricted, for example to planar cross-sections and plan views. The 3D capability allows visual displays to be produced upon similar lines to the 2D equivalent, i.e. colour coding of particles by threshold attribute filtering. However, incorporated is the facility to select appropriate cross-sections and perform rotations about the vertical axis (of symmetry for hopper flow and approximate symmetry for heap formation). Below, figure 4.17 shows the plan view of an evolving heap at a fixed point in time with a colour coded filter on lateral component of velocity applied. Only those particles within a certain distance from the surface of the heap are shown. The colour coding (in terms of velocity in this case is orange > yellow > green > blue. Discrete avalanching is shown by the "fingers" of green extending towards the edge.
Below, figure 4.18 shows a cross section of a heap again with colour coding by radial component of velocity. The particles included have centres within a slice through the middle of the heap of a selected width and rotated about the z axis by a selected angle. The colour coding (in terms of velocity) in this case is yellow > blue. It is emphasised that displays such as those of figures 4.17 and 4.18 show particles with centres with a stratum (figure 4.17) or cross-sectional slice (figure 4.18). The width of the stratum will dictate an apparent (and potentially misleading) "particle density". For example, figure 4.17 appears more dense than figure 4.18, but only because the stratum is wider.
For both plan views and vertical cross-sections, filtering of particles to be included can be on the basis of radial velocity, vertical velocity, rotational velocity, distance from the surface and distance from the base.
CHAPTER 5. APPLICATIONS OF THE 2D TOOLSET

5.1 Introduction

In section 5.2, segregation and mixing phenomena in poured binary heaps are investigated and mechanisms suggested for the different behaviour found for the low and high impact feed regimes. Because segregation during discrete avalanching is particularly identified in section 5.2, section 5.3 moves on to consider stress and voidage evolution in the low impact case. In both sections, attempts are made to couple variables in the context of discrete avalanching.

5.2 Flow regimes and segregation phenomena as a function of feed-rate

Recent published work on segregation and stratification is outlined in section 2.2 where the phenomena are found in a number of flow regimes and geometries. Mixtures of grain sizes tend to separate in response to many types of time dependent perturbation or agitation - an effect that is usually unwanted.

A lively debate concerning segregation and stratification phenomena has taken place recently in the granular literature where an underlying principle of much of the work seems to be that segregation is an innate property of granular mixtures and that it is in some sense unavoidable (e.g. Makse et al, 1998). This is certainly true if the mixture properties allow spontaneous percolation of fines through coarse. However, percolation can only take place for certain ratios of particle sizes and segregation is known to occur outside of these ratios. Baxter et al (1998) argue that controllable process conditions can be a strongly determining factor in segregation and that segregation may be prevented or suppressed by careful process design. It was not possible to determine the mechanism of segregation from the experiments involved in the work of Baxter et al because of the short time scale and lack of spatial resolution of
the observations. The GD simulations of this thesis allow such an investigation to be undertaken.

5.2.1 Scope of the investigation of segregation

In order to investigate segregation and mixing phenomena in a poured binary granular mixture, two different feed rate regimes have been considered, which are referred to as ‘low impact’ and ‘high impact’. Some periodic and intermittent phenomena are identified that might be important in determining the extent of mixing and segregation in real systems. In addition, segregation by self-diffusion for the low impact case is investigated in detail culminating in a proposed new mechanism for segregation.

5.2.2 Details of the simulations

The two dimensional simulations carried out employed a binary mixture of 8,500 particles (disks) of size ratio 3:1. The ratio of the number of particles of each type was, on average, 1:45 large to small particles, chosen randomly. The large particles occupied 16.8% of the covered area. Since segregation phenomena are the main focus, the possibility of bulk matrix percolation as a mechanism needs to be considered, and eliminated. Although percolation in two dimensions is not directly comparable with the situation in 3D, experimental investigations by Tüzün and Arteaga (1992) have shown that percolation in 3D requires a size ratio greatly in excess of 3:1 and one would expect 2D percolation to require even larger size ratios than in 3D. In fact, previous work in vibration-induced segregation has established that 2D binary mixtures require much greater size ratios than 3D mixtures in order to show similar behaviour, (12:1 in 2D rather than 3:1) (Duran et al, 1993). Thus, percolation can safely be discounted as a contributory mechanism for segregation in the simulations discussed here.

As mentioned in the previous section, two extreme case feed regimes are considered.
The “high impact case” involved discharge from a flat-bottomed ‘feed’ hopper with an orifice in the base of width 11 small particle diameters. The hopper was fixed in position about 100 small particle diameters above a horizontal plate. Groups of particles were periodically introduced near the top of the hopper, each particle being randomly positioned with a small random velocity along a horizontal line or ‘plug’. The plug descended in the hopper under gravity and when it had fallen a sufficient distance, based on the size of the largest particle, the next plug was introduced. The arrangement is shown in figure 5.1 where the feed plugs are clearly visible as lines of particles.

![Figure 5.1. The feed arrangement for the “high impact” simulations](image)

While the hopper was being filled, collisions between particles randomised the subsequent packing arrangement. For the “low impact case”, the top of the growing heap was continuously monitored and new particles were randomly placed with zero initial velocity as a horizontal plug about 6 particle diameters above the current top of
the heap. Monitoring dynamic attributes such as the top of a growing heap or the boundary of the sloping surface is not a straightforward matter. Sections 4.3.5 and 4.3.6 discuss methods and algorithms used. In the low impact scenario, the hopper feed procedure was not used. The particles only slowly moved away from the top of the heap, so that the intervals between the plug construction were much longer than in the high impact/ hopper feed case.

5.2.3 Results and discussion

In this section, the two-dimensional toolset is applied to the results of the Granular Dynamics simulations, particularly comparing the characteristics of heap evolution in low and high feed rate conditions.

5.2.3.1 Periodicity for a high impact feed regime

Heap evolution proceeds by a mechanism of surface avalanching and core consolidation. During an avalanche, the particles in the free-surface boundary region are highly thermalized. If the heap is relatively shallow, as in these simulations, the particles can migrate substantial lateral distances before coming to rest, hence lateral (i.e., horizontal) particle velocity components are significant and in fact will be a measure of avalanche activity. Lateral particle velocity components were investigated for the heap as a whole and for the left and right-hand halves of the heap separately. The study also considered layers at various depths within the heap (i.e., various perpendicular distances from the free surface). The high and low impact feed regimes show markedly different characteristics. Figure 5.2 shows a time series for the high impact case of the mean (absolute) lateral component of velocity vector of all particles ($v_x$) in the heap over a time period following an initial transient period of heap formation. Investigations must necessarily start at some arbitrary point in time when a heap is considered to exist. Clearly, due to the increasing heap volume, there is a dilution effect of significant activity over time. However, in figure 5.2 there is
considerable visual evidence of periodicity of lateral component of velocity in this high impact case.

![Figure 5.2. Time series of mean absolute lateral (horizontal) particle component of velocity, $v_L$, after initial transient phase of heap formation (high impact case).](image)

The components of periodicity within the series of figure 5.2 can be isolated by spectral analysis as described in section 4.6.1. The first stage of the process is the calculation of the autocovariance function according to equation (4.10). The second stage involves the calculation of the Fourier transform of the autocovariance function according to equation (4.11).
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Figure 5.3. Autocorrelation function \( r_k \) of the series given in Fig. 5.2 (high impact case).

Figure 5.4. Spectral density function \( I(f) \) relating to the series in Fig. 5.2 (high impact case).
Figure 5.3 shows the normalized autocorrelation function, \( r_h \), of the mean-velocity series given in figure 5.2 and calculated using equation 4.10. Figure 5.4 shows the power spectrum calculated using equation 4.11. The oscillations in the autocorrelation function, indicative of periodicity in the original series, appears as structure in the power spectrum. The peaks in this spectral density function correspond to the dominant characteristic frequencies inherent in the original signal. There is a strong peak in the spectrum at a frequency just above 0.05, which can be associated with the peaks in the original time series approximately 20 time units apart. In addition, there is a peak at a frequency of about 0.035 corresponding to peaks separated by about 29 time units. There appear to be two characteristic time scales for the ‘surges’ in the assembly dynamics with time constants of approximately 20 and 29. Possible causes for this periodicity will be considered later. Figure 5.5 shows a further resolution of the series of figure 5.2 into the components from the left and right sides of the heap. Clearly there is evidence of some symmetrical activity, although at certain time points there is evidence of a surge on one side of the heap but not on the other. In this particular simulation, more periodicity is apparent for the series from the right hand side of the heap. This dynamic asymmetry is considered to be an intrinsic feature of heap evolution and evidence for it will be shown in later sections.
The origins of the periodicity in the heap lateral velocity can be investigated by looking at activity within 'strata' parallel to the sloping surface of the heap. The strata investigated were approximately 5 small particle diameters wide measured perpendicular to the free surface. Strata positions and widths can only be quoted approximately as the particles that define the free surface are obviously not positioned nicely in a straight line and so a definition of "boundary" is necessarily arbitrary. Figure 5.6 compares, for the right hand side of the heap, the mean horizontal component of velocity at the free surface with that in a stratum approximately 15 small particle diameters below the surface. Because the peaks in the depth stratum are more pronounced than at the surface, it is clear that the periodicity originates from within the heap, although not surprisingly, the mean velocities are higher at the free surface.
where avalanching takes place. Additionally, it should be noted that the majority of depth stratum peaks precede those for the surface series.

Figure 5.6. Mean lateral component of velocity ($v_L$), for particles in the surface boundary layer five small particle diameters thick (full line) and in a stratum of equal width 15 small particle diameters from the surface (broken line) for the right side of the heap (high impact case).

5.2.3.2 Periodicity for a low impact feed regime

The equivalent analysis to figure 5.6 for the low impact case is shown in figure 5.7. In this case, the activity is concentrated on the surface and is significantly attenuated in the deeper stratum. Roughly the same number of particles is deposited in both cases (the high and low impact feed) by the end of the simulation. It should be emphasised that in order to make meaningful comparisons between figures 5.6 and 5.7, the time...
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axis has been compressed in figure 5.7 in order that the heap sizes are almost equal at the extreme left of each graph and at the extreme right. Clearly, for the low impact case, the time for the evolution of the heap will be significantly longer than for the high impact case.

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**Figure 5.7.** Mean lateral component of velocity, \(v_L\), for particles in the surface boundary layer five small particle diameters thick (full line) and in a stratum of equal width between 10 and 15 small particle diameters from the surface (broken line) for the right side of the heap (low impact case).

Figure 5.8 shows the power spectrum of the time series of figure 5.7 for the mean lateral velocity time series of the surface boundary layer. Once again, there are two distinct characteristic frequencies, this time at approximately 0.002 and 0.0055 inverse time units. However, it should be emphasised that the previous power spectrum in figure 5.4 (high impact case) used the average lateral velocity of the whole heap, whereas in figure 5.8 only the surface average lateral velocity was used. For the low
impact case, there is little evidence of periodicity over the whole heap, and any significant activity is confined to the free surface region. Nevertheless, the two quite different modes of activity for the two flow regimes seemingly share the characteristic of strong periodicity at two distinct (albeit different) frequencies.

![Figure 5.8](image)

**Figure 5.8.** Spectral density function of the surface stratum velocity series shown in Fig. 5.7 (low impact case).

Returning to the high impact case, there is significant periodicity in the mean lateral component of velocity bearing in mind that figure 5.2 applies to the whole heap. The plot here is of the average of the absolute velocities of the particles, and therefore cancellation between the left and right sides is not an issue. The times of maximum activity as shown in the time series are therefore candidates for further investigation. Use of the colour coded filtered display facility revealed some surprising phenomena with regard to mixing. The low impact case will be considered later in more detail. However, figures 5.9 to 5.11 and figure 5.13 below allow comparisons to be made between the two feed regimes for heaps of approximately equivalent size (numbers of particles).
5.2.3.3 Distinct regions/features in heaps for both feed rates

The application of particle displacement filters to the simulation data allowed ‘regions of stability’ to be identified for the high and low impact cases. The dark regions in figures 5.9(a) (high impact) and 5.9(b) (low impact) are composed of particles that move less than one particle diameter from the time of the snapshot to the end of the simulation. The high impact feed regime creates a highly mobile state throughout most of the heap, apart from near the base. In the low impact case there is a more substantial region of stability extending outwards from the centre, which broadly resembles the overall shape of the heap. This confirms the findings from the time series analysis that evolution of the low impact heap is confined to regions near the free surfaces. In contrast, very little of the high impact heap is stable except for a very small region towards the centre of the base. There is disruption of essentially the whole assembly. It is apparent that a wide range of boundary layer thicknesses can be created by varying the impact kinetic energy and particle flux.

Figure 5.9(a)

Figure 5.9(b)

Figure 5.9. “Regions of stability” (shaded dark) for (a) high impact and (b) low impact simulations. Stability is defined in terms of limited particle movement (less than one small particle diameter) from the time of the snapshot until the end of the simulation.
A second set of filters was used to identify and locate the most recent entrant particles within the heap at a given point in time. Figure 5.10 (a), for the high impact case, shows that new entrants embed themselves on entry, displacing existing particles and giving rise to a central ‘bowl’ of new particles. In the low impact case, shown in figure 5.10(b), the new entrants to the heap are more spread out and do not become initially trapped in the central region to the same extent as for the high impact case.

Applying a different set of filters, the high impact case is shown to be characterised by periodic pluming, where recent entrants are ejected from the bowl region towards the free surface. Figure 5.11 highlights those particles that have vertical accelerations and are moving upwards at the time. Reasonably centrally it can be seen that particles are moving upwards out of the bowl region towards the free surface. There is also a small plume on the right hand side of the heap. This “pluming” activity is highly intermittent and it appeared from inspection of sample snapshots similar to figure 5.11 that the
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phenomenon might be related to the periodic behaviour in the lateral velocity component demonstrated in figure 5.2 and previously discussed. Particle trajectory investigations revealed that many particles are projected upwards from the heap at the edge of the central “bowl” region.

Figure 5.11. An example of vertical “pluming”. The dark shaded particles are moving upwards and have an upwards acceleration (high impact case).

However, further investigation showed that the ‘pluming’ activity is considerably more frequent than the periodicity of mean lateral velocity ‘surging’ as identified by the spectrum of figure 5.4 and whilst more pronounced around the central bowl region, can be detected further towards the edge of the heap. For brevity, the original time series (of numbers of pluming particles) is not shown here, but figure 5.12 shows the frequency spectrum associated with this pluming. Initial investigations, by looking at a sample of snapshots, suggested that perhaps the pluming activity presaged lateral surging. However, comparisons between the two spectra do not suggest such a simple relationship. The tallest peak in figure 5.12 would seem to indicate periodicity of pluming at a frequency of about 0.16 (recall that the lateral velocity surges had lower frequencies of approximately 0.035 and 0.05). However, there are other potentially significant (though smaller) peaks at lower frequency that might be associated with the lateral velocity surges. The application here of time series (spectral) analysis is shown to over-rule what might result from just a visual inspection of time snapshots.
Figure 5.12. Power spectrum, $|f|$, of the vertical pluming (illustrated in Fig. 5.11) associated with the high impact simulation.

Lateral velocity surging has been cited as a characteristic of the high impact feed case. However, this is in the context of bulk lateral flow. (Figure 5.2 does not show a drop in mean lateral velocity below about 0.35. Associated with this bulk flow there is evidence of continuous avalanching and a reasonably well-defined horizontal velocity gradient, with increasing velocity towards the free surface. Figure 5.13 (a) for a point in time when the heap was quite well developed was derived by applying appropriate filters and illustrates the presence of a velocity gradient. In figure 5.13(a), the faster particles are coloured red, followed by yellow, then green and brown with the remaining particles coloured blue. By way of comparison, figure 5.7 shows that for low impact case, avalanches are more discrete in time. (The time series drops close to zero between peaks.) Additionally, as shown in figure 5.13 (b), avalanches in the low impact case are spatially localised. However, within the local avalanches there is still evidence of a velocity gradient. The presence of such a transient localised velocity gradient is likely to provide the mechanism for the segregation that is found in the low impact case. This will be discussed in the next section.
5.2.3.4 Evidence for segregation in the low impact case

The results from the two simulations discussed so far have illustrated some significant differences in the temporal evolution of heaps in the low and high impact cases. Shifting the attention to segregation and mixing phenomena in these cases, figures 5.14(a) and 5.14(b) show snapshots of the heaps at advanced stages in both the high and low impact simulations, respectively, with the large particles highlighted as light symbols against a black background. The total number of particles in each case was approximately the same. At first glance, it might appear that both are quite well mixed. However, closer inspection shows that for the high impact case there are more large particles in the middle of the heap. More importantly, for the low impact case, there are more large particles close to the base. These particles are evidence of segregation since they were at the bottom extreme edges when the heap was smaller. They became covered subsequently by later deposited particles as the heap grew outwards. From the evidence of section 5.2.3.3, they could only have reached this position by migrating down the free surfaces, not by penetrating through the bulk. It is commonly supposed
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that this migration is by rolling. This is further investigated in section 5.2.3.6. For the high impact case, there are relatively few large particles near the base; it seems that bulk mixing and convection in this case hindered any preferential movement of coarse particles towards the free surfaces or migrating down the sloping surfaces.

