The Application of Wavelet Transforms to Many-body Particle Interactions

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by

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Abstract

Wavelet transforms are used to explore the dynamic evolution of granular material by post-processing data from DEM simulations. Data sets generated from two different physical scenarios were analysed: particles in vibration cells and samples under compression.

It is shown how the wavelet multiresolution analysis (MRA) helps to reveal the particle motions within a vibration box subject to applied vibrations. Two combinations of amplitude and frequency vibration were applied in this work: low frequency with high amplitude and high frequency with low amplitude. Both cases give the same acceleration amplitude of approximately 7.8g where g is the acceleration due to gravity and both mono-sized particles and binary mixture were considered. The root mean square of the fluctuating velocity and the packing fraction of the two data sets are also consistent with the analysis results of the wavelets technique.

Furthermore, it is shown how the MRA techniques were used to capture the position of inhomogeneities in granular material response by analysis of data sets from simulations of biaxial and triaxial compression tests. In the case of biaxial compression, results from the wavelet analysis are compared with plots of the cumulative rotation of the particles. In the triaxial compression test where a bonded material is considered the wavelet analysis is compared with plots of the position of broken bonds in the sample.

Moreover, it is shown that the MRA techniques can aid in finding the time/strain scales on which significant events occur. This information could be used to determine how frequently to output data on stress, strain-rate (velocity) and packing voidage distributions during compression, shear and flow of the granular bulk. Furthermore, the wavelet technique should be considered for applications involving quantitative analysis of experimental data generated by the other advanced experimental techniques such as photo-elasticity and X-ray computed tomography techniques.
To Father and Mother.
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Chapter 1

Introduction

1.1 Introduction

Granular material is a collection of discrete, solid particles in a vacuum or interstitial fluid. A few examples include sand, stones, soil and plastics. Granular dynamics simulations are a very useful tool in providing information about the evolution of an assembly at the particle level. Known as a computer simulations technique for granular materials, the Discrete Element Method (DEM) has been well established for many years. The DEM simulation involves the motion of every particle in the flow and modeling each collision between particles and between particles and the environment. Consequently, a vast amount of data is available from DEM simulations. These data are mainly used to provide illustrative snapshots of the system at selected points in time.

The DEM simulations provide time-series data [81], such as particle positions, velocity or contact force and voidage. The abundance of time-series data from the computer simulation provides for a general mathematical framework for an analysis of the particle assembly evolution during the bulk flow.

Previously, Fourier transforms have been used to investigate periodicity in time-series. By applying the Fourier transforms [84], a power spectra plot reveals the peak frequency characteristics of the time-series. Although this method clearly allows the
dominant peak frequencies of the entire time series to be observed, the time information is lost. Specifically, it fails to capture the time of occurrence of specific peak frequencies as well as their length of duration. Spectral analysis is useful if a signal or time-series is stationary, that is constant in frequency components throughout time. However, many time-series in granular mechanics are non-stationary. A possible solution is to window the Fourier transform [35], thus allowing the localisation of non-stationary components of the signal. This approach is called the short-time Fourier transform. The frequency resolution in the short-time Fourier transform is influenced by the window length.

The wavelet transform (WT) technique is widely accepted as an alternative time-frequency analysis [52, 24, 37]. The wavelet transform can extract phenomena that are simultaneously localized in time and frequency using the scaling and/or translational functions of a local basic function called the mother wavelet. Smith et al. [42, 43] have demonstrated the potential of the discrete wavelet transform in granular material. They added wavelet analysis to their simulation post-processing toolset as an aid to coupling of time series variables in the context of localised defining events. They showed that correlation between time-lagged wavelet transform coefficients can be much more revealing than correlation functions derived from the original time series themselves, and that wavelet analysis has the potential to identify time constants in the absence of clearly defined periodicity. Moreover, they also demonstrated the enhanced capacities of their analysis toolset for three-dimensional data [44].

As illustrated by the power of the wavelet transform technique in previous works, ongoing developments of the wavelet transform in statistical post-processing of simulation data offer the possibility of real progress [81]. In this work, we explore the use of wavelet techniques to analyse data from two different physical scenarios: particle packing in a vibration cell and samples under compression.
CHAPTER 1. INTRODUCTION

1.2 Outline of the Thesis

This thesis is organised as follows:

Chapter 2 details the Discrete Element Method (DEM). The technical details of the interaction models for particle-particle are described. The details of the wavelet transforms are given in chapter 3 including a review of the application of wavelet transforms in other areas. Examples are given to show how the wavelet works with some different signals.

The results of analysis of data sets from simulation of particle packing in a vibration cell are presented in chapter 4. The data sets were provided by Professor A.B.Yu and Dr.K.J Dong at UNSW, Australia [78]. Two mono-sized cases and two binary mixture cases were analysed. In each group, different frequencies and amplitudes of vibration were applied: low frequency with high amplitude and high frequency with low amplitude. We show the analysis results both from the basic time-series analysis and from the wavelet analysis. Also, the fluctuating velocity, the granular temperature and the packing fraction were calculated in all cases.

Data from simulations of biaxial compression tests on dense two dimensional assemblies of disc were considered in chapter 5. The dense sample under planar biaxial strain exhibits a strain-softening type phenomena and a distinct localization post peak is evident [10]. As a consequence of the localizations, the post-peak response is not homogeneous throughout the specimen and the simulations are well-suited to assess whether wavelet analysis can effectively capture inhomogeneities in granular material response. There are two equivalent specimens with different numbers of particles: specimen A and specimen B. Three data sets were analysed, one from specimen A and two from specimen B. These data sets were provided by Dr.O’Sullivan from Imperial College.

Chapter 6 presents the results of the analysis of data sets which are results of a discrete element simulation of a triaxial compression test of a bonded material. These
data sets were provided by Geraldine Cheung, a PhD student from Imperial College. Three data sets were analysed. The first and the second data sets were identically generated but different data was saved in each case. The third data set was generated with the same parameters but with different initial positions for the particles.

Chapter 7 summarizes the results from this research and suggests potential improvements and extensions in future.
Chapter 2

The Discrete Element Method

2.1 Introduction

The flow of particulate materials is a critical part of many industrial and mining processes. For the simulation of granular flows, the Discrete Element Method (DEM) has been well established for simple flows for many years. DEM simulation involves the motion of every particle in the flow and modelling each collision between particles and between particles and the environment. The technique is essentially the same as the molecular dynamics (MD) method in which the particle trajectories are evolved in discrete time steps using a numerical integration of Newton's equations of motion.