Figure 5.14(a)

Figure 5.14(b)

Figure 5.14. Positions of the large (white symbols) and small particles (black background) at a point in time close to the end of the simulation. (a) for the high impact case and (b) for the low impact case.

Figure 5.15 presents the data in figures 5.14 (a) and (b) in another way. In each of the high and low impact cases, the heap is divided into horizontal strata, three small particle diameters in thickness. The percentage coverage by coarse particles in each stratum is given in the figure, for both high impact (grey) and low impact (black) cases. In the high impact simulation, the concentration of large particles adjacent to the base is very low; elsewhere the concentration is fairly uniform. For the low impact case, the proportion of large particles (by area) in the lowermost stratum (ca. 35%) is much higher than for the high impact case; otherwise, as for the high impact case, the heap is overall relatively “well-mixed”. Nevertheless, as discussed above, the markedly different coarse fractions in the lowermost regions of the heap are indicative of markedly different segregation behaviour for the two simulations.
Some evidence has now been provided to show that migration down the free surface might be the method by which large particles find their way to the bottom of the heap in the low impact case. However, this does not necessarily, in itself, constitute the complete mechanism of segregation. Clearly particles will, on impact, be on the surface and so, without other evidence, it is possible that the segregation demonstrated is due to rolling only. Using the analysis tool set, which filters on times of significant surface activity only, and in a stratum of suitable width to encompass the sizes of avalanches experienced, components of velocity vector perpendicular to the sloping surface for both large and small species were compared. The mean component for the large particles was approximately twice that for the small particles. Obviously, during an avalanche, the velocity vector of an avalanching particle will have a component perpendicular to the surface since, overall, the motion cannot be totally parallel to the free surface as ultimately the base gets in the way; but for large particles it is greater. The conclusion therefore is that whilst avalanching is taking place with a fairly well...
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defined velocity gradient (as evidenced in figure 5.13(b)), large particles have a propensity to migrate towards the free surface by a diffusive process of ‘kinetic sieving’. Rolling can be the secondary mechanism for large particles to reach the bottom of the heap, although this is considered in greater detail in section 5.2.3.6. The mean components of diffusive velocity were compared by a conventional (normal distribution) two sample (comparison of means) test. The resulting test statistic (from a large sample) was highly significant on a Null hypothesis that the population mean diffusional components of velocity for both species were equal.

5.2.3.5 The transition from the high to low impact regime

It has been established that segregation takes place for a low impact feed and that the highly agitated high impact feed regime seems to enforce mixing. It is instructive to investigate the transition between these two regimes. To accomplish this, a further simulation was carried out with a hopper fixed at a height of about 6 small particle diameters above the maximum height that the heap would ultimately reach. Thus in the early stages of evolution, the heap would be experiencing a high impact feed, whilst towards the end, the impact kinetic energy would be significantly lower, and tend towards the low impact limit. Figure 5.16 shows the mean (absolute) lateral component of velocity for this simulation, together with that of a high impact series similar to that already discussed, i.e. similar to figure 5.2. The new series is shown with a dotted line and has been scaled and translated on the time axis to be comparable with the high impact series on the basis of number of particles in the heap. (There will be a phase difference between the two series based upon the time for a particle to fall from the height of the higher feed hopper to that of the lower.) For the first part of the new series, the periodic surging activity closely follows that of the original high impact case but fails to show the last peak as the top of the heap approaches the hopper feed point. This is not to say that suddenly segregation will take place, but it appears to suggest that there is a fairly clear cut-off point in which the heap assembly evolution

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'switches' from the highly thermalized surging activity caused by high incident particle kinetic energy to a mechanism probably resembling that of the low impact case.

![Graph](https://via.placeholder.com/150)

**Figure 5.16.** Time series of mean absolute lateral (horizontal) particle component of velocity to compare lateral surging in the original high impact simulation (full line) and for the case when the hopper bottom was placed just above the ultimate top of the heap.
5.2.3.6 Segregation phenomena and diffusion in the low impact case

Thus far we have concluded that a greater preponderance of large particles near the base towards the end of the low impact simulation is evidence of segregation and that this segregation is initially by diffusion across a velocity gradient in the boundary layer. It is necessary to be confident that indeed it is shear-induced segregation that is being observed. Appendix B introduces the fundamental equations concerning segregation fluxes and diffusion. Essentially, it is necessary to be sure that segregation fluxes $J_{Di}$ (classical diffusion) and $J_{Pi}$ (percolation) make insignificant contributions. Percolation as a contributory mechanism of diffusion is discussed (and discounted) in section 5.2.2. Furthermore, results from simulations by Baxter (1998) have shown no evidence of percolation under similar conditions. In addition, the simulations involve a low number density of coarse particles and so percolation as a mechanism in these simulations can therefore be safely dismissed. Classical diffusion requires the presence of a concentration gradient. The random mixing of the feed precludes classical diffusion and so the flux for particle species should be given by equation B7 (in appendix B). However, as a secondary mechanism, classical diffusion can make a contribution following the setting up of a concentration gradient by the primary shear-induced mechanism (back diffusion). The explicit calculation of the transport coefficients appearing in the continuum equations B1-B7 is only possible by a detailed analysis of the micro-mechanics of particle assemblies, although coupling with continuum mechanics is not an easy task. This chapter proceeds to present further evidence associated with the diffusive segregation mechanism and attempts to couple the relevant variables in the context of the discrete (defining) events (e.g. avalanches) in the heap’s evolution.
On impact to the heap, particles will clearly be on the surface and so, without other evidence, it is possible that the segregation observed is due to rolling only. Rolling as a mechanism to propel large particles preferentially down the free surface would imply that large particles in the boundary layer would tend to have a higher component of lateral velocity. However, the reverse is found to be the case as demonstrated by figure 5.17 which shows a graph of a time series of spatial mean lateral velocity in the boundary layer for each of the two species. The mean velocity for the large species is shown to be generally lower. The apparent contradiction (that large particles are more likely to reach the base, yet on average travel slower than small particles) is resolved by investigating the distance travelled by both species whilst in the boundary layer.

Figure 5.18 clearly shows that the mean distance travelled by large particles whilst in the boundary layer is greater than for small particles. The reason why large particles tend to reach the base is that whilst they may have lower average velocities than the small species, they simply stay in the boundary layer longer and travel greater lateral distances, propelled by avalanches. Since small particles travel faster in the boundary layer, but travel a shorter distance it must be because they get covered by other particles and thus leave the boundary layer. The higher mean velocity is maintained by a replenishment of the small particles involved in avalanching.
There is now clear evidence that large particles have a tendency to remain in the boundary layer — presumably due to diffusion by kinetic sieving as other mechanisms have been suppressed. Further evidence for this diffusive mechanism is now presented.

Heaps present considerable difficulties with regard to the examination of diffusion (as compared, for example to flow in a hopper). The absence of a constraining geometry, and the fact that evolution of the heap involves defining events which move temporally (for example an avalanche) make averaging techniques difficult. Evidence for the underlying diffusion is given by examining components of velocity perpendicular to the sloping surface. It was found that during avalanche activity, large particles had a component of velocity normal to the free surface of about twice that of the small particles. This was shown (section 5.2.3.4) to be statistically very significant. However, in performing these calculations, assumptions of uniformity had to be made about the gradient of the sloping surface which will certainly be changing. Hard evidence of diffusion really requires the calculation of self-diffusion velocities and/or coefficients of self-diffusion. For an individual particle, the fluctuating velocity is defined as the vector difference $\mathbf{c} - \mathbf{u}$, between the velocity, $\mathbf{c}$, of that particle and the mean local velocity $\mathbf{u}$. Nikitidis et al (1998) describe the calculation of self-
diffusion velocities in hopper flow. However, for heaps there is a problem in defining a local (regional) mean velocity because the system boundary is moving. For example, an avalanche will move through a local region as it evolves. Taking a Lagrangian approach and following individual particles, the mean velocity local to each particle was calculated over particles whose centres were within a radius of 3.5 small particle diameters from the centre of a “test” particle. This defines a sufficiently large local region for both particle species. These local mean flows are certainly not uniform within avalanches as particles change direction on collision. The self-diffusion velocity in this case was taken as the component of fluctuating velocity perpendicular to the mean local flow. Considerations (by filtering) were restricted to particles that were on the right hand side of the heap and were clearly avalanching (moving outwards and downwards). A random sample of such avalanching particles was taken (at different times) and the mean self-diffusion (fluctuating) velocity for large and small particle species were compared. A conventional two sample $t$ test revealed that large particles do have a larger self-diffusion velocity which is significant at the 5% level. In fact, the mean self-diffusion velocity for large particles is more than twice that for small particles thus supporting the evidence in section 5.2.3.4 when velocity components perpendicular to the free surface were compared. However, the large standard deviations involved mean that the significance is only at 5%. The large standard deviations also signify that different particles of the same species have very different experiences during avalanching. These results are summarised in table 5.1.

<table>
<thead>
<tr>
<th>Particle size</th>
<th>Large</th>
<th>Small</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample size</td>
<td>386</td>
<td>1208</td>
</tr>
<tr>
<td>Mean self diffusion velocity</td>
<td>0.0129</td>
<td>0.0054</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>0.0666</td>
<td>0.0721</td>
</tr>
</tbody>
</table>

Null Hypothesis: Mean self diffusion velocities equal  
Alternative Hypothesis: Mean self diffusion velocity greater for large particles  
Significance Level: 5%  
Critical Region (one tailed) $T > 1.645$  
Observed $T$ statistic: 1.81  
Conclusion: Accept Alternative Hypothesis

*Table 5.1. $T$ test proving mean self-diffusional velocity is higher for large particles.*
The self-diffusion velocities calculated and the statistical test performed clearly demonstrate the diffusive mechanism of the observed segregation. It would have been helpful to proceed to calculate self-diffusion coefficients for the two species. McQuarrie (1976) has shown that the self diffusion coefficient (in two dimensions) can be expressed as an integral over time of the fluctuating velocity autocorrelation function (equation 4.8, presented again below for convenience). This material is covered in a little more detail in sections 3.4.1 and 4.4.1.

\[ D = \frac{1}{2} \int_0^\infty \langle C(0)C(r) \rangle \, d\tau \]  

(4.8)

In equation (4.8), \( D \) is the self-diffusion coefficient, \( \tau \) is the time lag between fluctuating velocities \( C \) and the angle brackets indicate averaging over different time origins. The integral in equation (4.8) is from 0 to infinity. In practice, it was found that the short time duration of avalanches in this case was insufficient for the calculation of the integral to sufficient accuracy. In fact, graphs of the fluctuating component of velocity (normal to the local mean flow) against time are quite oscillatory and result in an autocorrelation function which is itself oscillatory (e.g. figure 5.19). Clearly, the function would decay to zero given sufficient time but the discrete nature of avalanching in these simulations does not provide this time window. However, the work done in attempting to obtain the integral is not lost as it throws more light on the variability of the self-diffusion velocity as defined and illustrates why the standard deviations are high.
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Figure 5.19. Fluctuating velocity autocorrelation function calculated over an avalanche period for a selected large particle.

Figure 5.20. Spatial mean rotational velocity in the boundary layer 5 small particle diameters wide for small particles (full line) and large particles (broken line) for the right side of the heap (low impact case).

5.2.3.7 Coupling of velocity components using wavelets

Free surface rolling as the primary mechanism of segregation for the low impact case has been discounted. However rotation is certainly a potential candidate for investigation of the mechanism that instigates avalanching. A comparison between the large and small particle species is given in figure 5.20 which shows a time series of mean absolute rotational velocity in the boundary layer. Figure 5.20 demonstrates that large particles within the boundary layer experience much more extreme temporal variations in rotational velocity than small particles which is worth further
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investigation. The motion of an individual large particle which stays within the boundary layer and thus experiences avalanches was selected for further study and the motion of this particle, in terms of both translational and rotational components of velocity was analysed (figures 5.21 (a) and (b)). One realises the limitations of one particle statistics, but this section is included in order to demonstrate the capability of the wavelet transform in decomposing a signal (time series) into significant components of activity at different times and at different scales of scrutiny. For the selected large particle, time series of lateral and rotational components of velocity were wavelet transformed and the decompositions compared and correlated. Each scale of scrutiny gives rise to a set of wavelet coefficients that can be graphed. From just two time series, there are many graphs that might be presented. For the purposes of brevity, the lateral and rotational velocity component series and the wavelet decomposition for rotational velocity only are presented in figure 5.21.

Figure 5.21

(a) Lateral velocity component

(b) Rotational velocity component
Figure 5.21 (a) Lateral velocity component, (b) rotational velocity, (c), (d), (e): wavelet coefficients at scales 1, 2, 3 respectively for rotational velocity. Selected large particle.

Figure 5.21(a) of lateral velocity component and 5.21(b) of rotational velocity component show clearly that the selected particle experiences at least two significant avalanches. The two avalanche experiences clearly have very different characteristics. Figure 5.21(c) shows a graph of wavelet coefficients (for rotational velocity) at the
The purpose here is to investigate the influence of rotational activity in discrete avalanching and an obvious first step is to find the correlation of lateral velocity component (measuring strength of avalanching) with rotational velocity. Table 5.2 shows correlations between (absolute) values of lateral and rotational velocity components along with those of the wavelet coefficients at the three smallest scales of scrutiny; scale 1 is the smallest scale. Tabulated alongside the correlations is an indicative time scale of a single wavelet (the width of the triangular peak) at that scale of scrutiny. The shape of the Deslauriers-Dubuc (2,2) wavelet is shown in figure 4.8. Also tabulated alongside the correlations are the average and indicative maximum distances travelled by the particle during these time intervals (spanned by a wavelet).
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Clearly, the final (maximum distance travelled) column of the table refers to peaks of avalanche activity.

The wavelet coefficient correlation technique perhaps needs a little more explanation. Section 4.7.4 discusses this more fully. However a brief explanation is provided here in context. If a cross correlation coefficient between two series is calculated, then there are contributions to the coefficient from sections of the series which are of particular interest, but also from sections of the series which are of lesser interest. The sections of particular interest in this case are relatively isolated and discrete in nature. The purpose is to show that the wavelet transform is capable of isolating the details of interest which in this case involve relatively abrupt changes in the series. Interestingly, for the chosen particle, wavelet coefficients at the smallest scale of scrutiny correlate the lateral and rotational velocity components better (coefficient = 0.818) than the original series themselves (coefficient = 0.667). This indeed provides evidence of the discrete nature of the significant events in the two series being picked up at this smallest scale of scrutiny. The decreasing correlation of the wavelet coefficients as we move to coarser scales of scrutiny provides further evidence of the discrete nature of the avalanches under investigation.

5.2.3.8 Avalanche duration and location

It is clear from the discussions and evidence that discrete avalanching and the underlying mechanisms requires further study. In fact, the mechanics of assembly evolution is described by the frequency of avalanches, the size of the avalanche region and the rate of propagation of the advancing avalanche boundaries. Considerations now move from a “micro-description” of avalanching to a “macro-description”. With the shallow heap, surface lateral component of velocity is a suitable measure of avalanche behaviour. As a further stage in investigating the nature and mechanisms of avalanching, local average lateral surface velocities were calculated in a boundary layer 4 small particle diameters deep. Figure 5.7 in section 5.2.3.2 shows clearly that avalanche activity is pronounced in a boundary layer 5 small particle diameters deep
and so a width of 4 small particle diameters will pick up avalanche activity. A small sampling time interval of 0.2 reduced time units (about 0.002 seconds for small particle diameter 1mm) was used which gave just over 900 sets of (time referenced) local mean velocities equally spaced in time over the duration of the evolution of the heap. The results are best regarded as a rectangular array of mean velocities with the dimensions (array subscripts) being distance from the centre of the heap and time.

A suitable method of presenting the data (which is essentially grey scale values) is by a density map. Figure 5.22 is such a density map of absolute mean local lateral velocity where the lighter the shade of grey, the higher the velocity. Time is recorded on the vertical axis with the horizontal axis representing distance from a fixed reference point to the left of the heap (x=40 is the centre of the heap). The significant features of this “avalanche evolution plot” are the discrete (in time and space) and sometimes local character of the avalanches and the comparative asymmetry (sometimes there is an avalanche on one side of the heap whilst on the other side there is little activity). The horizontal span of the avalanches displayed in figure 5.22 demonstrate the long range connectivity of particle interactions, even at lengthscales comparable with the size of the heap. There is evidence of periodicity, though this is not necessarily regular. Figure 5.22 gives an alternative description of avalanching to the mean lateral velocity series of figure 5.7.
5.2.4 Summary of section 5.2

The 2D analysis toolset consists essentially of time series analysis components (in particular spectral analysis and the wavelet transform), visual display components and components related to statistical mechanics (for example to calculate diffusion coefficients). Each of these elements has been demonstrated to be revealing in the analysis of the dynamics of heap formation. It is evident that the application of these tools has extracted from the simulation data a more complete spatial and temporal resolution of the assembly than is possible by observing snapshots alone, and one in which some likely mechanisms of heap evolution have been identified. The periodicity of certain measurable phenomena (in particular components of velocity) has been quantified by means of spectral analysis and potential mechanisms contributing to segregation and mixing have been identified. The nature of discrete avalanching has been shown to be a complex bulk motion phenomenon which is discrete in time and space and involves elements of irregular periodicity but also asymmetry. The discrete wavelet transform has been shown to be potentially useful in
coupling variables (in this case components of velocity) in the context of time series characterised by fluctuations that are not periodic and for which Fourier techniques are inappropriate.