Discrete element methods have been extensively used for simulating a wide range of granular systems because they correspond to the discrete nature of the granulates. The DEM provides an invaluable method of investigating the particle-scale interactions underlying granular material response in a range of disciplines including chemical engineering [8, 46, 47, 78, 42, 43, 44], mechanical engineering [28] and soil mechanics [14, 40, 11, 13].

In pharmaceutical manufacture, for example, the DEM is used to investigate randomly packed particles in an attempt to model the process of pharmaceutical tablet manufacture by powder compaction [87, 74]. The DEM is also used in the industry of mining [62, 75], agriculture and food handling [6]. Furthermore, the technique has
been extensively used in the laboratory of particulate and multiphase processing to study the fundamentals of particulate matter at a particle scale [2]. This chapter briefly describes the contact model in the discrete element method.

2.2 Particle-particle interaction model

The choice of the particle-particle interaction is an important feature in a discrete element method. Most particles in a granular assembly will form contacts with several other particles. The contact interactions have elastic, kinetic energy damping and frictional components [47].

2.2.1 Normal elastic interaction

Three analytical forms of the normal interaction laws between the particles are considered in this section; these are the continuous interaction, the Hertzian interaction and Hooke's law.

Continuous interaction

For circular disc particles, the potential energy between two particles of diameter \(\sigma\) and a centre to centre distance \(r\) is given by:

\[
\phi(r) = \epsilon \left(\frac{\sigma}{r}\right)^n
\]

(2.1)

where \(\phi(r)\) is called the soft-sphere potential and \(\epsilon\) is a constant equal to the potential energy at \(r = \sigma\).

The normal force between the particles is given by:

\[
F_{N}^{C} = -\frac{d\phi(r)}{dr}.
\]

(2.2)

The particular value of \(n = 36\) was chosen in the work of Langston et al [47] to make a compromise; preventing excessive overlap without being too stiff. The interaction
between particles decays rapidly for values of $r$ greater than $\sigma$ and the interactions beyond a truncation separation distance $r_i = 1.2 \sigma$ are ignored.

**Hertzian interaction**

The normal force between the particles presented by Hertz is given as follows:

$$F_N^H = \frac{4}{3} E^* \sqrt{R} (\sigma - r)^{3/2}$$

$$\frac{1}{E^*} = \frac{1 - \nu_1}{E_1} + \frac{1 - \nu_2}{E_2}$$

$$\frac{1}{R} = \frac{1}{R_1} + \frac{1}{R_2}$$

where $E$ is Young’s modulus, $\nu$ is Poisson’s ratio, subscripts 1 and 2 indicate particles 1 and 2, $R$ is the contact radius of curvature. The Hertzian force varies as the $3/2$ power of overlap displacement.

**Hooke’s law**

The normal force can be obtained as follows:

$$F_N^S = k (\sigma - r)$$

where $k$ is a stiffness constant.

In all three cases the working values for the input parameters result in a normal stiffness that is quite soft when compared with real elastic contacts between particles. The respective normal stiffness is given by the derivative $(- \partial F/\partial r)$ which result in
\[ k_{\text{Hertz}} = 2E^* \sqrt{H} (\sigma - r)^{1/2} = \frac{3}{2} \frac{F_N^*}{(\sigma - r)} \] (2.4)

\[ k_{CI} = \epsilon n (n + 1) \left( \frac{\sigma}{r} \right)^n \frac{1}{r} = (n + 1) \frac{F_N^*}{r} \] (2.5)

\[ k_S = \frac{F_S^N}{(\sigma - r)}. \] (2.6)

### 2.2.2 Tangential Interaction

The tangential interaction, \( F_T^* \), is given by

\[ F_T^* = \mu F_N \left(1 - \left(1 - \frac{\delta_t}{\delta_{\text{max}}}\right)^{3/2}\right) \] (2.7)

where \( \delta_t \) is the total tangential displacement between the two surfaces from the point where they initially came into contact. The relative movement, \( \delta \) of the interacting surface within each time step is calculated and accumulated to the total displacement, \( \delta_t \). If |\( \delta_t | exceeds \( \delta_{\text{max}} \), the sliding occurs and \( \delta_t \) does not increase. The analytic form of equation (2.7) was first proposed by Mindlin and Deresiewicz [56].

### 2.2.3 Contact Damping

In order to allow energy dissipation through mechanical work, contact damping is incorporated in both the normal and tangential directions.

**Normal contact damping**

For a given point in time, the damping force during a contact is assumed to be proportional to the normal component of relative velocity of the two particles and conventionally, the damping force opposes the relative velocity. Thus the normal damping force is given by:

\[ F_D^N = (-c (v \cdot n)) n \] (2.8)

where \( c \) is a normal damping coefficient, \( v \) is the current relative velocity vector and...
n is the normal unit vector between the particle centres.

In many studies, such as the work of Langston [47] and the work of Baxter [30], the contact is approximated as a classical damped harmonic oscillator and \( c \) is a fraction of the critical damping parameter. This gives:

\[
m \ddot{r} + c \dot{r} + k r = F^N
\]  

(2.9)

where \( m \) is the particle mass, \( k \) is the current contact stiffness and \( F^N \) is the normal interaction load. The damping parameter is given by:

\[
\gamma = \sqrt{\frac{c^2}{4mk}}
\]  

(2.10)

where \( \gamma < 1, \gamma = 1 \) and \( \gamma > 1 \) respectively show that the contact is under-damped, critically damped and over damped. Letting \( c = c_c \) at critical damping and using equation (2.10), the critical damping coefficient is given by:

\[
1 = \sqrt{\frac{c_c^2}{4mk}}
\]

and \( c \) is assumed to be a proportion of \( c_c \). In the work of Baxter [30], \( c \) was chosen to be around 50% of \( c_c \).

To obtain \( c \), the contact stiffness, \( k \) has to be determined first. The stiffness in each contact model is given by equations 2.5–2.6.

**Tangential contact damping**

The basic formulation of the contact damping model is exactly as for the normal direction. The force is the product of a damping coefficient and the tangential com-
CHAPTER 2. THE DISCRETE ELEMENT METHOD

ponent of the relative velocity as follows:

\[ F_D^T = (-c_t(v \cdot t)) \cdot t \]  (2.11)

where the tangential damping coefficient is given by

\[ c_t = 2 \psi \sqrt{m k_t} \]

The tangential stiffness, \( k_t \) is obtained by differentiating equation (2.7):

\[ k_t = \frac{d F_T}{d \delta_T}. \]

Note that when gross sliding occurs, no tangential damping force is explicitly applied because the tangential stiffness goes to zero.

2.2.4 Particle Assembly Updating Scheme

The model simulates the flow of discs in two dimension or spheres in three dimension using an explicit time stepping numerical integration of force acting on the discs. At every time step, \( \Delta t \) the model calculates the resultant force and moment acting on each particle and generates its linear and angular accelerations. Numerical integration of velocities produces the positions and orientations of the particles for the next step. The Verlet algorithm is used as follows:

\[ \dot{\mathbf{r}}_{t + \frac{\Delta t}{2}} = \dot{\mathbf{r}}_t - \frac{\Delta t}{2} + \ddot{\mathbf{r}}_t \Delta t \]

\[ \ddot{\mathbf{r}}_t = \frac{F_t}{m} - \beta \dot{\mathbf{r}}_t \]

where \( \beta \), the global damping constant, is set to zero. Particle positions are updated according to

\[ \mathbf{r}_{t + \Delta t} = \mathbf{r}_t + \dot{\mathbf{r}}_{t + \frac{\Delta t}{2}} \Delta t. \]
Furthermore, a near-neighbour list scheme is employed in the simulation. The program records those particles with a separation distance less than a critical cut-off. In the work of Langston [46], they chose $r_0 = 1.8\sigma$. The particles within the near-neighbour list are searched to obtain the particles interaction. The neighbour list tables are updated when there is a possibility of the centre to centre distance between a pair of particles having reduced from being greater than $r_0$ to being less than $r_0$.

As described above in the simulation model, at every time step the positions and orientations of particles are updated, so there is a wealth of data available on a time referenced basis which has the potential to allow a quantitative analysis of dynamics of assembly evolution. Fourier transforms have been used as a tool for extracting local-frequency information from the signal. However, they have one major drawback that they cannot be used to approximate non-stationary signals. The Fourier representation only provides the spectral content with no indication about time localization of the spectral component. Since the wavelet transform can be used to analyse time series that contain non-stationary power at many different frequencies, it can be used as a tool to analyse the simulated data. The wavelet techniques are detailed in the next chapter.
Chapter 3

Wavelets

3.1 Introduction

The wavelet transform is a method of converting a signal or function into another form which either makes features of the original signal more amenable or allows the original data set to be described more succinctly. Wavelets are mathematical functions that decompose the signal or data into different bands of frequency. These mean each component can be studied separately with a resolution matched to its scale. The wavelet transforms overcome the limitation of the traditional Fourier methods in analysing physical situations where the signal is non-stationary or contains discontinuities and sharp spikes. Unlike Fourier analysis, wavelet analysis expands a function in term of wavelets, which are a series of translations and dilations of a basis function called a Mother wavelet. The wavelet function is localised in both space and scale.

There are two type of wavelet transforms: the continuous wavelet transform (CWT) and the discrete wavelet transform (DWT). This chapter describes the method of wavelet analysis. The continuous wavelet transform will be mentioned first in section 3.2 and then followed by the discrete type in section 3.3. Further details on the continuous wavelet transform can be found in [67, 16] and on the discrete wavelet transform in [45, 38]. Examples of both types will be presented in each section. The chapter ends with a review of the application of wavelet transforms.
3.2 The continuous wavelet transform

As mentioned in section 3.1, the wavelet transform unfolds a signal or data into different times (or spaces) and scales. To perform a wavelet transform we need a wavelet known as a mother wavelet or analysing wavelet. A wavelet or mother wavelet is a function \( \psi(t) \) satisfying certain mathematical criteria. Let us consider the function \( \psi_{(a,b)}(t) \), where \( \psi_{(a,b)}(t) \) is a family of functions defined as translations and re-scaling of the mother wavelet function \( \psi(t) \),

\[
\psi_{(a,b)}(t) = \frac{1}{\sqrt{|a|}} \psi \left( \frac{t - b}{a} \right). \tag{3.1}
\]

In the equation (3.1) \( a \) is a scaling parameter, \( b \) is a translation parameter and \( a, b \in \mathbb{R}, a \neq 0 \).

The continuous wavelet transform (CWT) of a continuous signal \( x(t) \) with respect to the wavelet function \( \psi_{(a,b)}(t) \) is defined as

\[
W(a,b) = \int_{-\infty}^{\infty} x(t) \psi^*_\psi_{(a,b)}(t) \, dt, \tag{3.2}
\]

where \( \psi^*_\psi_{(a,b)}(t) \) is the complex conjugate of \( \psi_{(a,b)}(t) \). In the equation (3.2), the product of wavelet and the signal are integrated over the signal range. Mathematically, this is called a convolution.

3.2.1 Properties of Wavelets

In order to be classified as a wavelet, a function must satisfy certain mathematical criteria. These are:

1. A wavelet must have finite energy:

\[
E = \int_{-\infty}^{\infty} |\psi(t)|^2 \, dt < \infty, \tag{3.3}
\]

where \( E \) is the energy of a function equal to the integral of its squared magnitude.
and the $|\cdot|$ represent the modulus operator.

2. Admissible Condition

A wavelet must satisfy the admissibility condition:

$$C_\psi = \int_0^\infty \frac{\hat{\psi}(f)^2}{f} \, df < \infty,$$  

(3.4)

where $\hat{\psi}(f)$ is the Fourier transform of $\psi(t)$. The admissibility condition implies

$$\hat{\psi}(0) = 0 = \int_{-\infty}^{\infty} \psi(t) \, dt.$$  

(3.5)

In equation (3.4), $C_\psi$ is called the admissibility constant.

3. Resolution of Identity

When the admissibility condition is satisfied, i.e., $C_\psi < \infty$, it is possible to find the inverse continuous transformation via the relation known as the resolution of identity,

$$x(t) = \frac{1}{C_\psi} \int_{-\infty}^{\infty} \int_0^\infty W(a, b) \psi_{a,b}(t) \frac{da \, db}{a^2}.$$  

(3.6)

3.2.2 The signal energy

The total energy contained in a signal, $x(t)$, is defined as

$$E = \int_{-\infty}^{\infty} |x(t)|^2 \, dt = ||x(t)||^2.$$  

(3.7)

The relative contribution of the signal energy contained at scale $a$ and location $b$ is given by the two dimensional wavelet energy density function:

$$E(a, b) = |W(a, b)|^2.$$  

(3.8)

A plot of $E(a)$ is known as a Scalogram.
The scalogram can be integrated across $a$ and $b$ to recover the total energy in the signal using the admissibility constant, $C_\psi$, as follows:

$$E = \frac{1}{C_\psi} \int_{-\infty}^{\infty} \int_{0}^{\infty} |W(a,b)|^2 \frac{da \, db}{a^2}. \quad (3.9)$$

The relative contribution to the total energy contained within the signal at a specific $a$ scale is given by

$$E(a) = \frac{1}{C_\psi} \int_{-\infty}^{\infty} |W(a,b)|^2 \, db. \quad (3.10)$$

Peaks in $E(a)$ highlight the dominant energetic scales within the signal.