In terms of the physics that governs the evolution of a poured granular heap, a number of important results have been demonstrated. With regard to segregation and mixing, it has been shown that the phenomenon of segregation on pouring is not an unavoidable consequence of particle geometry and size differences as had been previously conjectured (Makse, 1998), and that the process conditions, in this case feed rate, can be influential in controlling the extent of segregation. Further to this it has been shown that, for low impact feeds, whilst discrete avalanching is proceeding and there is a defined velocity gradient, large particles migrate preferentially towards the free surface. This process of kinetic sieving has been clearly demonstrated by a statistical \( t \) test to compare diffusional velocity in the two particle species. It might have been supposed that the next step in segregation would be rolling of the large particles down the free surface to the base. This would imply that the mean velocity of large particles in the boundary layer would be larger than for small particles. However, the reverse was found to be the case and evidence was presented to show that it is the propensity of large particles to remain in the boundary layer for longer that causes them to be propelled towards the base. This is not to say that rolling is not involved in segregation. However, rotation (as opposed to rolling) is shown to be important where changes in rotational velocity are more significant for large particles and are coupled with translational velocity in the context of the discrete defining avalanche events by the application of the wavelet transform. The wavelet transform is shown to be capable of determining the scale of defining events (disturbances in the time series) during the evolution of the heap.

The simulations studied involved approximately 8,500 particles. In two dimensions, this gives a reasonable heap size for probing and investigation. The principle conclusion in terms of process engineering that segregation can be prevented by a suitably high feed rate must be considered against the size of "real" industrial
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stockpiles. The simulations described probably represent the situation near the peak of a large heap. Sufficiently far away from a high impact feed region, it is possible that discrete avalanching with consequent segregation may well take place. Full thermalisation of a large heap by feed impact alone is clearly impracticable. However, one clear conclusion is that discrete avalanching may well be accompanied by particle size segregation.

It is emphasised that whilst the toolset has been applied to simulated data sets, the analyses are equally applicable to data obtained by experimentation.
5.3 Stress and voidage distribution and evolution in heap evolution

Section 5.2 has provided ample evidence that the evolution of a poured granular heap proceeds by a process of avalanching. Furthermore it has been shown that for the low impact feed case, avalanching is discrete in time and space so that an investigation into the coupling of assembly variables is not a simple matter. In a section 5.2.3.7, the application of the wavelet transform was shown to be capable of coupling variables during discrete avalanching. However, considerations were restricted to rotational and translational components of velocity only. However, fundamental to the dynamics of the heap evolution will be the build-up and relaxation of compressive and shear stresses with associated changes in voidage and velocity profiles. It is these aspects of heap evolution that now receive focus.

5.3.1 Stress and heap evolution

The ultimate purpose in applying wavelet analysis to stress, strain rate (velocity) and voidage is to begin the development of a constitutive framework for the evolution of bulk flow. The focus of the analysis is on regions close to the free surface boundary of the heap which experience the avalanching behaviour. This is then contrasted this with the stresses experienced by elements buried deeper in the heap. The majority of the work involves an Eulerian approach where the experience of static cells is investigated as particles flow through. However, this work is supported by some Lagrangian analysis where the experience of a particle is followed as it moves through the heap.

The low impact “trickle feed” simulation characterised by discrete avalanching and studied extensively with regard to velocity components was further investigated with regard to voidage and stress evolution. Both of these quantities are necessarily defined by a local averaging procedure and more detail is presented on this in sections 4.3.3 and 4.3.4. The size of local regions for the calculation of average voidage and stress require some consideration. The process of averaging must involve the application of a spatial grid to the output, so that any particle is tagged as being within a grid cell if its
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centre is within that grid cell. The cell size needs to be small enough to pick up significant local activity, but not so small as to pick up only noise. However, it should not be so large as to average out significant local variations. If we consider in particular the case of voidage, if the grid cell is very small compared to the size of particles, then in the extreme, values of voidage will be 100% if the grid cell is in a region of space between particles and 0% if the cell is placed on top of a particle. On the other hand, if the cell is large compared to the size of particles, then the derived local voidage may well be just the bulk voidage. A particular consideration involved in the choice of cell size is that it must be small enough to allow the investigation of activity within the boundary layer of significant avalanche activity which was found to be of the order of 12 small particle diameters as discussed later in section 5.3.4. A square cell with sides of length equal to 4 small particle diameters was chosen which allows an investigation at different depths within the boundary layer but which is sufficiently large to contain enough particles for stress and voidage calculations to be meaningful.

5.3.2 Determination of voidage

Section 4.3.3 discusses methods to determine voidage and in particular justifies the application of the methods used here. For the Eulerian investigations, area packing in each grid square is accumulated from the contributions of particles that overlap the square. Each small particle carries with it a 99 by 99 square grid allocation of points, centred on the particle. Of these 99x99=9801 points, those covered by the particle score 1 and those not covered score 0 in a 99 by 99 array. A similar procedure was applied to the size 3 particles. Thus two arrays were set up at the beginning of the programming code. The appropriate array then follows any particle as it moves through the domain of the simulation and at any time it is a relatively short computation to attribute those points of coverage to grid cells by a simple modular arithmetic technique and thus arrive at local packing (and therefore its reverse, voidage). Figure 5.23 shows a schematic of a grid cell with part of a particle covering some of the cell area with test points (at a coarse spacing for illustrative purposes). The points shown
would be accumulated with those provided by other particles overlapping the cell to allow a percentage coverage of the cell to be determined. The values obtained with this voidage calculation are comparable with those quoted by German (1989), thus validating the procedure.

*Figure 5.23. Illustrative voidage test points within a grid cell*

In order to adopt a Lagrangian approach, the voidage experienced by a particle as it moves through the heap is required. Section 4.3.3 discusses the problem of step changes in grid cell voidage as a particle moves between cells. Such step changes will be picked up by the wavelet transform that will be applied and would generate results which are just artefacts of the voidage calculation procedure. The annular voidage measure described in section 4.3.3 was used in the Lagrangian analyses and involved a circle of equally spaced points around the test particle with a radius 20% greater than that of the test particle. The percentage of these test points not covered by other particles is a measure of the test particle’s freedom to move and is referred to as “the annular voidage measure”.
5.3.3 Determination of components of the stresses tensor

Section 4.3.4 describes the method of calculating local stress based upon the accumulation of forces on local particles. Stress is calculated over the same grid cell system as local voidage and the subscript convention is such that the first subscript refers to a plane normal to the axis referred to by the subscript and the second subscript refers to the direction of the stress. \( \sigma_{yx} \) is therefore shear stress in a plane normal to the \( y \) direction but acting in the \( x \) direction. The equations used to calculate stresses are numbered 4.3 to 4.6 in section 4.3.4.

All quantities derived from the simulation are in reduced units which are briefly described in appendix A2. All stresses derived from equations 4.3 to 4.6 are therefore in reduced units. Conversion to SI units requires only the specification of the small particle size. In illustration, for 1mm. diameter small particles, any stress graphed or discussed in later sections would need to be multiplied by 7.7 to be in SI units (Nm\(^{-2}\)).

5.3.4 Rotation of axes

The simulation code was written with the \( x \) co-ordinate direction horizontal and the \( y \) co-ordinate direction vertical. However, the evolution of the heap is by avalanching down the free surface. The slope obviously fluctuates slightly over time, but a representative sloping surface angle was chosen by calculating surface gradients at sample times and then averaging. This allowed transformation to a new set of axes with the \( x \) direction down the right hand slope and the new \( y \) direction perpendicular to this. The transformation with a clockwise axis rotation of \( \theta \) is performed by the transformation equations numbered 4.1 and 4.2 and given in section 4.3.1.

In these investigations, after the rotation of co-ordinate axes, only particles on the right hand side of the heap were considered. Working in the transformed co-ordinate system,
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the transformed $x$ velocity is now an avalanche velocity and meaningful velocity gradients and appropriate components of normal and shear stresses for the investigation of coupling can be more readily calculated. Henceforth, stress subscripts are in this transformed co-ordinate system and avalanche velocity is the velocity component in the transformed $x$ direction. Figure 5.24 shows a schematic to illustrate the transformation of axes and the location of test cells for further investigations.

![Figure 5.24. A schematic to illustrate the new rotated co-ordinate system and positioning of test cells used for investigation of velocity, stress and voidage.](image)

5.3.5 The depth of the avalanche boundary layer

In section 5.2.3.3 (figure 5.9 (b)), evidence was provided to show that for the low impact feed regime, there is a fairly well defined region of stability below the surface of the heap with avalanche activity taking place in a boundary layer. However, the depth of this active boundary layer was not specifically investigated. By calculating the average velocity of particles at different depths from the surface (averaged over the duration of the simulation), it was found that below about 12 small particle diameters from the surface, average velocity was very small and so investigations of avalanche
activity can be confined to a boundary layer of approximately this depth. This is not to say that below the boundary layer particles are not experiencing changes effected by the heap evolution as will be evidenced later.

5.3.6. Results and discussion

Separate investigations were performed on the stress distributions for the static region of the heap and for stress and strain rate evolution coupling with voidage for the active boundary layer. It is emphasised that the discrete wavelet transform can only be applied to series of lengths which are powers of 2. To allow for comparison with correlations of wavelet transforms, calculation of correlation coefficients for any un-transformed series have also been restricted to a length which is an appropriate power of 2, in this case 256.

The results from the simulations can be scaled to apply to different grain sizes. The code produces output in terms of “reduced units” (appendix A2) based upon the diameter of the small particle and simulation output was sampled every 2 reduced time units. With regard to time and units, a number of issues in terms of clarity of presentation arise, for example, wavelet scale and associated time lags at different scales. Table 5.3 gives a conversion between wavelet scale, sampled time units, reduced time units and illustrative “real time” in seconds for 1mm small particle diameter. All time series graphs have sampled time along the horizontal axis (every 2 reduced time units) which corresponds to about 0.02 seconds for small particle diameter equal to 1mm. With regard to explaining how the wavelet transform operates, it is much easier to work in unit (sampling time) increments.
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<table>
<thead>
<tr>
<th>Wavelet scale</th>
<th>Sampled time unit</th>
<th>Reduced time unit</th>
<th>Time in seconds for 1 mm small particle diameter</th>
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<tr>
<td></td>
<td>8</td>
<td>16</td>
<td>0.16</td>
</tr>
</tbody>
</table>

Table 5.3. Conversion between wavelet scales and time units.

Whilst the principal concern is with fluctuations in voidage, the actual voidage values that are reported and discussed in this section require a little more consideration. German (1989) gives voidage values for different granular arrangements. The lowest voidage possible for hexagonal close packed disks of equal size is 9.3%. However, random packings result in voidages in excess of this limiting value. Assemblies are likely to progress via agitation from a loose random packing of 27% voidage to a dense random packing of 18% voidage. Obviously, within any bulk, there will be local variations around these values. The simulation model (appendix A1) encompasses “particle overlap” which allows a realistic representation in terms of frictional engagements of particles. The voidages calculated in these simulations are therefore likely to be somewhat lower than for a real granular system. However, for the fines continuous mixture, they are within the limits discussed above.

5.3.6.1 Stress distributions in the static regions of the heap

In section 5.2.3.3 the shape of the static region of the low impact feed heap was investigated and shown to resemble the shape of the heap as a whole (see also Smith et al, 2001). The outer regions form a boundary layer where particle movements are significant. The static region of the heap will clearly have lower values of voidage than the avalanching outer regions. The coupling of stresses with voidage was investigated and some evidence was found that over a very large number of sampled points in the static region, high stress is associated with low voidage, though with a very wide scatter. However, the situation is rather more complicated and interesting.
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Figure 5.25. Scatter of high values of normal stress against voidage for a period towards the end of the simulation. (1 reduced stress unit = 7.7 Nm⁻²).

Figure 5.26. Distribution of normal stress ($\sigma_{xx}$) towards the end of the simulation. The right hand side of the heap is shown. The lighter circles indicate cells (regions) of highest stress – not particles. The legend indicates regions with stresses above the quoted percentile. A,B,C,D identify the high stress cluster at voidage just above 15%.
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Figure 5.25 shows the scatter of just the largest compressive stresses $\sigma_{xx}$ (in excess of 25 reduced units) against voidage. It appears from the scatter that high values of stress are associated with particular discrete values of voidage. For example at voidage just above 15%, there is a fairly sharp peak in the scatter with an absence of points either side of this peak. There appear to be perhaps 5 or so specific voidages which are supporting high stresses in this range. Other localised “peaks” appear if the threshold of minimum stress is relaxed below 25 reduced units. It should be noted that the scatter of figure 5.25 involves both a time and spatial sampling and so without further investigation it is possible that each peak is associated with a specific cell with the large number of observations over the time of the simulation and the variation in voidage over time giving rise to the observed shape of the peak. However, further investigation revealed that the peak in question involves 8 cells with 4 providing most of the points. The positions of these 4 cells are labelled A,B,C,D in figure 5.26 which shows the normal stress ($\sigma_{xx}$) distribution in the right hand half of the heap towards the end of the simulation by grey scaling with lighter colour representing higher stress. Clearly these 4 cells are in a stratum which is approximately parallel to the free surface. Further investigation showed that some of the peaks in figure 5.25 do result from a large number of time samples for a single cell that experiences sustained high normal stresses. However, there appears to be some evidence that certain specific voidages are capable of supporting high normal stresses, perhaps due to particular local stable crystalline arrangements as the cells do appear in the same stratum.

Figure 5.26 shows percentile ranges of the distribution of normal stresses, $\sigma_{xx}$, in the right hand side of the heap by means of grey scaling. The positions of the circles are based upon the cell centres over which stresses were calculated. The circles are not equally spaced because transforming back to the original cartesian co-ordinate system involved only integer co-ordinates. The lighter circles (indicating cell centres) with the highest normal stress seem to fall along a line sloping parallel to the free surface of the heap with lower normal stresses below this line. Section 5.2.3.3 discussed a “region of stability” in terms of particle movements (see also Smith et al, 2001), where by stable (at a point in time) we meant that particles translated only a very short distance...
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(arbitrarily a maximum of one small particle diameter) from then onwards. However, figure 5.26 seems to provide evidence of a rather smaller passive region deeper in the heap bounded by the line of maximum normal stress. Above the line of maximum stress, regions of equal stress are approximately in strata parallel to the free surface as shown by grey scaling.

5.3.6.2 Stress and voidage evolution in the static regions of the heap

With regard to the evolution of stresses, the experience of a cell that ultimately supports high normal stresses (cell C in figure 5.26) was further investigated. Figure 5.27 graphs the normal stress $\sigma_{xx}$ and voidage over time for this cell. Clearly the normal stress increases with time as the cell becomes more and more buried. However, voidage clearly settles to a stable value. With regard to "regions of stability", the term stable does not imply that key attribute values remain constant. Indeed figure 5.27 suggests that there is connectivity over a considerable number of particles as the stress does continue to increase for the duration of the simulation.

Figure 5.27. Normal stress ($\sigma_{xx}$) and voidage evolution for a cell that experiences high stress (cell C in figure 5.26). (1 reduced stress unit = 7.7 Nm$^{-2}$ for 1mm diameter small particles).
5.3.6.3 Strain and voidage coupling in the evolving boundary layer

Avalanche activity is clearly measured by the component of particle velocity down the slope of the free surface. Having transformed the co-ordinate system by rotation, this avalanche velocity is the transformed $x$ velocity component. The simulation output has been adapted to include average cell values such as components of velocities, voidage and components of stress. A suitably placed cell was selected (called test cell 1, shown in figure 5.24) that would experience a number of avalanches during the time of the simulation and ultimately finds itself buried to a depth of more than 4 small particle diameters (the grid size used for averaging). Figure 5.28 is a graph showing voidage and avalanche velocity for test cell 1. The initial time of zero is taken as the cell is just receiving the first flow of particles and hence has a very high voidage. Thereafter the voidage drops as the cell fills to time approximately 70 from where investigation of the series starts. It is clear that voidage does fluctuate with avalanche activity and that these fluctuations are of the order of 10%. It is generally accepted that the initiation of granular flow involves a degree of dilation (see for example Tüzün et al, 1988) and so the observation is in agreement with the results of previous studies. However, the precise nature of the coupling between voidage and avalanche velocity is not clear from a visual inspection of the graphs although it may appear that voidage fluctuations occur shortly before peaks of avalanche activity in some cases.
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Figure 5.28. Avalanche velocity and voidage for test cell 1 (the deeper test cell).