### 3.2.3 The inverse wavelet transform

The inverse wavelet transform is defined as

$$x(t) = \frac{1}{C_\psi} \int_{-\infty}^{\infty} \int_{0}^{\infty} W(a,b) \psi_{a,b}(t) \frac{da \, db}{a^2}. \quad (3.11)$$

This allows the original signal to be recovered from its wavelet transform by integrating over all scales and locations, $a$ and $b$. If we limit the integration over a range of $a$ scales rather than all $a$ scales, we can perform a basic filtering of the original signal. The signal reconstructed by limiting the range of $a$ scales is given by

$$x(t) = \frac{1}{C_\psi} \int_{-\infty}^{\infty} \int_{a_*}^{\infty} W(a,b) \psi_{a,b}(t) \frac{da \, db}{a^2}. \quad (3.12)$$
3.2.4 Examples of continuous wavelet transform

There are a large number of wavelets to choose for using in analysis. The best one for a particular application depends on both the nature of the data and what we require from the analysis. The Mexican hat wavelet is chosen to illustrate analysing the signal in this section. The following examples are implemented in MATLAB.

The Mexican hat wavelet is defined as

\[ \psi(t) = (1 - t^2) e^{-t^2/2} \]  

\[ (3.13) \]

As it is described before, equation (3.13) is the mother wavelet or analysing wavelet. The Mexican hat wavelet is shown in figure 3.1

![Figure 3.1: Mexican hat](image)

Let us consider the four cycle sinusoidal signal shown in figure 3.2(a). The signal was equally sampled for 1000 sample points and then the Mexican hat wavelet was applied to the signal. In figure 3.2(b) we have a surface plot of \( W(a, b) \). This may also be represented by a 2D plot that is colour-coded according to the value of \( W(a, b) \), shown in figure 3.2(c).

How can the large undulations be explained? To explain this, we refer to equation (3.2). The value of transform convolution depends on the location and dilation of the wavelet. If the wavelet matches the shape of signal well at a specific scale and location, then a large transform value, a wavelet coefficient, is obtained.
(a) The signal: four cycles of sinusoid

(b) Surface plot of $W(a,b)$

(c) Wavelet transform plot

Figure 3.2: Wavelet transform plot of four cycles of a sinusoid
Let us consider a signal that is more complicated than the first one. The signal is composed of two sinusoidal waveforms, a sum of two sinusoids of frequencies of 4Hz and 20Hz. Again, the signal was sampled for 1000 data points. The Mexican hat wavelet was applied to decompose the signal. Figure 3.3(a) shows a plot of signal and Figure 3.3(b) show three dimensional plot of the wavelet coefficients with location $b$ and scale $a$. The 2D plot that is colour-coded according to the value of $W(a,b)$ is shown in Figure 3.3(c). The figure clearly shows the ability of the transform to decompose the signal into its separate components. The transform has unfolded the signal to reveal its two constituent waveforms.
Figure 3.3: Wavelet transform plot of two combined sinusoids


3.3 The discrete wavelet transform

In this section we consider the discrete wavelet transform (DWT). Similar to the continuous wavelet transform, the DWT is a process of determining how well a series of wavelet functions represent the signal being analyzed. The result is a bank of coefficients associated with two parameters, dilation and translation. In the last section, the wavelet function was defined at scale $a$ and location $b$ as

$$\psi_{(a,b)}(t) = \frac{1}{\sqrt{|a|}} \psi \left( \frac{t-b}{a} \right). \quad (3.14)$$

In this section the wavelet transform of a discrete time signal, $x(t)$, is considered where discrete values of the dilation and translation parameter are used.

The wavelet transform is evaluated at discrete scales and translations. The discrete scale is expressed as $a = a_0^j$, where $j$ is integer and $a_0 > 1$ is a fixed dilation step. The discrete translation factor is expressed as $b = k b_0 a_0^j$, where $k$ is integer. The translation depends on the dilation step, $a_0^j$. The corresponding discrete wavelets are written as:

$$\psi_{(j,k)}(t) = \frac{1}{\sqrt{a_0^j}} \psi \left( \frac{t-kb_0 a_0^j}{a_0^j} \right). \quad (3.15)$$

We choose $a_0 = 2$ so that the sampling of the frequency axis corresponds to dyadic sampling. For the translation factor we choose $b_0 = 1$ so that we also have dyadic sampling of the time axis. This power-of-two logarithmic scaling of both the dilation and translation steps is known as the dyadic grid arrangement.

The Haar transform is selected to illustrate how the DWT work. Also, a different wavelet was applied to a number of synthetic signals through examples. Moreover, the basic concepts are introduced.
3.3.1 The scaling function and the wavelet function

The scaling function is associated with the smoothing of the signal, given by

\[ \phi_{j,k}(t) = 2^{-j/2} \phi(2^{-j}t - k) \]  

(3.16)

It has the property \( \int_{-\infty}^{\infty} \phi_0(t) dt = 1 \). Also, the wavelet function is given by

\[ \psi_{j,k}(t) = 2^{-j/2} \psi(2^{-j}t - k) \]  

(3.17)

The scaling function can be convolved with the signal to produce approximation coefficients as follows:

\[ s_{j,k} = \int_{-\infty}^{\infty} x(t) \phi_{j,k}(t) dt. \]  

(3.18)

The wavelet function can be convolved with the signal to produce wavelet or detail coefficients as follows:

\[ d_{j,k} = \int_{-\infty}^{\infty} x(t) \psi_{j,k}(t) dt. \]  

(3.19)

Discrete dyadic grid wavelets are commonly chosen to be orthonormal. These wavelets are both orthogonal to each other and normalized to have unit energy. This is expressed as

\[ \int_{-\infty}^{\infty} \psi_{j,k}(t) \psi_{j',k'} dt = \begin{cases} 1 & \text{if } j = j', k = k' \\ 0 & \text{otherwise.} \end{cases} \]  

(3.20)

We can represent a signal \( x(t) \) using a combined series expansion using both the approximation coefficients and the detail coefficients as follows:

\[ x(t) = s_{j,k} \phi_{j,k} + \sum_{j=1}^{j} \sum_{k=1}^{2^{j-1}} d_{j,k} \psi_{j,k}(t). \]  

(3.21)

The scaling equation and scaling coefficient

The scaling equation describes the scaling function \( \phi(t) \) in term of contracted and shifted versions of itself as follows:

\[ \phi(t) = \sum_{k} c_k \phi(2t - k) \]  

(3.22)
where \( c_k \) is the scaling coefficient that must satisfy the following constraint:

\[
\sum_k c_k = 2. \tag{3.23}
\]