Figure 5.29. Avalanche velocity and voidage for test cell 2 (the test cell nearer the surface). Dotted arrows point to referenced avalanches.
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<table>
<thead>
<tr>
<th></th>
<th>Lag 1</th>
<th>Lag 2</th>
<th>Lag 3</th>
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</tr>
<tr>
<td>Scale 3</td>
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<td>0.48</td>
</tr>
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</table>

Table 5.4. Time equivalent in seconds (for 1mm diameter particle) when lagging (shifting) wavelets at different scales.

<table>
<thead>
<tr>
<th>Correlation between wavelets at</th>
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<th>scale 3</th>
</tr>
</thead>
<tbody>
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</tr>
<tr>
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<td>0.41</td>
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</tr>
<tr>
<td>lag 1</td>
<td>0.15</td>
<td>lag 1</td>
</tr>
<tr>
<td>unlagged</td>
<td>0.19</td>
<td>unlagged</td>
</tr>
</tbody>
</table>

Table 5.5. Lagged correlations between wavelet coefficients for avalanche velocity and voidage for test cell 1 (the deeper test cell).

Figure 5.30. Time series plots of wavelet transform coefficients at scale 3 for avalanche velocity and voidage with unit forward shift of voidage coefficients so that avalanche velocity coefficient is matched with a preceding voidage coefficient.
Correlation studies are now used in an attempt to couple the two series in figure 5.28, but using wavelets as well as the original time series. Also correlations for lagged (shifted) wavelet coefficients will be considered. To avoid confusion concerning the units involved, refer to table 5.3 which gives a conversion into reduced time units and ultimately into seconds (for 1mm small particle diameter) between the wavelet scales used and the sampling time interval for the original time series. For example, the bottom line of the table means that a scale 3 wavelet spans 8 sampling time intervals which is 16 reduced time units equivalent to (about) 0.16 seconds for 1mm diameter small particles. Table 5.4 converts into seconds (for 1mm diameter small particles) the time involved in lagging (shifting) wavelets at different scales. For example, a scale 3 wavelet with a lag of 2 is equivalent to a time shift of 0.32 seconds (for 1mm diameter small particles).

A simple attempt using Pearson's product moment correlation coefficient (equation 4.12) to correlate the two series of figure 5.28 gives a non-significant result. Over a suitable 256 length sample starting at about sampling time = 70 and encompassing the significant avalanches, the correlation coefficient is 0.05 and even working with absolute values it is 0.02. Applying equation 4.13 (lagging one or other series) did not reveal any more significant correlation. However applying the wavelet transform to both series and attempting to correlate the coefficients, something of the nature of the coupling is revealed. At wavelet scale 1, the correlation between wavelet coefficients (absolute values) is -0.03. At scale 2 it is 0.19 and at scale 3, 0.16. These values are obviously not significant. However, for scale 2 wavelets, applying equation (4.13) (for a lagged correlation) with lag \( t = 2 \) (i.e. shift the voidage set of wavelet coefficients forward by two places so that we are correlating disturbances in avalanche velocity with disturbances in voidage at two wavelet times scales previously) then a significant correlation coefficient (of 0.32) is obtained. With lag \( t = 3 \) (a further shift and correlation coefficient calculation), the correlation coefficient is 0.41. There is also a significant correlation at lag \( t = 1 \) for scale 3 wavelets (of 0.52). A summary of the results is given in table 5.5 where the significant correlations are emboldened. It is again emphasised that in this table, correlation at lag \( n \) using equation 4.13, means that
before the correlation coefficient is calculated, the voidage wavelet coefficients are shifted forward \( n \) places so that a particular velocity wavelet coefficient is lined up with the voidage coefficient \( n \) wavelet scale points previous. It is also emphasised that the amount of the lag in terms of the sampling interval needs to be scaled by the "width" of the wavelet: 2 for a scale 1 wavelet, 4 for a scale 2 wavelet, 8 for a scale 3 wavelet etc. (see table 5.4).

The emboldened values of increased correlation coefficient in table 5.5 are consistent in that a scale 3 wavelet is twice as wide as a scale 2 wavelet and the size of its unit shifts are also double. One would therefore expect to see some agreement between a scale 3 wavelet lagged once and a scale 2 wavelet lagged twice. The emboldened values are all significant (on a null hypothesis of no correlation). There is therefore evidence of a coupling between fluctuations in the two series characterised by wavelets at scales 2 and 3 but such that the coupling is for a lag of about 8 sampling time points on the original time scale. (Recall that a scale 3 wavelet scales across \( 2^3 \) time points). 8 sampling time points would correspond to about 0.16 seconds for 1mm diameter small particles.

One must take care when interpreting correlation coefficients as the nature of the scatter may not support the simple association that might appear to be the case on face value of the coefficient. Of the 32 wavelet coefficients at scale 3, only some with significant values will be detecting the few (short time span) disturbances in a series. The remainder will take small values. A correlation coefficient calculated between two such sets of coefficients will reflect the degree to which the few significant coefficients line up. Figure 5.30 shows the time series graphs of avalanche velocity transform coefficient (at scale 3) and unit shifted voidage transform coefficient (again scale 3) together, i.e. on the same time graph, the values that constitute the significant emboldened correlation coefficient of 0.52 (at scale 3, lag 1). One can clearly see where the significant values correspond. However, there are times when there is a significant value in one series but not in the other. It is emphasised that since absolute values of wavelet transform coefficients are being correlated, disturbances (localised
short term periodicity) in the two series are being coupled, but that a phase coherence is not implied. In this particular case, the argument is that the wavelet transform is providing evidence that when short term fluctuations in avalanche velocity occur, there is significant evidence of preceding short term fluctuations in voidage at the same scale. In principle, the wavelet transform correlation technique could be applied to actual (not absolute) values of transform coefficients when phase coherence would be identified.

Test cell 1 used to generate the data for the graph in figure 5.28 becomes full at about sampling time =70 and so by the time of later avalanches, for example just before time=250, it is buried a few particle diameters below the surface. It is instructive to also consider the cell immediately above this one (called test cell 2, shown in figure 5.24). Figure 5.29 graphs voidage and avalanche velocity for test cell 2 which becomes full around time 175. After this time there are four significant avalanches indicated by arrows. Interestingly, the avalanche just before sampling time 250 is as sharply defined in figure 5.28 (test cell 1), but the others (at about 210, 280 and 330) whilst clearly defined in figure 5.29 (test cell 2) are much less so in figure 5.28. The depth of the avalanching region is clearly different for different avalanches.

5.3.6.4 Stress evolution in the boundary layer

Figures 5.31 and 5.32 show the evolution of normal and shear stresses for the two adjacent test cells over the same time scale as for figures 5.28 and 5.29. Both graphs show a gradual overall increase in normal stresses ($\sigma_{xx}$ and $\sigma_{yy}$). Shear stress $\sigma_{yx}$ appears to become stationary after initially increasing (in the negative sense). $\sigma_{xy}$, shear stress in the $y$ direction stays close to zero. This is to be expected as in the rotated coordinate system, the rotated $y$ direction is perpendicular to the flow. Visually comparing figures 5.28 and 5.29 with figures 5.31 and 5.32, it appears that avalanche activity between times 70 and 350 (when rather more discrete and identifiable avalanches occur) is more pronounced in test cell 2 (figure 5.29) than in test cell 1.
which is deeper in the heap. However, peaks in the stress graphs that correspond are more easily identifiable in the series for test cell 1 (figure 5.31). This perhaps suggest that the triggering catastrophic events that set off avalanches are a little below the surface, but that the subsequent avalanche activity is more pronounced near the surface. Arrows in figures 5.29 and 5.31 indicate the approximate times of the avalanches. A visual inspection of figure 5.31 seems to show that at about the time of an avalanche, absolute value of shear stress $\sigma_{yx}$ (it is always negative) drops significantly towards zero before peaking at a maximum value. The second and third avalanches arrowed reveal that the peak in shear stress $\sigma_{yx}$ is a little after the peak in avalanche velocity. So, it appears that at the onset of an avalanche, the shear stress drops, presumably due to an associated fluctuation in voidage. Once flow is initiated, shear stresses increase to a peak and then fall back somewhat after the avalanche. The normal stress $\sigma_{xx}$ seems to follow avalanche activity as well, again peaking after the avalanche. It would appear from an inspection of both figures 5.31 and 5.32 that the series for shear stress $\sigma_{yx}$ seem to settle down to a limiting mean value (obviously with significant variations at times of avalanche activity). However, for both normal components of stress ($\sigma_{xx}$ and $\sigma_{yy}$), the series show an increasing trend (again with significant variations at times of avalanche activity). This would appear to provide evidence that after each avalanche, the packing settles into an ordering that is capable of supporting greater normal stresses.
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Figure 5.31. Normal and shear stresses for test cell 1 (the deeper test cell). (1 reduced stress unit = 7.7 \text{ Nm}^{-2} \text{ for 1mm diameter small particles). For ease of identification, \( \sigma_{xy} \) is the plot tracking the time axis. Arrows highlight referenced avalanche times.

Figure 5.32. Normal and shear stresses for test cell 2 (the cell nearer the surface). (1 reduced stress unit = 7.7 \text{ Nm}^{-2} \text{ for 1mm diameter small particles). For ease of identification, \( \sigma_{xy} \) is the plot tracking the time axis.
Clearly, visually there appears to be a coupling of avalanche velocity (particularly on the surface, test cell 2) and stresses a little below the surface (test cell 1). In an attempt to throw light upon the nature of this coupling, the discrete wavelet transform was applied to avalanche velocity (test cell 2) and to normal stress $\sigma_{xx}$ and shear stress $\sigma_{yx}$ in test cell 1. The transforms failed to reveal a significant correlation between shear stress $\sigma_{yx}$ and avalanche velocity. However, correlations between normal stress $\sigma_{xx}$ and avalanche velocity were investigated at different lags. Table 5.6 shows the results where, as described previously, lag means correlating the transform coefficients of velocity with later transform coefficients of normal stress.

<table>
<thead>
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<th>Correlation between wavelets</th>
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<th>scale 3</th>
</tr>
</thead>
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<td>lag 2</td>
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</tr>
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<td>lag 1</td>
</tr>
<tr>
<td>unlagged</td>
<td>0.11</td>
<td>unlagged</td>
</tr>
</tbody>
</table>

Table 5.6. Lagged correlations between wavelet coefficients for avalanche velocity in test cell 2 (the upper test cell) and normal stress, $\sigma_{xx}$, in test cell 1 (the deeper test cell).

The wider (larger scale) wavelet at scale 3 picks up a significant correlation both unlagged and at lag 1, whilst the scale 2 wavelet picks up significant correlation at lag 1. These results are consistent in pointing to an association between peaks in the velocity series and those in the stress series about 8 sampling time points later. 8 sampling time points corresponds to about 0.16 seconds for 1mm diameter small particles. A possible interpretation here is in terms of a relaxation time constant following avalanche activity.

5.3.6.5 Focus on avalanche activity

To get a better appreciation of what is happening during an avalanche, two short sections of some of the series in figures 5.28, 5.29, 5.31 and 5.32 are magnified for
visual inspection. There is clearly an avalanche at around sampling time 245. Figure 5.33 shows a short section of the series for avalanche velocity for test cell 1, avalanche velocity for test cell 2 and normal stress $\sigma_{xx}$ and shear stress $\sigma_{yx}$ for test cell 1. It can be seen that there are two drops (in the negative sense) in shear stress during the avalanche followed by an increase at the end. Normal stress peaks about 11 sampling time points after the avalanche which is in broadly in agreement with the wavelet analysis. Figure 5.34 focuses in on the avalanche just before sampling time 300. This avalanche has twin peaks (for surface velocity) which appear somewhat spread out at the scale of this figure. However, one can clearly see shear stress dropping during the avalanche and then rapidly peaking. Normal stress follows a very similar pattern to shear stress in this case.

![Graph showing stresses and avalanche velocity](image)

*Figure 5.33. Stresses and avalanche velocity for test cell 1 (the deeper test cell) for the avalanche near sampling time 245.*
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Figure 5.24. Stresses and avalanche velocity for test cell 1 (the deeper test cell) for the avalanche near sampling time 300.

5.3.6.6 A Lagrangian perspective on strain/voidage coupling

An alternative to the Eulerian approach taken thus far, i.e. observing the experience of a fixed cell as granules flow through, is to follow the experience of individual particles. However, as has been discussed above, cell average values can present a problem in terms of discontinuities as a particle moves from one cell to the next. In particular, with regard to voidage, the “annular voidage measure” discussed previously (section 5.3.2) is used. The percentage of annulus points around the test particle not covered by another particle is a measure of voidage around the test particle – i.e. a measure of its freedom to move. A particular particle that moved through the test region (test cell 1) that we have already used for our Eulerian analyses was followed. The particle experiences a number of avalanches and so is suitable for the purpose. Figure 5.35 shows a graph of avalanche velocity and both the annular and cell voidage measures, though it is again noted that abrupt changes in cell voidage are likely as the particle moves between cells. Visually, it looks as though the annular voidage measure is related more to avalanche velocity than the cell voidage measure. As before an attempt
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was made to correlate the original series themselves and see whether the wavelet transform throws more light on the relationship. The correlation coefficient calculated between avalanche velocity and annular voidage measure (over a suitable 256 point sample length) is 0.245 and for absolute values of both series it is 0.29. However, the wavelet coefficients (absolute values) at scale 1 give a correlation coefficient of 0.59 which is quite significant. The fact that wavelets at the smallest scale are the ones identifying correlations is indicative of particles during an avalanche experiencing disturbances at a smaller scale (greater frequency) than is picked up by the Eulerian (cell average) approach.

![Figure 5.35. Avalanche velocity and cell and annular voidage measures following a test particle.](image)

In the earlier discussion, an attempt was made to try to explain how the wavelet transform focuses on significant events (at a particular scale) within a series and figure 5.30 was used in illustration. It is probably instructive at this point to look at the scatter of wavelet coefficients that in this case gave rise to a correlation coefficient of 0.59. Figure 5.36 shows this scatter. Inspection of figure 5.36 shows a large number of points near the origin corresponding to points in the series where little of interest is
happening (for both series). There is clearly a fair amount of scatter, but the significant value of the correlation coefficient derives from the 7 or so points farthest from the origin towards the top right of the scatter. It is emphasised that our interpretation of a significant correlation coefficient between sets of wavelet transform coefficients concerns the capacity of the transform to focus in on the few defining events (in this case avalanches) at a particular scale whilst filtering out regions of the series where little is happening. In this case, it is revealed that there is a considerable coupling of avalanche velocity with annular voidage measure over the limited number of points relating to defining events (perhaps 7 or so over the sample length of 256).

Given that there is a significant correlation between scale 1 wavelet coefficients for avalanche velocity and annular voidage in this case which is greater than the correlations that we have calculated thus far, this result is interpreted as pointing to an experience of individual particles which are avalanching which is not picked up by the Eulerian approach. It seems that local agitations involving individual particles that facilitate avalanching are at a finer scale (greater local frequency) than the voidage changes detected on a cell average basis. This would appear to indicate that a small change in local average voidage (calculated on a cell basis) may allow greater changes in freedom to move for individual particles. It was mentioned that visually (cell) voidage changes of the order of 10% seem to accompany avalanches. The experience of individual particles can clearly be rather more than 10%.
5.3.7 Summary of results from section 5.3

Stress and voidage propagation in the static and avalanching regions of an evolving heap have been investigated. With regard to the non avalanching regions of the heap, it has been shown that a stratum parallel to the free surface supports the highest level of normal stress (directed parallel to the free surface). Above and below this stratum, normal stresses are less. Further to this, evidence has been presented that certain granular arrangements are particularly capable of supporting high normal stresses.

It has been shown that at the times of the defining events of heap evolution, shear and normal stresses peak and relax during a short interval of peak avalanche velocity with some evidence of a normal stress relaxation time constant of the order of 0.16 seconds for 1mm diameter small particles. Whilst normal stresses might relax during an avalanche, they do rise over time as the re-packing of the material allows support of these greater stresses. The behaviour of shear stresses is perhaps less clear, but there is
some evidence that shear stresses drop (in magnitude) during an avalanche and peak afterwards.

With regard to the avalanching regions, a relationship between local voidage and avalanche velocity has been pointed to which involves a time lag such that avalanche velocity changes are associated with voidage changes some time earlier. The time lag is of the order of 0.16 seconds for 1mm diameter small particles.

The difference between the Eulerian and Lagrangian approaches to post simulation processing have been described and the importance of performing both has been demonstrated. In particular, the Lagrangian approach reveals that significant disturbances at the particle level may be of a much shorter scale (greater local frequency) than for local cell averages and in particular that voidage changes experienced by individual particles may be rather larger than those calculated as averages over cells of the size of a few small particle diameters.

Most significantly, the capacity of the wavelet transform to provide a focussed probing into the time localised but significant defining events in the evolution of a granular assembly has again been shown.
CHAPTER 6. APPLICATIONS OF THE 3D TOOLSET

6.1 Introduction

Two dimensional models are obviously capable of simulating much larger geometries than three dimensional models and given the constraints in computer processing power, this is a considerable advantage. However, there is always the potential for phenomena which might manifest themselves in two dimensions to be attenuated in three dimensions because of the greater capacity for energy dissipation and also because particles can move in the extra dimension. To the extent that it is possible, 3D analyses supporting the work done on 2D heaps will now be reviewed. In addition, segregation by self-diffusion during 3D hopper discharge will be investigated.

6.2 Investigation of avalanche activity for 3D heap formation

The simulations in 2D have shown some interesting results in terms of heap evolution by continuous avalanching in the high impact feed case and by discrete avalanching in the low impact feed case. In particular, the toolset has been used to reveal evidence of periodicity in avalanching (for the high impact case) and has been useful in coupling variables in the context of discrete avalanching events (for the low impact case). The active regions of the heap have also been interpreted visually by the 2D filtered display capability. Whilst the results of these simulations have direct application to some real industrial process such as heap formation between retaining walls or the stacking of cylinders (e.g. bottles, cigarettes), clearly real 3D heaps will behave somewhat differently to 2D heaps partly because of the freedom of particles to move in the extra dimension (e.g. perpendicular to the line of greatest slope), but also because as particles move away from the centre of the heap, the volume available to them for translation becomes progressively greater (i.e. the circumference of the circle in plan view becomes larger). Particles will thus potentially interact with a greater number of other particles and so there is a greater potential for the dissipation of energy. It is therefore important to perform (as far as is possible) equivalent analyses in 3D to those carried out in 2D by way of comparison and validation.
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The 3D simulation (as with the 2D case) involved a continuous interaction (CI) model as described in appendix A1 and whilst there is obviously a greater degree of sophistication, in principle, the algorithms are similar. For the 3D simulations, the feed rate was controlled by the diameter of the orifice of a feed hopper. The simulation performed for the investigation described below was “low impact”, though in practice not as low as the trickle feed for the 2D heap. Particles fell a short distance from the feed hopper to a flat surface constructed of small particles. The geometry of the arrangement including the feed hopper is shown in figure 6.1. The binary feed consisted of 5% by number of large particles which had a diameter twice that of small particles. A size ratio of 3:1 in 3D as used in the 2D simulations would have created difficulties in sizing grids for Eulerian analyses. The distribution of particles was suitably randomised during the hopper fill.

![Figure 6.1 the geometry of the 3D heap simulation, showing the position of the test cell.](image-url)
The output of the simulation as in the 2D case is essentially multivariate time series of particle attributes such as components of position and velocity vectors. This data was again recorded in a database from where the 3D analysis tools can be applied (in terms of investigating plan views, rotated cross sections etc.). With regard to an Eulerian approach, where the application of some form of grid cell averaging is required, some post-simulation capability is afforded from the database values recorded. However, with regard to stresses, these need to be calculated within the simulation, which requires the imposition of a grid co-ordinate system at the time of the simulation. Given the size of the simulation, this meant that with regard to stress investigation, an arbitrary cross section through the centre of the heap was investigated. The 2D work described in section 5.3.5 included some investigations into the coupling of voidage with stresses and avalanche activity. Unfortunately, even with approximately the same number of particles in the simulation, the dimensions of the heap are considerably smaller which makes the determination of a meaningful voidage (especially in the boundary layer) impractical.

The analysis is therefore in two parts, a Lagrangian part where particles may be followed as they move in all three dimensions and an Eulerian part restricted to the chosen fixed cross section. Where a one dimensional wavelet transform is applied, it is the same as that applied to data derived from the two dimensional simulations and described in appendix E, i.e. the transform utility for which the code was written from scratch. Where a two dimensional wavelet transform is applied it is the Daubechies (2) transform provided by the Matlab © Wavelet Toolbox; the two dimensional transform utility developed from scratch is in pilot form only.

6.2.1 Experience of particles – the Lagrangian approach

As in the 2D case, suitable database indexes were used in order to identify particles that spent a significant time in the active boundary layer and are thus suitable for investigation. In all figures, time is in reduced units as described in appendix A2.
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Translational velocity units are small particle diameters per time unit. Sampling was every 0.6 time units starting at an arbitrary point in time when a heap was beginning to form. Sampling time relates to this sampling, i.e. 1 sampling time unit = 0.6 reduced time units.

Figure 6.2 below is a graph of vertical velocity component for a selected small particle that spends much of its time in the boundary layer. Whilst the mean vertical (z) velocity is negative, the nature of the avalanching is such that the particle vertical component of velocity oscillates rapidly between a positive and a negative direction. For this reason, for this shallow heap, vertical velocity will therefore not be used to measure avalanche activity for an individual particle.

![Figure 6.2, Vertical component of velocity plotted against time for a selected small particle that remains in the boundary layer](image)

Figure 6.3 below is a time series graph of radial velocity and rotational velocity, for the same small particle as represented in figure 6.2. Clearly the nature of avalanching experienced by the particle is different from the two dimensional case discussed.
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extensively in section 5.2. Here there is evidence of rather more avalanches over the duration of the simulation. One would expect to have avalanches of shorter duration (and so more of them) because of the greater capacity for energy dissipation for the three dimensional case. Given that the heap is smaller than for the 2D studies, the particle clearly experiences more avalanches in its progress down the boundary layer close to the sloping surface.

Radial velocity (as opposed to vertical z velocity) will be used as a measure of avalanching because of the very oscillatory nature of z velocity (as evidenced in figure 6.2) for this relatively shallow heap. For the two dimensional simulations, an investigation was performed into the coupling of rotational with avalanching velocity and the same will be done here. Visually, it is difficult to detect a distinct coupling of the two plots in figure 6.3. In fact, over a suitable 256 sample length section, the product moment correlation coefficient (equation 4.12) is -0.1. However, after performing the discrete wavelet transform on the two series (over the same 256 sample length), there is a correlation of absolute values of wavelet coefficients at scale 1 of
0.33. Though small, this value is significant and indicates that rotational velocity and radial (avalanche) velocity show some degree of coupling but on the basis of discrete changes as represented by wavelet coefficients at scale 1.

For the two dimensional heap, it appeared (section 5.2.3.7) that rotational velocity was more important in terms of avalanching for the larger particles and the wavelet transform was shown to be helpful in coupling rotational and avalanche velocity. For this three dimensional simulation, a suitable large particle was selected for investigation. Figure 6.4 shows graphs of radial (avalanche) velocity and rotational velocity for this particle. Rotational velocity shows rather fewer peaks than was the case for the small particle (in figure 6.3). As with the small particle, the correlation between the two series is negligible (a value of $-0.09$). However, absolute values of wavelet transform coefficients at scale 1 reveal a correlation of 0.35 with a value of 0.41 for scale 2. Given the slightly different feed rate, it would be difficult to attempt to make direct comparisons with the 2D case. However, the evidence here is supportive of the conclusions from the 2D simulations, i.e. that the coupling of rotational and translational velocity during discrete avalanching is in terms of disturbances at an identifiable local time scale. Again, the wavelet transform is shown to be capable of coupling series in the context of the perturbations within.
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Radial velocity
Rotational velocity

Figure 6.4, Radial velocity and rotational velocity for a selected large particle that remains in the boundary layer plotted against time

6.2.2 Eulerian investigation of components of velocity and stress during avalanching

A cell was selected for the investigation of variables associated with avalanching. The position of the cell (figure 6.1) was approximately \( x=9, z=5 \) (units are small particle diameters) within the cross-section selected for investigation. Given that the cell is within a cross-section through the heap (with \( y=0 \)), one would expect avalanche activity to be reflected in terms of \( x \) and \( z \) components of velocity. (For an Eulerian cell based approach, average \( z \) velocity must not be discounted on the basis of the Lagrangian evidence of figure 6.2). Figure 6.5 below shows a graph of mean \( z \) component of velocity (downwards positive), mean \( x \) component of velocity and mean \( y \) component of velocity.
The mean $z$ component of velocity is on average less than the mean $x$ component of velocity as one would expect with a fairly shallow heap. However, the mean $y$ component (which is perpendicular to the radial flow direction) is often significant, indicating that the avalanche is often not straight down the radial direction, i.e. the direction of greatest slope. However the graph of $y$ component of velocity component does show evidence of stationarity around a mean value of zero. The evidence therefore is that some avalanches sweep clockwise (in plan view) whilst others sweep anti-clockwise, a phenomenon that has been observed in real, large industrial stockpiles.

One would perhaps expect simple correlations to exist between $z$ and $x$ components of velocity. In fact over a suitable 256 sample length series, the correlation between $x$ and $z$ components of velocity is $-0.09$ (i.e. negligible). However, if absolute values are taken then the correlation rises to $0.33$. Figure 6.5 clearly shows both positive and negative $z$ component of velocity and so there is some association between vertical velocity (whether up or down) and $x$ velocity (which is always to the right). If avalanching was straight down the sloping surface then one would expect a strong
correlation between $x$ and $z$ velocity components. The evidence here is that avalanching in 3D is rather more complex with the freedom to move in the $y$ direction decreasing the coupling between $x$ and $z$ velocity components. Both $x$ and $z$ velocity series were wavelet transformed and an investigation was made into correlations between wavelet transform coefficients. However the best correlation was 0.29 for wavelets at scale 3 and so in this case, the wavelet transform did not reveal any further information. The significant peak in $z$ mean velocity in figure 6.5 around time 75 requires some explanation as it indicates the contents of the cell moving quite rapidly upwards. Section 6.2.3 addresses this issue.

An interesting aspect of the graph in figure 6.5 is that $y$ velocity component is very oscillatory. Again, the correlation between $z$ velocity and $y$ velocity is negligible (0.07) and for absolute values it is only 0.17. However, wavelet transforms at scale 3 show a correlation of 0.38. The conclusion is that avalanche activity is to some extent associated with lateral velocity ($y$ velocity component) but on the basis of distinct changes as detected by the wavelet transform at scale 3.

The main conclusion from this short section is that all three cartesian components of velocity play a part in avalanching and that for a real heap avalanching is likely to be very much a three dimensional phenomenon.

6.2.3 Stress components during avalanching

Investigations associated with stresses are again focussed on the selected test cell represented in figure 6.1. The usual subscript notation for components of stress is adopted where, for example, $\sigma_{xz}$ refers to stress in a plane normal to the $z$ direction but acting in the $x$ direction. Figure 6.6 shows a graph of the three normal components of the stress tensor over the same time interval as figure 6.5.
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Figure 6.6. Components of compressive stress, $\sigma_{xx}$, $\sigma_{yy}$ and $\sigma_{zz}$ for the test cell plotted against time.

The extreme perturbations at around time = 76 are associated with a z component of velocity (in figure 6.5) which is negative (upwards) and as discussed previously is associated with an avalanche that whilst moving radially outwards, forces the local particles upwards. Under such circumstances one would expect high compressive stresses, especially $\sigma_{xx}$ which is indeed the case. However, the general trend of compressive stresses is gradually to increase. This phenomenon was demonstrated in the 2D case (section 5.2.5.4) where increases in stress followed by a relaxation were shown to occur around the time of an avalanche. As in the two dimensional case, the test cell becomes buried as the simulation proceeds and there is a consequent overall increase in compressive stress though this is less clearly demonstrated due to the relatively smaller scale of the 3D simulation.
Applications of the 3D toolset

Figure 6.7. Components of shear stress, $\sigma_{zx}$ and $\sigma_{zy}$, for the test cell plotted against time.

Figure 6.7 shows a graph of two components of shear stress, $\sigma_{zx}$ and $\sigma_{zy}$. $\sigma_{zy}$ shows evidence of stationarity as one would expect as the main direction of flow is in the $x$ direction. However, there are at least two significant peaks associated with strain in the $y$ direction. Average shear stress $\sigma_{zx}$ shows signs of slightly increasing (on average) over time which is similar to the two dimensional case (sections 5.3.6.4, figures 5.31, 5.32). There are clearly significant peaks in the stress graph and so as in the 2D case, an attempt was made to investigate the association of stresses with components of velocity.

6.2.4 Stress coupling with velocity components

For the cross-sectional slice under investigation, $x$ velocity component has been shown to be the best measure of avalanche activity. The correlation between $x$ velocity component and $\sigma_{zx}$ over a suitable 256 sample length section of the series was found to be negative (-0.28). One would expect this, since presumably normal stresses build before an avalanche and relax during the avalanche. This was shown to be the case for
2D simulations (section 5.3.6.4). However, the nature of the build-up and relaxation of normal stresses is more clearly shown by looking at the wavelet transforms of stress components and velocity. The same 256 sample sections of the time series were submitted to the Deslauriers-Dubuc 2,2 wavelet transform as was used for the 2D simulations. Little is revealed from the wavelets at scales 1 and 2. However, at scale 3 a significant correlation is found. Table 6.1 shows the correlation at different lags between absolute wavelet coefficients for normal stress $\sigma_{nx}$ and $x$ component of velocity (representing avalanching). In this case a lag of +1 means that the $x$ velocity wavelet coefficient is being correlated with the stress wavelet coefficient one sampling time earlier.

<table>
<thead>
<tr>
<th>lag</th>
<th>correlation</th>
</tr>
</thead>
<tbody>
<tr>
<td>-3</td>
<td>0.37</td>
</tr>
<tr>
<td>-2</td>
<td>0.14</td>
</tr>
<tr>
<td>-1</td>
<td>0.01</td>
</tr>
<tr>
<td>unlagged</td>
<td>0.24</td>
</tr>
<tr>
<td>1</td>
<td>0.51</td>
</tr>
<tr>
<td>2</td>
<td>0.01</td>
</tr>
</tbody>
</table>

*Table 6.1. Lagged correlations between scale 3 wavelet coefficients of $x$ velocity component and normal stress, $\sigma_{nx}$*

The largest value of 0.51 at lag 1 would appear to indicate that there is some association in disturbances in the two series as detected by wavelets at scale 3 but such that disturbances in the normal stress series precede those in the $x$ velocity series. This relates to a time constant of the order of 8 sampling time units which converts to approximately 0.05 seconds for 1mm diameter small particles. There is also a correlation of 0.37 at lag -3 indicating a relationship (though less strong) between avalanche activity and a later build up of compressive stresses. The time constant here is the same as that found in the 2D case, i.e. of the order of 0.16 seconds for a small particle diameter of 1mm. In the context of compressive stress build-up after an avalanche, there is therefore supporting evidence in 3D for the conclusions reached in 2D (section 5.2.5.4). Inferring results from 2D simulations to real 3D processes
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requires some caution. Evidence has been provided here that some results do translate into 3D, but that other mechanisms can be at play for the 3D case.

However, returning to the 0.51 correlation (at lag 1) indicating a relationship between fluctuations in compressive stresses and later avalanche event, some explanation is required as this might appear to be contradictory to the results from 2D simulations for which there was no evidence of such an association. For the three dimensional case, given the ability of particles to move more freely, there is perhaps a greater propensity for abrupt changes in compressive stresses at the initiation of an avalanche whereas in the 2D case the release is perhaps constrained to be more gradual.

As mentioned previously, one must take care in interpreting correlations between wavelet coefficients. Figure 6.8 shows the $x$ velocity transform coefficients (multiplied by 100 to be on a similar scale to those of the stress transform) along with $\sigma_{xx}$ transform coefficients shifted (one scale 3 sampling point before) giving rise to the 0.51 correlation in table 6.1. The significant contributions to the correlation coefficient come from points in the series where peaks correspond. Clearly this happens at two or three main points in the series. However, there are times when one series is peaking and the other is not.
6.2.5 Investigation of the avalanching surface

In the previous sections, the Eulerian analyses were based upon a cross-sectional slice through the heap. Attention now moves to consider the whole avalanching surface. Using the 3D display component of the toolset, a visual analysis of avalanche activity at different points in time was performed by applying suitable filters. The distance from the “notional” surface is recorded on the database for each particle at all sampling times. A filter was applied to restrict the display to particles that were less than two small particle diameters from the surface, thus certainly restricting considerations to particles within the boundary layer. With no further filter applied, the particles were coloured blue. Three further filters were successively applied for radial particle velocity greater than 0.1, 0.2 and 0.3 (small particle diameters per time unit) respectively. The colours applied were respectively green, yellow and red; i.e. the
particles with greatest radial velocity (>0.3) are coloured red, those particles above 0.2 but less than or equal to 0.3 are coloured yellow and so on. Localised avalanching is clearly shown to take place with a number (perhaps six or so) avalanches taking place at any one time. Figure 6.9 is the display for (absolute) sampling time 420 which is towards the end of the simulation. Absolute sampling time starts before a heap has started to form. As one would expect, there is a region in the centre of faster moving particles as this where the feed stream impacts. However, as mentioned, there is evidence of localised avalanche activity in perhaps 6 or so locations. It is emphasised that figure 6.9 shows all particles whose centres are within two small particle diameters of the notional surface. Apparent void spaces towards the centre are a consequence of the algorithm used to determine the notional surface. Views such as these are intended to show spatial velocity distributions only.