In order to create an orthogonal system we require that

\[
\sum c_k c_{k+2k'} = \begin{cases} 2 & \text{if } k' = 0 \\ 0 & \text{otherwise.} \end{cases} \tag{3.24}
\]

The wavelet equation

The same coefficients are used to produce the wavelet equation. We can define the wavelet function as

\[
\psi(t) = \sum_k (-1)^k c_{N_k-1-k} \phi(2t - k) \tag{3.25}
\]

where \( N_k \) is a finite number of scaling coefficients. The coefficients used for the wavelet function are written more compactly as

\[
b_k = (-1)^k c_{N_k-1-k} \tag{3.26}
\]

where the sum of all coefficients \( b_k \) is zero. The equation (3.25) can be rewritten as

\[
\psi(t) = \sum_{k=0}^{N_k-1} b_k \phi(2t - k). \tag{3.27}
\]

3.3.2 Wavelet energy

The total energy of the discrete signal is equal to

\[
E = \sum_{i=1}^N (x_i)^2 \tag{3.28}
\]

which is equal to the sum of squared detail coefficients over all scales plus the square of the remaining approximation coefficients, \( s_j \), as follows:

\[
E = s_j + \sum_{j=1}^J \sum_{k=1}^{2^j - j} (d_{j,k})^2 \tag{3.29}
\]
In fact, the energy contained within the transform vector at all stages of the multiresolution decomposition remains constant. This is an important property of the Haar transform. It conserves the energies of signals.

3.3.3 The Haar transform

We now illustrate the discrete wavelet transform via a procedure using the Haar wavelet. Figure 3.4 shows the Haar wavelet.

For the Haar wavelet, the scaling coefficients are $c_0 = c_1 = 1$. These coefficients are obtained from solving equation (3.23) and (3.24) simultaneously, so the scaling equation is given by

$$\phi(t) = \phi(2t) + \phi(2t - 1).$$

The Haar wavelet equation can be obtained by using equation (3.25) and the equation is

$$\psi(t) = \psi(2t) + \psi(2t - 1).$$

A discrete signal $x(t)$ is an ordered sequence of real or complex numbers of length $N$ which is represented as
\[ x = (x_1, x_2, x_3, \ldots, x_N). \]

The Haar transform decomposes a discrete signal into two subsignals of half its length. One subsignal is a running average and the other is a running difference.

Let us begin with the average from the first-level Haar transform, which is denoted by

\[ s_1 = (s_{1,1}, s_{1,2}, \ldots, s_{1,N/2}). \]

The first value \( s_{1,1} \) is calculated by taking average of the first pair of the signal \( x(t) : ((x_1 + x_2)/2) \), and then multiplying by \( \sqrt{2} \). The next values are calculated the same way, so the formula for the values of \( s_{1,m} \) is

\[ s_{1,m} = \frac{x_{2m-1} + x_{2m}}{\sqrt{2}} \quad (3.32) \]

for \( m = 1, 2, 3 \ldots N/2 \).

The other subsignal is the difference, which is denoted by

\[ d_1 = (d_{1,1}, d_{1,2}, \ldots, d_{1,N/2}). \]

The first value, \( d_1 \) is calculated by taking the difference of the first pair of the signal \( x(t) : ((x_1 - x_2)/2) \), and then multiplying by \( \sqrt{2} \). Similarly, the next values are computed the same way. The values of \( d_{1,m} \) are calculated according to the following formula:

\[ d_{1,m} = \frac{x_{2m-1} - x_{2m}}{\sqrt{2}} \quad (3.33) \]

for \( m = 1, 2, 3 \ldots N/2 \).

The Haar transform is performed in several levels. The first level is the mapping \( H_1 \) defined by

\[ x : H_1 \rightarrow (s_1 | d_1) \quad (3.34) \]
The second level is then performed by computing $s_2$ and $d_2$. To obtain $s_2$ and $d_2$, equation (3.32) and (3.33) are applied to the values of $s_1$ respectively. Then the second-level Haar transform of $x$ is the signal

$$(s_2 | d_2 | d_1).$$

The $j$-level can be done and the result is

$$(s_j | d_j | ... | d_2 | d_1),$$

where $j$ is the highest level when $N = 2^j$.

### 3.3.4 Haar wavelet

The first-level Haar wavelets used to transform the signal $x$ can be defined as

$$W_{1,1} = \left( \frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}, 0, 0, \ldots, 0 \right)$$

$$W_{1,2} = \left( 0, 0, \frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}, \ldots, 0 \right)$$

$$W_{1,N/2} = \left( 0, 0, \ldots, 0, \frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}} \right)$$

The equation (3.33) can be summarized in terms of scalar products with the first-level Haar wavelets:

$$d_{1,m} = x \cdot W_{1,m}$$

for $m = 1, 2, 3 \ldots N/2$.

Similar to the differences $d_m$, the averages $s_m$ can be expressed in terms of scalar products:

$$s_{1,m} = x \cdot V_{1,m}$$
for \( m = 1, 2, 3 \ldots N/2 \).

\( V_{1,m} \) are the first-level Haar scaling signals and they are defined as

\[
\begin{align*}
V_{1,1} &= \left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0, 0, \ldots, 0 \right) \\
V_{1,2} &= \left( 0, 0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, \ldots, 0 \right) \\
V_{1,N/2} &= \left( 0, 0, \ldots, 0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \right). 
\end{align*}
\]  

(3.38)

The idea discussed above extends to every level. For instance, the difference of the second-level Haar transform of signal \( x \) is

\[
d_{2,m} = x \cdot W_{2,m} \quad (3.39)
\]

and the average is

\[
s_{2,m} = x \cdot V_{2,m} \quad (3.40)
\]

for \( m = 1, 2, 3 \ldots N/2 \).

### 3.3.5 Multiresolution analysis

This section will show how discrete signals are synthesized by beginning with low resolution and adding on detail to create higher resolution until getting the finest resolution. This is known as multiresolution analysis (MRA).

To synthesize the signal, we need the inverse Haar transform. Referring to the the mapping \( H_1 \) in equation (3.34), its inverse map the transform signal \( (s_1 \mid d_1) \) back to the original signal \( x \), via the following formula:

\[
x = \left( \frac{s_{1,1} + d_{1,1}}{\sqrt{2}}, \frac{s_{1,1} - d_{1,1}}{\sqrt{2}}, \ldots, \frac{s_{1,N/2} + d_{1,N/2}}{\sqrt{2}}, \frac{s_{1,N/2} - d_{1,N/2}}{\sqrt{2}} \right) \quad (3.41)
\]

To define the first level Haar MRA, we make use of equation (3.41) to express the signal \( x \) as the sum of two signals:
The two signal are called the approximations and the details respectively. That is, we have

\[ x = A1 + D1 \] (3.42)

where \( A1 \) is called the first approximation and is defined by

\[ A1 = \left( \frac{s_{1,1}}{\sqrt{2}}, \frac{s_{1,1}}{\sqrt{2}}, \frac{s_{1,2}}{\sqrt{2}}, \frac{s_{1,2}}{\sqrt{2}}, \ldots, \frac{s_{1,N/2}}{\sqrt{2}}, \frac{s_{1,N/2}}{\sqrt{2}} \right) \] (3.43)

and \( D1 \) is called the first detail and is defined by

\[ D1 = \left( \frac{d_{1,1}}{\sqrt{2}}, \frac{-d_{1,1}}{\sqrt{2}}, \frac{d_{1,2}}{\sqrt{2}}, \frac{-d_{1,2}}{\sqrt{2}}, \ldots, \frac{d_{1,N/2}}{\sqrt{2}}, \frac{-d_{1,N/2}}{\sqrt{2}} \right). \] (3.44)

The approximations and the details can be expressed in terms of scaling signal and wavelets as

\[
A1 = s_{1,1}V_{1,1} + s_{1,2}V_{1,2} + \ldots + s_{1,N/2}V_{1,N/2}
\]

\[
D1 = d_{1,1}W_{1,1} + d_{1,2}W_{1,2} + \ldots + d_{1,N/2}W_{1,N/2}.
\]

Applying formulas in the equation (3.36) and (3.37) to these last two equations, we can rewrite them as follows

\[
A1 = (x \cdot V_{1,1})V_{1,1} + (x \cdot V_{1,2})V_{1,2} + \ldots + (x \cdot V_{1,N/2})V_{1,N/2}
\]

\[
D1 = (x \cdot W_{1,1})W_{1,1} + (x \cdot W_{1,2})W_{1,2} + \ldots + (x \cdot W_{1,N/2})W_{1,N/2}.
\]
The last two formulas show that the approximation is a combination of the Haar scaling signal, with the values of the first average subsignal as coefficients; and that the detail is a combination of the Haar wavelets, with the values of the differences as coefficients.

The idea of the first level MRA can be extended to the higher level. For example, the second level MRA of signal $x$ can be expressed as

$$x = A_2 + D_2 + D_1$$

(3.47)

where $A_2$ is the second approximation and $D_2$ is the second detail.

In general, if the number $N$ of signal values is divisible $j$ times by two, then a $j$-level MRA is

$$x = A_j + D_j + \ldots + D_1.$$  

(3.48)

3.3.6 Daubechies wavelets

In this work, a member of Daubechies wavelets, Daub2 or db2 used in Matlab is used as a mother wavelet. Figure 3.5 show the db2 wavelet.

![Figure 3.5: db2 wavelet.](image)
The Daubechies are used most often for detecting localisation[48] of disturbance signals. The Daubechies wavelet transforms are defined in the same way as the Haar transform, but the scaling equation and wavelet have slightly longer support, i.e., they produce averages and differences using a few more values from the signal.

The Daub2 wavelet

Let us consider the signal $x(t)$ which is an $N$ values signal where $N = 2^J$, the result of the first-level transform is $(s_{1,k}, d_{1,k})$, where

$$s_{1,k} = x \cdot V_{1,k} \tag{3.49}$$

and

$$d_{1,k} = x \cdot W_{1,k}, \tag{3.50}$$

for $k = 1, 2, \ldots, N/2$.

Similar to the Haar case, the $j$-level transform is obtained by applying the $j$-level transform to the preceding approximation coefficients. The difference between the Haar transform and the Daub2 transform is the scaling function and wavelet function.

The constraints that determine the Daub2 scaling coefficients and wavelets are equation (3.22)-(3.26) and

$$\sum_{k=0}^{N_k-1} (-1)^k c_k k^m = 0. \tag{3.51}$$

Thus the scaling equation of Daub2 is

$$\phi(t) = c_0 \phi(2t) + c_1 \phi(2t - 1) + c_2 \phi(2t - 2) + c_3 \phi(2t - 3) \tag{3.52}$$

and the corresponding wavelet function is

$$\psi(t) = c_3 \psi(2t) + c_2 \psi(2t - 1) + c_1 \psi(2t - 2) + c_0 \psi(2t - 3) \tag{3.53}$$

Using equation (3.22) - (3.24) we get
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\[ c_0 + c_1 + c_2 + c_3 = 2 \]  
(3.54)

and

\[ c_0^2 + c_1^2 + c_2^2 + c_3^2 = 2. \]  
(3.55)

Letting \( m = 0 \) and \( m = 1 \) in the equation (3.51), we get

\[ c_0 - c_1 + c_2 - c_3 = 0 \]

and

\[ -c_1 + 2c_2 - 3c_3 = \text{respectively.} \]

The four coefficients that satisfy the above equations are

\[ c_0 = \frac{1 + \sqrt{3}}{4\sqrt{2}}, \quad c_1 = \frac{3 + \sqrt{3}}{4\sqrt{2}}, \quad c_2 = \frac{3 - \sqrt{3}}{4\sqrt{2}}, \quad c_3 = \frac{1 - \sqrt{3}}{4\sqrt{2}}. \]

These coefficients are called the scaling coefficients. We can obtain the wavelets by using the equation (3.53) and the wavelet coefficients are

\[ b_0 = \frac{1 - \sqrt{3}}{4\sqrt{2}}, \quad b_1 = \frac{-3 + \sqrt{3}}{4\sqrt{2}}, \quad b_2 = \frac{3 + \sqrt{3}}{4\sqrt{2}}, \quad b_3 = \frac{-1 - \sqrt{3}}{4\sqrt{2}}. \]

The first-level Daub2 scaling signals used to transform the signal \( x \) can be defined as

\[
\begin{align*}
\mathbf{V}_{1,1} & = \begin{pmatrix}
\frac{1 + \sqrt{3}}{4\sqrt{2}}, & \frac{3 + \sqrt{3}}{4\sqrt{2}}, & \frac{3 - \sqrt{3}}{4\sqrt{2}}, & \frac{1 - \sqrt{3}}{4\sqrt{2}}, & 0, & 0, & \ldots, & 0
\end{pmatrix} \\
\mathbf{V}_{1,2} & = \begin{pmatrix}
0, & 0, & \frac{1 + \sqrt{3}}{4\sqrt{2}}, & \frac{3 + \sqrt{3}}{4\sqrt{2}}, & \frac{3 - \sqrt{3}}{4\sqrt{2}}, & \frac{1 - \sqrt{3}}{4\sqrt{2}}, & \ldots, & 0
\end{pmatrix} \\
\mathbf{V}_{1,N/2} & = \begin{pmatrix}
0, & 0, & \ldots, & 0, & \frac{1 + \sqrt{3}}{4\sqrt{2}}, & \frac{3 + \sqrt{3}}{4\sqrt{2}}, & \frac{3 - \sqrt{3}}{4\sqrt{2}}, & \frac{1 - \sqrt{3}}{4\sqrt{2}}
\end{pmatrix}.
\end{align*}
\]  
(3.56)