Figure 6.9. Colour coded plan display of the boundary layer (at absolute sampling time 420, towards the end of the simulation) showing radial particle velocity; colour coding is red> yellow> green> blue.
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An alternative view of avalanching is provided by a cross-section display which is an option within the same display utility of the 3D toolset. Figure 6.10 is a vertical cross-section through the heap shown in plan view in figure 6.9. In this figure, the depth of the central active region is clearly shown, but also some discrete avalanching. The colour coding is the same as for figure 6.9.

![Figure 6.10. Colour coded cross-section showing radial particle velocity at absolute sampling time 420; colour coding is red > yellow > green > blue.](image)

The situation a little later at absolute sampling time 425 shown in figure 6.11 is a little different. There is some activity in regions that were active at time 420, but also some activity in different places. This accords with the evidence presented previously that avalanching in 3D is more frequent and of shorter duration.
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Figure 6.11. Colour coded plan display of the boundary layer at absolute sampling time 425 showing radial particle velocity, colour coding is red> yellow> green> blue.

Similar displays to figure 6.11 at later times also revealed local discrete avalanching but in different places.

6.2.6 Application of the two dimensional wavelet transform in region identification

Avalanching is clearly the mechanism by which the heap evolves. The one dimensional wavelet transform has been shown to be capable of coupling discrete disturbances in time series derived from an individual test cell. However, figures 6.9 and 6.11 show that at any one time, a number of avalanches may be taking place and so the ideal analysis would involve all surface cells and over all sampling times. Further refinements would ideally involve restricting considerations to avalanching regions which themselves would need to be identified. The size of the 3D simulations severely restricts the capacity for revealing the potential of the two dimensional
wavelet transform in this respect. However, the analyses described below do point to the usefulness of the 2D transform for larger data sets.

The analyses that follow apply to the surface boundary layer at a time later on in the simulation. The two dimensional wavelet transform requires that a square matrix of numbers is submitted to the transform and of course the boundary layer particles are not spaced equally over a co-ordinate plane (as shown in figures 6.9 and 6.11). To facilitate the application of a two dimensional wavelet transform, a 32 by 32 grid cell system was applied to the surface. The square cells were of side 2 small particle diameters and the mean radial velocity of particles within these cells but in the boundary layer (2 small particle diameters deep) was calculated. The matrix of numbers therefore represented the mean radial velocity in square cells across the surface. The 32 by 32 matrix is represented by grey scaling in figure 6.12 where lighter colours represent greater radial velocity. This was done since a suitable representation of two dimensional wavelet transform coefficients is by such a grey scaling. The centre of the figure has faster moving particles as was shown in figures 6.9 and 6.11. However, there are clearly regions of avalanching visible where there are localised bright squares.
A two dimensional wavelet transform was applied to the grid average radial velocities represented in figure 6.12 and grey scale images of the transform coefficients are shown in figures below. It must be remembered that the two dimensional wavelet transform performs a decomposition in terms of horizontal, vertical and diagonal detail and that any one or a combination of these might identify disturbances that relate to avalanches. The scale 1 wavelet transform coefficient for the two dimensional transform are represented in figures 6.13, 6.14 and 6.15. A 32 by 32 matrix submitted to a two dimensional transform results in 16 by 16 arrays of transform coefficients. This is clearly small bearing in mind that the one dimensional transforms were applied to series of length 256 or more. Scale 2 wavelet coefficients in this case would be represented in 8 by 8 matrices which would be very unlikely to be revealing. However, there is evidence that a small number of scale 1 coefficients are located in positions which represent edges in the radial velocity representation of figure 6.12. An example
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is figure 6.13 (diagonal detail) where 3 centrally placed light squares would seem to surround the central faster moving region in the centre of the heap. The lighter squares in figures 6.14 and 6.15 can also be related to avalanching regions of figure 6.12. It is emphasised that the horizontal, vertical and diagonal decomposition performed by the 2D wavelet transform) essentially relates to "edge detail". Edges in this context refer to perturbations in radial velocity over 2D space. It is important to recognise that, compared to the application of the one dimensional transform, this is no longer a time base analysis but a 2D spatial analysis.

*Figure 6.13. Grey scale representation of diagonal detail wavelet transform coefficients at scale 1. The lighter colours represent greater values.*
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Figure 6.14. Grey scale representation of horizontal detail wavelet transform coefficients at scale 1. The lighter colours represent greater values.

Figure 6.15. Grey scale representation of vertical detail wavelet transform coefficients at scale 1. The lighter colours represent greater values.
6.2.7 Radial and angular velocity coupling using two dimensional wavelet transform.

In the analysis of section 5.2.3.7 for the two dimensional low impact feed heap, the one dimensional wavelet transform was shown to be a useful tool in coupling rotational and translational velocity in the context of discrete avalanching. As mentioned above, some progress can be made in coupling variables for the three dimensional simulation by correlating (one dimensional) wavelet transforms of time series, in particular with regard to the examination of the (Eulerian) experience of a selected test cell. However, it would be advantageous to be able to perform a correlation analysis that is essentially two dimensional, for example by looking at the experience of a set of adjacent cells (one dimension) over time (the other dimension). The alternative of course is to apply the analysis to a two dimensional surface. The two dimensional wavelet transform may have application in this circumstance and what follows demonstrates the potential usefulness of correlation studies on two dimensional wavelet transforms.

In the same was as mean cell values for radial velocity were calculated (section 6.2.6) and represented by grey scaling in figure 6.12, figure 6.16 below represents mean rotational cell velocities in a similar fashion.
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The most significant feature of figure 6.16 is that larger values of rotational velocity are not apparent until some distance from the centre of the heap. This is in sharp contrast to figure 6.12 for radial velocity where the greater mean velocities are towards the centre. The particles must enter the heap with very small angular velocities and it is only when particles have progressed some distance from the centre that rotation begins to play a significant part. Looking at the regions of high angular velocity (white squares), it would appear visually that there is some correspondence with radial velocity in terms of avalanching away from the centre of the heap. An obvious starting point would be to calculate the correlation coefficient between radial and angular velocity. However, restricting the calculation to cells that actually contain particles, the product moment correlation coefficient (using equation 4.12) is \(-0.27\). On face value this might be interpreted as implying that rotational activity occurs more in slower moving (non-avalanching) regions. However, the reason is that the high values of radial velocity towards the centre of the heap correspond to near zero values of angular velocity, thus leading to a negative correlation. In an attempt to focus in on

Figure 6.16. Grey scale representation of boundary layer rotational velocity where lighter colours represent greater rotational velocity.
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avalanche activity and its association with angular velocity, both arrays (of radial and rotational velocity) were submitted to a two dimensional wavelet transform and the transform coefficients correlated.

Figure 6.17 below shows wavelet transform coefficients for diagonal detail at scale 1 for the transform of rotational velocity.

![Wavelet Transform Coefficients](image)

*Figure 6.17. Grey scale representation of diagonal detail wavelet transform coefficients (for rotational velocity) at scale 1. The lighter colours represent greater values.*

The location of the larger coefficients does not seem to correspond well with radial velocity or the wavelet transform thereof. Indeed, the correlation between wavelet coefficients at scale 1 is 0.01 (i.e. completely insignificant). It appears that in this case diagonal detail is not helpful in coupling radial and rotational velocity. However, moving to horizontal detail transform coefficients, the situation is a little different. Figure 6.18 shows level 1 horizontal detail coefficients for the wavelet transform of rotational velocity.
Figure 6.18. Grey scale representation of horizontal detail wavelet transform coefficients (for rotational velocity) at scale 1. The lighter colours represent greater values.

Whilst not necessarily in terms of the brightest colours, there is perhaps visually more evidence of an association with horizontal detail for the radial velocity transform. Indeed, in this case, the correlation coefficient over a rectangular region defined by the curved boundary of the heap gives a value of 0.39. Given that the boundary of the heap is curved, some check must be made into the contribution of corresponding zeros in the two arrays being correlated. In fact, with all such pairs removed from the calculation, the correlation is still 0.32 over a sample size of 142. This value is significant. (The critical 5% one tailed value for 40 pairs is 0.30). Whilst in an ideal world one would like to see higher values of correlation coefficients, the two dimensional wavelet transform is still shown to be capable of coupling variables in the context of the disturbances found in two dimensional data.
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With regard to vertical detail, an equivalent correlation coefficient was calculated. The correlation coefficient was 0.21. Though small, this value is significant (at the 5% level) for the sample size and indicates some (though slight) coupling of the wavelet coefficients at scale 1.

6.2.8 Summary of section 6.2

Discrete avalanching has been shown to take place during simulated 3D heap formation. However, the avalanching is rather more frequent and of shorter duration than was found for the 2D case. The one dimensional wavelet transform has been shown to be capable of coupling disturbances in avalanche velocity with normal stress and showing agreement with the equivalent analysis performed on 2D simulations. The 3D filtered display capability has been shown to be helpful in demonstrating the frequent and discrete avalanches that take place in 3D and in showing the depth of activity with the cross-sectional display utility. The two dimensional wavelet transform has been applied to two dimensional grid cell averaged data and whilst it must be stressed that the arrays being transformed are very small, the two dimensional transform is shown to be capable of extending the capacity of the toolset in terms of coupling discrete disturbances in process variables. However, the fact that the transform partitions into horizontal, vertical and diagonal detail makes for a rather more difficult interpretation than is the case for the one dimensional transform. It is emphasised that the two dimensional transform in this case performed a spatial as opposed to a time based decomposition.
6.3 Diffusion phenomena during hopper discharge

The investigation of the flow field within a discharging hopper is clearly extremely difficult. Cleaver and Nedderman (1993) describe experiments involving tracer particles introduced amongst the feed before discharge. However there were implicit assumptions necessary regarding the radial flow of particles. Nikitidis et al (1998) conducted non-invasive probing of the discharge of a binary mixture using gamma-ray tomography where large particles were found to migrate across a presumed velocity gradient within the conical section. In this section, a 3D investigation by simulation into self-diffusion activity was performed partly in order to attempt to confirm the results of Nikitidis et al, but also to confirm and extend the 2D results of section 5.2.3.6 relating to self-diffusion.

6.3.1. Computational details for 3D hopper discharge

The simulation involved the discharge of a binary mixture of 10,000 particles with a size ratio of 2:1 with 5% of large particles by number. The hopper was cylindrical with a conical discharge section. The arrangement is shown as a schematic (not to scale) in figure 6.19. The cylindrical diameter was 20 small particle diameters and the half angle of the conical section was 20 degrees narrowing to a discharge orifice of 8 small particle diameters. The co-ordinate system for the simulation used a z axis as the vertical line of symmetry through the hopper. The x and y axes formed a plane 30 small particle diameters below the hopper orifice. In figure 6.19, the y axis is pointing out of the paper. A cross sectional slice of width 3 small particle diameters centred on a diameter of the hopper was selected for investigation by restricting attention to y co-ordinates between -1.5 and +1.5. Due to axial symmetry, any results should be generally applicable. Initial particle positions within the hopper were randomised and the fill was allowed sufficient time to settle before the bottom orifice was opened to initiate flow. The CI model for particle interactions was the same as for the 3D heap investigations of section 6.2 and described in appendix A1.
For the purposes of investigating diffusion, a transformation by rotation (using the transformation matrix of section 4.3.1) was performed in the $x_z$ plane so that the new (transformed) $z$ direction was parallel to the left-hand hopper wall (in the cross-section of investigation). Thus the transformed $x$ velocity component becomes a diffusional component across a presumed main direction of flow (at least near the wall). The main focus of investigation was a test cell near the hopper wall (bounded in red in figure 6.19) and of size $2 \times 5$ (in the rotated $x$ and $z$ directions) and 3 deep. (Units are small particle diameters.) With regard to the investigation of diffusion, a mean flow direction must be identified. Obviously at the hopper wall, flow must be parallel to the wall and so for the initial investigations this was taken as the reference mean flow direction, though clearly, in this small scale simulation the direction of flow can change significantly over short distances.

![Test cell bounded red. Inner & outer cells bounded black.](image)

*Figure 6.19. The feed hopper showing the test cell, inner and outer cells and rotated co-ordinate axes (not to scale).*
6.3.2 Results and discussion

6.3.2.1 The presence of a velocity gradient

Segregation by self-diffusion requires the presence of a velocity gradient. The mean flow in the transformed $z$ direction was calculated over a $3 \times 3$ (small particle diameter) grid system within the cross-section selected for study. Figure 6.22 represents these local mean components of velocity by means of grey scaling (of circles) at a suitable point in time during steady state flow after the initial transient period. The lighter the shade of grey, the higher is the mean component of velocity in the cubic cell. It is emphasised that the component of flow velocity represented in figure 6.22 is that parallel to the left hand hopper wall within the cross section of study and so only the left hand side of this diagram should be considered — and in fact towards the centre of the hopper the mean flow would be expected to be vertically downwards. The position of the test cell is approximately indicated in figures 6.19 and 6.22. Clearly (figure 6.22) the cell is shown to be in the presence of a velocity gradient at this time (i.e. lighter colours away from the wall). The same was found to be the case at other test times. However, to be sure that the velocity gradient is sustained, a further investigation involved calculating the mean flow component of velocity in two further test cells, centred 1 unit nearer the wall and 1 unit nearer the centre, i.e. sitting on the test cell edges. These two cells are indicated in figure 6.19 and are bounded in black. Figure 6.21 graphs the mean component of velocity parallel to the hopper wall for these two extra test cells. The difference between the two plots therefore represent the velocity gradient across the primary test cell. The early part of the graph shows the initial transient phase before steady state flow is established. Thereafter a velocity gradient is clearly present to provide the driving force for diffusion of large particles towards the centre which is later shown to be the case.
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Figure 6.20. Cell mean component of velocity perpendicular to the conical wall against time for large and small particles.

Figure 6.21. Cell mean component of velocity parallel to the conical wall against time for outer test cell (near wall) and inner test cell (towards centre).
Figure 6.21 also demonstrates that the flow velocity (as measured by the component parallel to the hopper wall) is quite oscillatory and in fact the two graphs do not necessarily show local maxima and minima at the same time. One would perhaps expect very strong correlation between the two series. However, the correlation (discarding the initial transient period) is 0.39 which though significant indicates that surges in neighbouring regions are not necessarily occurring at the same time. It would be interesting to investigate the frequency of the apparent surging. Figure 6.23 gives the power spectrum (calculated using equations 4.10 and 4.11) for the “inner cell” series of figure 6.21. The range over which dominant frequencies exist is approximately 0 to 0.7. Clearly, the lower significant frequencies relate to the evident surging activity. The fact that there are clearly a number of constituent frequencies might appear not to be particularly informative. However, diffusional motion across the velocity gradient is investigated later when the power spectrum is found to be in agreement with that associated with surging.
6.3.2.2 Diffusion across a presumed flow direction

Returning to consider diffusion across the main direction of flow, it is emphasised that the flow direction (in the transformed co-ordinate system) is specified as being parallel to the left-hand hopper wall (conical section). Even with a simulation of 10,000 particles, in 3 dimensions only quite small geometries are possible and within the conical section of the hopper, flow directions will change considerably over relatively small distances. For example, at the approximate height of the test cell, moving from the wall to the centre is only about 7 small particle diameters and one would expect the mean flow direction to change by 20 degrees. The relatively small diffusional components of velocity against a presumed direction are therefore likely to be masked by contributions from the mean flow if it is not exactly in the prescribed direction and some further explanation is required in order to interpret results.

Figure 6.20 shows time series of mean $x$ component of velocity in the test cell for both particle species – i.e. the component of diffusional velocity across a presumed

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*Figure 6.23. Power spectrum for bulk surging in the conical section of the hopper (inner test cell)*
direction of flow (assumed parallel to the wall). The two series both have a mean value which is negative for the reason described above, i.e. the mean flow is not actually parallel to the hopper wall and has a significant component against the presumed diffusional flow direction. The mean component of velocity across the presumed flow direction is -0.040 for large particles and -0.052 for small particles. The mean value for large particles is found to be statistically significantly larger than for small particles using a conventional t test. The interpretation of this result is that diffusion across the velocity gradient for large particles is responsible for the difference. However, this is supported by a visual inspection where for large particles the graph of figure 6.20 is above that for small particles for most of the time and in fact significant sections of positive diffusional velocity are predominantly for the large particles. The section of the graph for large particles which follows the time axis (between times 20 and 30 approximately) is when there are no large particles in the cell.