\( \mathbf{W}_{1,m} \) are the first level Daub2 wavelets and they are defined as
3.3.7 Examples of Discrete wavelet transform

A signal $x(t)$ composed of three different frequencies sinusoids is now given as the first example as follows:

$$x(t) = \sin(5t) + \sin(50t) + \sin(200t).$$

The signal consists of 1000 data points and at values of $t=n\Delta t = 1, 2, 3, \ldots, 1000$ where $\Delta t = 0.001s$. This means that the number of data points in one period for the frequency 5 component is 200, for the frequency 50 component is 20, and the frequency 200 component is 5.

Figure (3.6) shows the result of DWT using Daub2. The original signal is plotted as shown in Figure 3.6(a) and Figure 3.6(b)–(f) show the details at scale $\text{D}1$–$\text{D}4$ and the approximation at scale $\text{A}4$ respectively. It can be seen that the slow, medium and rapid sinusoids appear most clearly in approximation $\text{A}4$, detail $\text{D}4$, and detail $\text{D}2$ respectively. This example shows that how the DWT can identify the different frequencies in the signal.

In order to compare the wavelet technique with the Fourier transform, the discrete Fourier transforms was applied to the signal. Frequency components of the signal are shown in Figure 3.7

$$W_{1,1} = \begin{pmatrix} 1 - \sqrt{3} & -3 + \sqrt{3} & 3 + \sqrt{3} & -1 - \sqrt{3} \\ 4\sqrt{2} & 4\sqrt{2} & 4\sqrt{2} & 4\sqrt{2} \end{pmatrix}, 0, 0, \ldots, 0$$

$$W_{1,2} = \begin{pmatrix} 0, 0, 1 - \sqrt{3} & -3 + \sqrt{3} & 3 + \sqrt{3} & -1 - \sqrt{3} \\ 4\sqrt{2} & 4\sqrt{2} & 4\sqrt{2} & 4\sqrt{2} \end{pmatrix}, \ldots, 0$$

$$W_{1,N/2} = \begin{pmatrix} 0, 0, \ldots, 0, 1 - \sqrt{3} & -3 + \sqrt{3} & 3 + \sqrt{3} & -1 - \sqrt{3} \\ 4\sqrt{2} & 4\sqrt{2} & 4\sqrt{2} & 4\sqrt{2} \end{pmatrix}.$$ \hspace{1cm} (3.57)
Figure 3.6: The result from analysis of a sum of sines using Daub2. (a) shows the signal $x(t)$ versus the time, (b)–(e) show the MRA of the signal at scale $D_1$–$D_4$ versus time, (f) shows a plot of the approximation at scale $A_4$ versus time.

Figure 3.7: The analysis result by the Fourier transforms.
In the first example the signal is stationary, so the discrete Fourier transforms can clearly show the frequency components in the signal. Let us consider another synthetic signal $x(t)$ which is also composed of three different frequencies sinusoids but for different time intervals as follows:

$$x(t) = \begin{cases} 
\sin(5t) & \text{if } 0 \leq t \leq 500 \\
\sin(50t) & \text{if } 501 \leq t \leq 750 \\
\sin(200t) & \text{if } 751 \leq t \leq 1000 .
\end{cases}$$

Figure 3.8 shows the result of DWT using Daub2. The discontinuity points of the signal can be seen in the detail $D_2$. It is also clearly seen in the detail $D_1$ if the scale of Y axis is made smaller. The signal is decomposed into different bands of frequencies as can be seen in the detail $D_2$, $D_4$ and the approximation $A_4$.

Figure 3.8: The result from analysis of a sum of sines using Daub2. (a) shows the signal $x(t)$ versus the time, (b)-(e) show the MRA of the signal at scale $D_1$-$D_4$ versus time, (f) shows a plot of the approximation at scale $A_4$ versus time.
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The result of the discrete Fourier transforms is shown in Figure 3.9. Frequency components of a signal are clearly seen but it does not show the discontinuities and when these frequencies occur.

Figure 3.9: The analysis result by the Fourier transforms.

This example shows that wavelet transform is greatly superior to Fourier transform in analysis of non-stationary signals. The Fourier transform tells us how much of each frequency exists in the signal but it does not tell us at which time each frequency occurs.
3.4 Wavelet cross-correlation

3.4.1 Cross correlation

Cross correlation is a standard method of estimating the degree to which two series are correlated. Consider two series \( X(i) \) and \( Y(i) \) where \( i = 1, 2, ..., n \). The cross correlation \( r \) at lag \( d \) is defined as

\[
r(d) = \frac{\sum(x_i - \bar{x})(y_{i-d} - \bar{y})}{\sqrt{\sum x_i^2 - n\bar{x}^2} \sqrt{\sum y_{i-d}^2 - n\bar{y}^2}}
\]  

(3.58)

3.4.2 Wavelet cross correlation

The cross-correlation between wavelet coefficients of two signals over time delay \( \tau \) at scale \( j \) is defined as

\[
\rho_{j,\tau} = \frac{\sum_k (d_x(j,k) - \bar{d}_x(j,k))(d_y(j,k+\tau) - \bar{d}_y(j,k))}{\sqrt{\sum_k (d_x^2(j,k) - n\bar{d}_x^2)(\sum_k (d_y^2(j,k+\tau) - n\bar{d}_y^2))}}
\]  

(3.59)

where \( d_x(j,k) \) and \( d_y(j,k) \) are respectively the wavelet coefficients of signal \( x \) and \( y \) at scale \( j \) and \( \tau \) denotes the delay between two signals or time lagging.
3.5 The application of wavelet transform

Wavelets have been used by many different researchers to study different kinds of signals or data [66]. This includes aperiodic, noisy, intermittent or transient signals. For example, in geological work, the technique has been used for denoising noisy data [76, 7]. Also, it has been proved to be a very powerful tool for characterizing and detecting behaviour over a wide range of time scales [25, 64]. Lockwood et al. [51] has applied the wavelet transform in an attempt to detect long-period components early in a seismogram. The wavelet has potential application to the rapid identification of large earthquakes with high tsunami potential. Also, the wavelet analysis presents a useful way of observing the varying spectral (time-frequency) components of a seismogram. The wavelet method is able to simultaneously pick up both high- and low-frequency arrivals.