Summarising the results of this section, Figure 6.21 shows that over the duration of the simulation, there is a flow velocity gradient across the test cell. Within the test cell the diffusional components of velocity (across the presumed flow direction) are found to be significantly different for large and small particles. The difference in the mean values is due to a greater tendency of large particles to migrate across the velocity gradient (towards the greater flow velocity). The velocity gradient is present to provide the driving force for diffusion of large particles towards the centre of the hopper.

6.3.2.3 Diffusion across a local flow (velocity) gradient

The evidence for diffusion in the above section is sound. However, because of the small size of the hopper and the (quite significant) changes in radial flow direction in adjacent cells, the evidence is somewhat “disguised”. The simulation was re-run, but this time with a calculation of the mean components of velocity in the test cell for all particles and for large and small particles separately. Thus the instantaneous mean fluctuating (diffusional) components of velocity of both large and small particles
Applications of the 3D toolset

perpendicular to the instantaneous mean flow can also be calculated. It is emphasised here that a flow direction is determined at each sampling time, not presumed as in section 6.3.2.2. The large number of time samples allow the calculation of a paired t test to determine whether large particles have a greater tendency to migrate across the velocity gradient. Over the period of flow, the mean velocity gradient (derived from the two series of figure 6.21) is of the order of 0.05. The test is significant and the details are given below.

Large particles: mean diffusional velocity = 0.0556
Standard deviation = 0.0498

Small particles: mean diffusional velocity = -0.0000767
Standard deviation = 0.0028

Null hypothesis: No difference in diffusional velocity
Alternative hypothesis Large particles have greater diffusional velocity
Paired t test
Sample size 474
Test statistic = 2.34
Significance of test statistic 0.01 (i.e. 99%)

The standard deviations here are high. However, statistically, large particles have a mean diffusional velocity across the local mean flow (and towards the hopper centre) which is larger than that for small particles. Clearly, if large particles are on average diffusing in one direction, then small particles must on average be migrating the other way. We have many more small particles in this simulation and so in terms of absolute values, the mean diffusional velocity will be much less.

Bringing together the results of this section and section 6.3.2.2, however a local flow direction is defined, there is statistically significant evidence of large particle species diffusing across a velocity gradient and towards the centre of the hopper. The results from this 3D hopper flow simulation therefore support the conclusions reached by Nikitidis et al (1998) derived from tomographic experiments.
6.3.2.4 The fluctuating velocity autocorrelation function and self diffusion coefficients

In section 5.2.3.6, segregation by self-diffusion in 2D avalanching heaps was investigated where the mechanisms other than kinetic sieving were shown not to be contributory. The analysis involved an attempt to derive self-diffusion coefficients by way of an integral of the fluctuating velocity autocorrelation function. It was found that the function did not decay sufficiently rapidly for the integral to be reliably determined because of the short time duration of avalanches in the 2D simulation.

The calculation of self-diffusion coefficients here in the context of hopper discharge would certainly complement the results that have been demonstrated thus far. Restricting the investigation to the test cell (which is known to have a maintained flow velocity gradient) the focus is on those particles which have a long residence time in the test cell. The data was held in a relational database and it was a relatively easy task to derive a table of particle residence times within the test cell. From this table it was possible to select suitable particles for an autocorrelation study.

To ensure greater precision, the Lagrangian approach (following individual particles) really requires that the local mean velocity components are calculated over a suitable sized region that follows the particle in its travel. In fact, the local mean components of velocity were calculated over neighbouring particles within 3 small particle diameters of that particle. In this case, the fluctuating component of velocity towards the centre of the hopper was output as a time series for selected particles. The fluctuating velocity autocorrelation function was then calculated with the intention of deriving the self diffusion coefficient as a numerical integral of this function (equation 4.8). However, the autocorrelation functions for most particles were found not to decay to zero sufficiently quickly to allow calculation of the integral. For a selected large particle, figure 6.24 plots the fluctuating velocity, and figure 6.25 plots the (normalised) autocorrelation function.
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Figure 6.24. Fluctuating component of velocity towards the hopper centre for a selected large particle.

Figure 6.25. The normalised fluctuating velocity autocorrelation function (derived from figure 6.24).
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Clearly the autocorrelation function of figure 6.25 has not settled to zero within the time of residence within the test cell. However, the function is highly oscillatory itself, as indeed is the original fluctuating velocity series itself. Other velocity traces for other particles gave evidence of periodicity though some did not. It would be illustrative in this instance to derive the power spectrum (as the Fourier transform of the autocovariance function using equations 4.10, 4.11) for periodicity of fluctuating velocity for this particular particle. The power spectrum is shown in figure 6.26.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{power_spectrum.png}
\caption{Power spectrum of fluctuating component of velocity for a selected large particle.}
\end{figure}

There are 4 significant peaks at frequencies of approximately 0.004, 0.013, 0.028 and 0.04 with the last significant peak at a frequency of about 0.75. If a comparison is made with figure 6.23, the spectrum for surging within the conical section of the hopper evidenced in figure 6.21, it is found that dominant frequencies are in a very similar range – and in fact some are very close. The unfortunate circumstance that the fluctuating velocity autocorrelation functions do not decay due to the inherent periodicity has been discussed. However, there is now some degree of explanation as to why this is so. The periodic braking and accelerating in the bulk flow will clearly
provide an opportunity for a change in the nature of the diffusional flow. The large standard deviations in fluctuating component of velocity is now explained in terms of an inherent periodicity whereby the direction of diffusion changes. However, on average, diffusion of large particles is preferentially towards the centre of the hopper as proved by t-tests on mean fluctuating velocities.

It is unfortunate that the autocorrelation functions that we have derived do not decay sufficiently to allow the determination of self diffusion coefficients. Figure 6.27 shows the fluctuating velocity component for another selected large particle.

![Fluctuating velocity component for a second selected large particle.](image)

Again, the autocorrelation function fails to decay to zero sufficiently quickly. In this particular circumstance a justification can be clearly given. Two regions of the graph (labelled A and B) have a similar slope. When these short sections are involved in the autocorrelation calculation (in this case with a lag of about 11) their product contribution will be very significant (the two lagged sections are very highly correlated). So, in the presence of pronounced periodicity, we are unable to use the
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autocorrelation method of deriving self-diffusion coefficients. However, it is emphasised that different particles have different experiences.

6.3.3 Summary of section 6.3

Summarising, the results of this section, there appears to be inherent periodicity within various different velocity components within the conical section of the hopper. The bulk flow shows clear evidence of periodicity at a limited number of distinct frequencies. Interestingly, the periodicity of diffusional particle velocity is in the same frequency range. Diffusion across a velocity gradient has been shown to take place by the application of some simple statistical tests, thus confirming the results found in 2D simulations of heap formation but also confirming the experimental results of Nikitidis et al (1998) at the mid-plane of an axially symmetric hopper. Unfortunately, self-diffusion coefficients could not be calculated from the results of the simulation studies due to the inherent periodicity of fluctuating components of velocity.
CHAPTER 7. CONCLUSIONS AND OPPORTUNITIES FOR FURTHER WORK

7.1 Principal results and conclusions

Before the work done in order to complete this thesis, most conclusions drawn from the results of granular dynamics simulations have been on the basis of visual observation of static displays. Little has been done by way of investigating the temporal nature of granular assemblies and in coupling important variables especially in the context of discrete events.

Whilst essentially static in nature, in conjunction with the time series techniques developed, the filtered visual display capability in both 2D and 3D has been shown to be useful in investigating boundary layer flow in avalanching heaps. In particular, the nature of the velocity gradient in 2D for a low impact feed stream was shown to be sufficiently well defined to support segregation by self-diffusion of particle species. In addition, particle trajectories were supportive of the conclusion that for a high impact feed heap, bowling in the central region was associated with lateral surging that seemed to enforce mixing of particle species. In 3D, the discrete (but frequent) nature of avalanching was demonstrated using the filtered display capability and some insight was given into the velocity profile in a cross-section through the heap which showed some evidence of a velocity gradient during discrete avalanching, but also revealed the dissipative nature of avalanching in 3D.

The essentially time series based analyses have been particularly revealing in terms of the dynamics of granular flow in the context of the discrete events which govern the evolution of granular assemblies. Self-diffusion of particle species has been shown to take place in 2D low impact feed heaps where, furthermore, a mechanism by which segregation takes place has been suggested. Larger particle species were found to be more likely to remain in the avalanching boundary layer and so find their way to the bottom of the heap. This mechanism was shown to favour the migration of large
particles towards the bottom of the heap despite their lower average lateral velocity. Without the detailed analyses performed here, surface rolling would have been presumed to be the prevailing mechanism. It is known that phenomena that manifest themselves in 2D are often attenuated in 3D. However, evidence of segregation by diffusion in the presence of a velocity gradient was found in the conical section of a hopper for the 3D case. This result also supports the conclusions reached experimentally by others using tomographic techniques. The calculation of self-diffusion coefficients requires the integration of the fluctuating velocity autocorrelation function. However, for both 2D heaps and 3D hopper flow, the VACF did not decay sufficiently to perform the interval. However, flow during discharge from the 3D hopper was shown to be characterised by periodic surging and spectral analysis revealed that the periodicity of this surging was in a similar range to that for the fluctuating velocity.

Spectral analysis applied to the time series for a high impact feed stream in the 2D case has revealed a regular periodicity of lateral surging associated with a cratering at the point of impact of the feed stream. This behaviour was found to abruptly shut off as the impact velocity is reduced, providing evidence of at least two distinct flow regimes.

In terms of the discrete nature of the events which characterise granular flow, in particular for heaps, the one dimensional discrete wavelet transform has been shown to be capable of identifying the time location and scale of events such as avalanching. However, in addition, coupling of process variables by correlation of wavelet coefficients has been shown to be a useful aspect of wavelet analysis. The extension of this concept to correlation of lagged wavelet coefficients has pointed to a method of determining time constants in the context of irregular discrete events. Within the size constraints on the geometry imposed by 3D simulations, the potential for the two dimensional wavelet transform to be applied in a similar fashion to the analysis of surface data such as boundary layer mean velocity components has been demonstrated.
Conclusions and opportunities for further work

In summary, the development of a toolset for the focussed probing of large time dependent data sets such as those resulting from granular dynamics simulations has been shown to be helpful in unravelling the underlying physics.

7.2 Potential for future research

This thesis has focussed largely on heap formation with some investigation of hopper flow. The nature of heap formation is such that many different phenomena (e.g. avalanching, cratering, flow against a fixed base) can be present within the unconstrained geometry. In many ways this diversity allows the researcher freedom to investigate in a variety of areas (e.g. diffusion, stress evolution, avalanche investigation, moving boundaries). However, the transient nature of the defining events involved brings difficulties in analysis. For example, diffusion has been shown to contribute to segregation effects but the relatively short duration of avalanche events means that there is insufficient time to allow the integration of a velocity autocorrelation function and hence obtain diffusion coefficients. Also, the moving heap (surface) boundary makes for difficulties in terms of Eulerian analyses. In terms of finally tying down these analyses, there is the potential to focus the work more precisely on some of these aspects. For example if a simulation can be devised that maintains a velocity gradient (such as those investigated here) for sustained periods then an appropriate diffusion coefficient could be calculated. Also, whilst significant, the coupling of process variables such as voidage, stress and velocity in the context of discrete events has been on the basis of correlations of the order of 0.4 or 0.5 meaning that for some avalanches the association is there, but for others it is not. Further studies which extend the time span of the analyses (presumably larger simulations) would be helpful here. Not all avalanches are the same, which would be a reason for the values of correlation coefficients obtained. In a longer time span investigation, there is a greater chance of finding repeat events and greater patterning.
Conclusions and opportunities for further work

The simulations studied were also for a fixed size ratio and fines proportion. There is scope here to investigate the diffusional properties of different binary mixtures (and indeed ternary and other mixtures) to extend the formalism. Whilst the simulations here have involved up to 10,000 particles, in terms of real industrial processes there is ultimately a question of scale in applying the results that have been clearly demonstrated. For example, the periodic surging evident in the high impact heap that seemed to enforce mixing might be a phenomenon restricted to small region close to the feed point. Up-scaling of the investigations to determine the likely impact on real processes is likely to be a fruitful area of new research.

Perhaps the most novel aspect of the work in this thesis is the application of the discrete wavelet transform (mainly the 1D transform, but some 2D applications). The wavelet transform is certainly capable of representing the “signature” (in terms of characteristic local frequencies) of defining events. In terms of a predictive capability (e.g. for avalanche events) there is the potential to take the work further and also to investigate other families of wavelets in this context. With regard to the 2D wavelet transform (as with other aspects of extending the work), it is ultimately a matter of performing larger simulations to allow the interpretation of larger grey scale images.

The post-simulation analysis toolkit presented here is equally applicable for the quantitative analysis of experimental data that might be generated by non-invasive techniques such as x-ray and gamma ray tomography. Such microstructural data sets of internal stress and flow fields are appropriate input data for the analyses presented in this dissertation. Powerful mathematical toolkits capable of distilling quantitative information on the underlying physics of granular systems is a much welcome addition to the arsenal of techniques available to research in this area.
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Appendices

Appendix A. The CI simulation model and reduced units

A1. Technical details of the CI simulation

The technical features of the Granular Dynamics (GD) simulation model used in the thesis are the same as those described by Baxter et al (1997). The potential energy between a particle pair is given by the short-range repulsive (SRP) analytic form, \( \phi(r) = \varepsilon (\sigma/r)^n \) where \( r \) is the centre-to-centre separation of the pair and \( \sigma \) (small particle diameter) and \( \varepsilon \) (potential energy at \( r=\sigma \)) respectively set the distance and energy scales of the interaction. The parameter, \( n \) is the characteristic particle index which describes the ‘hardness’ of the interaction. In these simulations, the pair potential is defined to give unit repulsive force at an inter-particle separation of \( r=\sigma \). Given definitions of the small particle diameter \( \sigma \), the interaction index \( n \) and the gravitational constant \( g \), the quantities mass, time, energy and force can be derived. Restricted rotation of the grains is included in the model by tangential or “frictional” forces, the upper limit of which is given by Amonton’s law of friction, \( \mu F_N \), where \( \mu \) is the Coulomb friction coefficient, and \( F_N \) is the normal force derived from the pair potential, \( \phi(r) \). It is more realistic to base these frictional ‘engagements’ on the history of the contact and not simply the current velocity, which would mean the sign of the tangential force would unrealistically reflect the current, rapidly varying, relative velocity of the grains. The frictional algorithm incorporates a memory of the past deformation history of each contact by accumulating a tangential displacement, which builds up over the duration of the contact as described by Baxter et al (1997).
Appendices

A2. Reduced units

The results from the simulations are given in terms of reduced units which can be converted to conventional units given values for \( n, \sigma, g \) and particle density \( \rho \). Table A1 below defines the quantities mass, time, energy and force in terms of these.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length</td>
<td>( \sigma )</td>
</tr>
<tr>
<td>Mass</td>
<td>( \pi \sigma^3 \rho/6 )</td>
</tr>
<tr>
<td>Time</td>
<td>( \sigma^{1/2} \rho^{-1/2} )</td>
</tr>
<tr>
<td>Energy</td>
<td>( \pi \sigma^4 \rho g/6n )</td>
</tr>
<tr>
<td>Force</td>
<td>( \pi \sigma^3 \rho g/6 )</td>
</tr>
</tbody>
</table>

Table A1: Mass, Time, Energy and Force in terms of defined units

Much of this thesis has concerned time series for which the reduced time unit is \( \sigma^{1/2} g^{1/2} \). For a particle of diameter 1mm, this means that 1 reduced time unit is equal to 0.0101 seconds.
Appendix B. Equations governing diffusion

The basic equations to be solved to yield a continuum description of granular flow are the mass conservation equation, the linear momentum conservation equation and the kinetic energy conservation equation. For a first order description, we have:

\[ \text{Flux} = \text{transport coefficient} \times \text{driving force} \quad \text{B1} \]

where the driving force is a local gradient of a thermodynamic variable. With regard to the investigation of segregation, the concern is with mass conservation. The conservation of mass equation is

\[ \frac{\partial n}{\partial t} + \nabla \cdot (nv) = 0 \quad \text{B2} \]

where \( n \) is the number density (i.e. concentration) and \( v \) is velocity.

Consider a mixture of grain sizes (species) in an assembly. Applying equation 2 for species \( i \) in a mixture, we have

\[ \frac{\partial n_i}{\partial t} + \nabla \cdot (n_i[v + v_i]) = 0 \quad \text{B3} \]

where \( n_i \) is the concentration of \( i \), \( v \) is the bulk velocity and \( v_i \) is the drift velocity of species \( i \). Of course, the sum of these equations applied to each species should equal the overall conservation equation (2). The drift velocity will be a function of contributing diffusional components. Assuming that these diffusional components are additive, then we have

\[ v_i = v_{Di} + v_{Si} + v_{Pi} \quad \text{B4} \]
where:
$v_{Di}$ is the drift velocity of $i$ due to classical diffusion, i.e. flow down a gradient of concentration of $i$.
$v_{Si}$ is the drift velocity of $i$ due to shear-induced segregation, i.e. the flow of particles across gradients of bulk velocity.
$v_{Pi}$ is the drift velocity of $i$ due to spontaneous percolation of fines in a mixture through the coarse phase.

The segregation fluxes are related to the drift velocities by

$$J_i = n_i v_i = n_i (v_{Di} + v_{Si} + v_{Pi}) = J_{Di} + J_{Si} + J_{Pi} \quad \text{(B5)}$$

Each flux is derived from the transport equation (1). The diffusive flux is a product of a characteristic diffusion coefficient ($D_i$) and a concentration gradient:

$$J_{Di} = -D_i \nabla n_i \quad \text{(B6)}$$

For shear-induced flux, it is suggested that the driving force is a gradient in bulk velocity and that the transport coefficient is a granular viscosity $\eta_i$ for species $i$ in the mixture. The resulting relationship (normalising the velocity gradient by dividing by $v$) is

$$J_{Si} = \eta_i \frac{\nabla v}{v} = \eta_i \nabla (\ln v) \quad \text{(B7)}$$
Appendices

Appendix C. Quadtree and Octtree Representation

Below is a 2D Black and white image in an 8 by 8 grid.

Splitting the figure into 4 (4 by 4) quadrants, the SE quadrant is a white leaf node and the SW quadrant is a black leaf node. The NE and NW quadrants are both split onto 4 (2 by 2) quadrants. The process is repeated until all leaf nodes have been reached. The quadtree for this figure is given below.

```
NE SE SW NW
(W) (B) (W) (W)
```

```plaintext
B W W B B W W B
```
Three dimensional black and white images can be similarly represented by octtree, where a cube is divided into 8 sub-cubes, which are further sub-divided until all leaf nodes have been found.

Quadtree and octtree representation allow a reduction in the amount of storage required for an image. More importantly in this report they allow the location by size of binary regions of uniformity. Computer representation of tree structures is via pointers, although they can be implemented in conventional array structures.
Appendices

Appendix D. Routines for calculating Autocorrelations and Spectral Densities

These routines were implemented in Borland Delphi ©, but are presented here in pseudocode form in order to allow implementation in other platforms. Variable frequency numerator specifies the number of frequencies analysed. Variable frequency division defines the smallest frequency analysed.

****** calculate mean and variance
max_ctr=ctr
tot=0
sqtot=0
for i=1 to max_ctr
    tot=tot+x[i]
    sqtot=sqtot+x[i]*x[i]
next
mean=tot/max_ctr
autocorr_denom=sqtot-max_ctr*mean*mean

****** calculate autocovariances in autocov[]
for lag=0 to max_ctr
    runtot=0
    for t=1 to (max_ctr-lag)
        runtot=runtot+(x[t]-mean)*(x[t+lag]-mean)
    next
    if lag=0
        autocov0=runtot/max_ctr
    else
        autocov[lag]=runtot/max_ctr
    endif
next

****** calculate spectral densities
for i=1 to freq_numerator
    freq=i/freq_division
    runtot=0
    for k=1 to freq_numerator - 1 do
        runtot=runtot+autocov[k]*cos(2*pi*k*freq)
    next
    spectrum[i]=(1/(2*pi))*(autocov0+2*runtot)
Appendices

Appendix E. The C++ class for the one-dimensional wavelet transform

The class itself is as below in C++ code. However, the public routines are described below this in generalised pseudo-code so that implementation in another platform could be more easily done. Within the class, the filters are currently hard coded.

E1. The one dimensional wavelet transform class

class wavelet_transform
{
private:
    int l;
    float*transform,*reconstruct,*signal,*sampled,*upsampled;
    float *scalefacts,*newscalefacts,*wavelets,*newwavelets,*tempscalefacts;
    float *lowfilt,*highfilt,*lowsynthfilt,*highsynthfilt;
    int ctr,i,n,power,sampsize,highoffset,lowoffset,lowfiltno;
    int highfiltno,pos,increm;

public:
    wavelet_transform(float arrinl[],int lin)
    {
        l=lin;
        signal = new float[l+1];
        for (int i=0;i<=l;i++) signal[i]=arrin1[i];
        transform = new float[l+1];
        reconstruct = new float[l+1];
        sampled = new float[l+1];
        upsampled = new float[l+1];
        scalefacts = new float[3*l+1];
        newscalefacts = new float[3*l+1];
        wavelets = new float[3*l+1];
        newwavelets = new float[3*l+1];
        tempscalefacts = new float[3*l+1];
        float low [] = {0,-0.125,0.25,0.75,0.25,-0.125};
        float high [] = {0,0.25,-0.5,0.25};
        float lowsynth [] = {0,0.5,1.0,0.5};
        float highsynth [] = {0,0.25,0.5,-1.5,0.5,0.25};
        lowfilt=new float[6];
        highfilt=new float[4];
        lowsynthfilt=new float[4];
        highsynthfilt=new float[6];
        for (int ii=0;ii<=5;ii++)
        {
            lowfilt[ii]=low[ii];
            highsynthfilt[ii]=highsynth[ii];
        }
    }
}
if (ii<=3)
{
    highfilt[ii]=high[ii];
    lowsynthfilt[ii]=lowsynth[ii];
}

~wavelet_transform()
{
    delete [] signal;
    delete [] transform;
    delete [] reconstruct;
    delete [] sampled;
    delete [] upsampled;
    delete [] scalefacts;
    delete [] newscalefacts;
    delete [] wavelets;
    delete [] newwavelets;
    delete [] tempscalefacts;
    delete [] lowfilt;
    delete [] highfilt;
    delete [] lowsynthfilt;
    delete [] highsynthfilt;
}
void filter(float arrin[], float arrout[], float filt[], int arrlen, int filtlen, int offset);
void periodise(float [], float [], int, int);
void sample(float [], float [], int);
void zeroarray(float [], int);
void totransform(float [], float [], int);
void upsample(float [], float [], int, int);
void build(float [], float [], float [], int, int);
void makescalefacts(float [], float [], int, int);
void makewavelets(float [], float [], int, int);
void disparray(String, float []);
float* forwardO;
float* inverseO;
float* inversewave(int);
E2. Wavelet transform pseudocode

**Routine Forward**

<table>
<thead>
<tr>
<th>Signal</th>
<th>vector to be transformed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scalefacts</td>
<td>vector of scaling factors</td>
</tr>
<tr>
<td>Newscalefacts</td>
<td>vector of new scaling factors</td>
</tr>
<tr>
<td>Wavelets</td>
<td>vector of wavelet coefficients</td>
</tr>
</tbody>
</table>

Periodise signal to vector scalefacts

```plaintext
i=0;
power=1;
sampsize=n;
ctr=0;
while (power<n) //forward transform
  increment ctr
  power=power*2;
  zero array newscalefacts
  zero array wavelets
  routine filter(scalefacts,newscalefacts,lowfilt)
  routine filter(scalefacts,wavelets,highfilt)
  zero array sampled
  routine sample(newscalefacts,sampled)
  zero array scalefacts
  routine periodise(scalefacts,sampled)
  zero array sampled
  routine sample(wavelets,sampled)
  for i=1 to n/power
    increm=power/2;
    pos=(i*increm)+1-increm
  next
  pos=n/power
  routine totransform(transform,sampled,pos)
Endwhile
transform[1]=scalefacts[n+1]
return transform
```

produces newscalefacts
produces wavelets
sample newscalefacts
array sampled is
periodised to scalefacts
sample wavelets to sampled
place sample wavelet coefficient in transform
last remaining value
Routine Inverse

Zero array reconstruct
Zero array scalefacts
Zero array wavelets

scalefacts[n+1]=transform[1];
wavelets[n+1]=transform[2];
i=0
power=1
sampsize=n
temp=1;
while power<n)
    i=i+1
    power=power*2;
    Routine upsample(scalefacts,upsampled,power/2,n)
    Routine periodise(scalefacts,upsampled,power,n/power)
    Zero array newscalefacts
    Routine filter(scalefacts,newscalefacts,lowsynthfilt)
    Routine upsample(wavelets,upsampled,power/2,n)
    Routine periodise(wavelets,upsampled,power,n/power)
    Zero array newwavelets
    Routine filter(wavelets,newwavelets,highsynthfilt)
    Zero array reconstruct
    Routine build(reconstruct,newscalefacts,newwavelets,n,power);
    Zero array scalefacts;
    Routine makescalefacts(reconstruct,scalefacts,power,n)
    Zero array wavelets
    Routine makewavelets(transform,wavelets,power,n);
Endwhile
return reconstruct;
**Routine Sample**

Input arguments arrin[], arrout[], samplen

swap=true;
arrpos=1;
zero array arrout
for i=1 to samplen
  if (swap)
    arrout[arrpos]=arrin[i+samplen]
    arrpos++;
    swap=false;
  else
    swap=true
  endif
next

**Routine Filter**

Input Arguments arrin[], arrout[], filt[], arrlen, filtlen, offset

Arrlen - length of (periodised) signal to filter
Filtlen - length of filter
Offset - positions the filter for convolution

no_loops=arrlen+1-filtlen;
for i=1 to no_loops
  temptot=0;
  for j=1 to filtlen
    temptot=temptot+arrin[i+j-1]*filt[j];
  next
  arrpos=i+offset;
  if (arrpos>0 and arrpos<=arrlen)
    arrout[arrpos]=temptot;
  endif
next
Routine Build

Input arguments arrout[], arrin1[], arrin2[], n, arrlen

for i=1 to arrlen
    arrout[i]=arrin1[n+i]+arrin2[n+i];
next

Routine makescalefacts

Input arguments arrin[], arrout[], num, n
for i=1 to num
    arrout[n+i]=arrin[i];
next

Routine makewavelets

Input arguments arrin[], arrout[], num, n
for i=1 to num
    arrout[n+i]=arrin[num+i];
next

Routine periodise

Input arguments largearr[], smallarr[], currlen, mult
ctr=0;
for j=1 to 3*mult signal periodised threefold
    for k=1 to currlen
        ctr=ctr+1
        largearr[ctr]=smallarr[k]
    next
next

Routine upsample

Input arguments arrin[], arrout[], samplen, n
Zeroarray arrout
for i=1 to samplen
    arrout[i*2-1]=arrin[n+i]
next
Appendices

Routine to transform

Input arguments arrout[], arrin[], pos
for i=1 to pos
    arrout[pos+i]=arrin[i];
next
Appendix F. Pseudocode for the two-dimensional wavelet transform

The pseudocode below is for a pilot separable two dimensional transform. The pilot has been tested for a square image of size 8 by 8 including full reconstruction. The routines called such as periodise and filter are those described for the one dimensional wavelet class in appendix E. Each iteration produces sub-images highhigh (diagonal detail), highlow (vertical detail), lowhigh (horizontal detail). What remains is the scaling factor array which is passed through the next iteration.

```
lowfiltno=5;
highfiltno=3;
highoffset=-2;
lowoffset=0;
n=8;
zero2Darray(transform,9);
power=1;
sampsize=n;
while (power<n/4)
    ***** forward transform
    power=power*2;
currszie=(n*2)/power;
    ***** low pass
    ****** row sequence section
    zero2Darray(temp2D,9);
    for (int i=1;i<=currszie;i++)
        zeroarray(signal,9);
        for j=1 to currszie
            signal[j]=image2D[i][j]
        next
    periodise(scalefacts,signal,currszie,power/2)
    zeroarray(newscalefacts,25)
    filter(scalefacts,newscalefacts,lowfilt,24,5,2)
    zeroarray(sampled,9)
    sample(newscalefacts,sampled,n)
    for (int j=1;j<=currszie/2;j++)
        temp2D[i][j]=sampled[j]
    next
    ****** column sequence section
    zero2Darray(lowlow,9);
    zero2Darray(lowhigh,9);
    for (int j=1;j<=n/2;j++)
```
zeroarray(signal,9);
for i=1 to currsise
    signal[i]=temp2D[i][j]
next
periodise(scalefacts,signal,currsise,power/2)
****** lowpass section on columns
zeroarray(newscalefacts,25)
filter(scalefacts,newscalefacts,lowfilt,24,5,2)
zeroarray(sampled,9)
sample(newscalefacts,sampled,n)
for i=1 to currsise/2
    lowlow[i][j]=sampled[i]
next
****** highpass section on columns
zeroarray(wavelets,25)
filter(scalefacts,wavelets,highfilt,24,3,2)
zeroarray(sampled,9)
sample(wavelets,sampled,n)
for (int i=1 to currsise/2
    lowhigh[i][j]=sampled[i]
next
****** end low pass
****** high pass
****** row sequence section
zero2Darray(temp2D,9);
for i=1 to currsise
    zeroarray(signal,9)
    for j=1 to currsise
        signal[j]=image2D[i][j]
    next
    periodise(scalefacts,signal,currsise,power/2)
    zeroarray(newscalefacts,25)
    filter(scalefacts,newscalefacts,highfilt,24,3,2)
    zeroarray(sampled,9)
    sample(newscalefacts,sampled,n)
    for j=1 to currsise/2
        temp2D[i][j]=sampled[i]
next
next
****** column sequence section
zero2Darray(highlow,9)
zero2Darray(highhigh,9)
for j=1 to n/2
    zeroarray(signal,9);
for i=1 to currsize
    signal[i]=temp2D[i][j]
next
periodise(scalefacts,signal,currsize,power/2)
****** lowpass section on columns
zeroarray(newscalefacts,25)
filter(scalefacts,newscalefacts,lowfilt,24,5,2)
zeroarray(scaled,9)
sample(newscalefacts,sampled,n)
for i=1 to currsize/2
    highlow[i][j]=sampled[i]
next
****** highpass section on columns
zeroarray(wavelets,25)
filter(scalefacts,wavelets,highfilt,24,3,2)
zeroarray(scaled,9)
sample(wavelets,sampled,n)
for i=1 to currsize/2
    highhigh[i][j]=sampled[i]
next
****** end low pass
for i=1 to currsize/2
    for j=1 to currsize/2
        image2D[i][j]=lowlow[i][j]
    next
next
****** now place sub-images into transform
for i=1 to currsize/2
    for j=1 to currsize/2
        transform[i][j]=lowlow[i][j]
next
****** top left
for (int j=1;j<=currsize/2;j++)
    transform[i][j]=lowlow[i][j]
next
****** top right
for j=1 to currsize/2
    transform[i][j+currsize/2]=highlow[i][j]
next
****** bottom left
for j=1 to currsize/2
    transform[i+currsize/2][j]=lowhigh[i][j]
next
next
for i=1 to currsiz/2
    ***** bottom left
    for j=1 to currsiz/2
        transform [i+currsiz/2][j+currsiz/2]=highhigh[i][j]
    next
next
endwhile
Appendix G, Publications Summary


L. Smith and U. Tüzün (2002), Stress, voidage and velocity coupling in an avalanching granular heap, Chemical Engineering Science, (Accepted for publication July, 2002).
Appendix H. The multi-resolution wavelet transform

As compared to the Fourier transform, wavelet basis functions are localised and are generated from two mother functions, a scaling function, \( \phi(x) \), and its wavelet counterpart, \( \psi(x) \), which satisfy the following conditions

\[
\int_{-\infty}^{\infty} \phi(x)\,dx = 1, \quad \int_{-\infty}^{\infty} \phi(x)\psi(x)\,dx = 0, \quad \int_{-\infty}^{\infty} \psi(x)\,dx = 0 \quad (H1)
\]

A unique feature of the mother functions is that they must be localised, i.e. non-zero only in a finite domain. This property is called compact support:

\[
\phi(x) \equiv 0, \psi(x) \equiv 0, \text{ if } x \leq a \text{ or } x \geq b; \quad b > a. \quad (H2)
\]

All basis functions are generated by translation and dilation of the two mother functions:

\[
\phi_{j,k}(x) = 2^{j/2} \phi(2^j x - k), \quad \psi_{j,k}(x) = 2^{j/2} \psi(2^j x - k) \quad (H3)
\]

It is further required that all scaling functions and wavelet functions at a common level (i.e. same level of dilation) are mutually orthogonal:

\[
\int_{-\infty}^{\infty} \phi_{j,k}(x)\phi_{l,m}(x)\,dx = \delta_{j,l} \quad (H4)
\]

\[
\int_{-\infty}^{\infty} \phi_{j,k}(x)\psi_{l,m}(x)\,dx = 0, \text{ for all } j, k, l, m \quad (H5)
\]

\[
\int_{-\infty}^{\infty} \psi_{j,k}(x)\psi_{l,m}(x)\,dx = \delta_{j,l,i,m} \quad (H6)
\]

where \( j, k, l, m \in \mathbb{Z} \) (i.e. they are integers).

A further condition applies to Daubechies wavelets:

\[
\int_{-\infty}^{\infty} \psi(x)\,dx = 0, m = 0, 1, \ldots, M - 1 \quad (H7)
\]

Functions that satisfy equation (H7) are said to have \( M \) vanishing moments. The more vanishing moments the smoother (more differentiable) the wavelet is. Greater smoothness brings with it a wider supporting domain.