The wavelet analysis is also widely used in medical studies [83, 80], for example, using multiresolution wavelet analysis techniques and using the features of signals studied to train a neural network for detection of Alzheimer’s disease [68]. Addison et al. [3] has attempted to utilize wavelet techniques in the analysis of biomedical signals including ECGs. Furthermore, the technique has been used for classifying patients into different groups [86, 29]. For example, Thurner et al. [79] has applied multiresolution wavelet analysis to the sequence of times between human heartbeats (R-R intervals) and have found a scale window, between 16 and 32 heartbeat intervals, over which the widths of the R-R wavelet coefficients fall into disjoint sets for normal and heart-failure patients. This has enabled them to correctly classify every patient in a standard data set as belonging either to the heart-failure or normal group with 100% accuracy, thereby providing a clinically significant measure of the presence of heart failure from the R-R intervals alone. Comparison is made with previous approaches, which have provided only statistically significant measures. Also, it has been found that the wavelet technique is very useful to improve the performance of epileptic seizures prediction [61].

As wavelets have the ability to localize a time series in time-scale space, the the-
ory has been used in financial analysis [36, 90]. Ramsey [70, 69] has proposed that wavelets may well be able to provide new insights into the analysis of economic and financial data. The most important property of wavelets for economic analysis is decomposition by time-scale. Economic and financial systems, like many other systems, contain variables that operate on a variety of time-scales simultaneously so that the relationships between variables may well differ across time-scales.

The relationships in time frequency space between two time series also interests many researchers. Grinsted et al. [23] have used the cross wavelet transform and wavelet coherence for examining relationships in time frequency space between two time series. They have demonstrated how phase angle statistics can be used to gain confidence in causal relationships and test mechanistic models of physical relationships between the time series. Smith and Tuzun [42, 43, 44] have applied wavelet transforms to investigate the disturbances in time series data which result from granular dynamics simulation. They have demonstrated the capability of the wavelet transform to decompose a signal into significant components of activity at different times and at different scales of scrutiny. Time series of lateral and rotational components of the velocity of a selected particle were wavelet transformed and the decompositions compared and correlated. They found an interesting result that for the chosen particle, the wavelet coefficients for the lateral and rotational velocity component at the smallest scale of scrutiny correlate better than the original series themselves.
Chapter 4

Particle packing in vibration cell

4.1 Introduction

This chapter shows results of the analysis of data sets received from Professor A.B. Yu and Dr. K.J. Dong at UNSW, Australia. These data sets result from a simulation study of the packing of spherical particles by the application of a vertical vibration. The analysis results of one preliminary data set and four further data sets are presented: two mono-sized spherical particles data sets and two binary mixture data sets. The preliminary data set was only used to show visual aids of the simulation because of the small number of time steps.

The chapter begins with an overview of work on vibration of granular materials in section 4.2. A brief discussion of the simulation model used by Prof. Yu's group is given in section 4.3. Further details can be found in [78]. The analysis results of the preliminary data set are presented and then followed by the analysis results of the two mono-sized cases and the two binary mixture cases in section 4.4–4.6 respectively. The chapter ends with a summary and conclusion.
4.2 Overview of work on vibration granular materials

The behaviour of granular particles contained in a vibration box has shown a variety of phenomena [15]. In a two dimensional system, different types of convection cells were observed by Gallas et al. [21]. Lee [33] observed heap formation in two dimensional granular media simulations for two systems, one with constant vertical shear and the another with a vibrating bottom and sidewalls. The effect of the vibration amplitude \( A \) was examined. He found that if \( A \) is small (\( \Gamma < 1 \), where \( \Gamma \) is the ratio of the acceleration of the bottom to the acceleration due to gravity), there is no net shear force and as a result no convection. In contrast, he found heap and convection even for \( \Gamma < 1 \) when they fixed the sidewalls and vibrated only the bottom. He also studied the time-averaged behavior of the two-dimensional system using numerical and analytic methods by using molecular dynamics simulation [49]. The time-averaged value of the density, the granular temperature fields and the height expansion which is the rise of the centre of mass due to the vibration scale in the variable \( x = A f \), where \( f \) is the frequency of the vibration. Furthermore, the time-dependence of the system was studied [34]. He found that the temporal fluctuations of the height expansion and pressure scale in \( A f \) while no scaling was found for the fluctuations of granular temperature and the vertical velocity.

For the three dimensional system, a deep bed of granular material (more than 6 layers of particles) subjected to vertical vibration was experimentally investigated [85]. Several phenomena were observed depending on the amplitude of excitation. This included heaping, surface wave and arching. A microscopic behaviour of granular materials subjected to vibration was also investigated by Lan and Rosato [89] using three-dimensional granular dynamic simulations. They found that the characteristic of the bed was different depending on the strength of the applied floor acceleration, \( \Gamma = A \omega^2 \). The temperature is a maximum at the floor and monotonically attenuates upward while the solid fraction profile peaks at some intermediate depth. Furthermore, a vibration amplitude also plays an important role to the bed character. Remond [72] has shown that a large vibration amplitude (\( > d/10 \)), where \( d \) is a particle diameter, lead to a crystallization of the system whereas a small vibration amplitude
(< d/40) induces an efficient compaction of the packing.

Size segregation is an interesting phenomenon when a mixture of particles of the same material but different sizes are shaken in the container. Large particles rise to the top known as a Brazil nut effect (BNE). Rosato et al. [71] have shown a dynamical picture of the segregation process by using a Monte Carlo simulation method to study the size segregation in two space dimensions. They explained the segregation process by a process of void filling. During the shaking of granular mass, the large particles are moved up as the smaller particles fill voids created beneath them. Using the molecular dynamics simulations, Poschel et al. [77] have found that the rising of larger particles is accompanied by the existence of convection cells even in the case of lowest possible frequencies. The convection can be trigged by the larger particle itself. The possibility of rising through this mechanism strongly depends on the depth of the larger particle. Also, a two-dimensional event-driven (ED) simulation code has been developed by Sanders et al. [73] to show that for both single and multiple intruders the BNE is dominated by a buoyancy-like effect. They have found that the mean position of a single intruder is governed by the buoyancy-type effects. A system of many neutrally buoyant intruders also exhibits strong collective behavior that results in clustering or sideways segregation.

In a three-dimensional container, Jason et al. [22] reported the first three-dimensional molecular dynamics simulation of particle segregation by shaking. Two different containers were considered: one cylindrical and another one with periodic boundary conditions. Simulations were done for small particles and a single big test sphere. Also, Möbius et al. [54] have tracked the intruder particle in the presence of granular convection produced by vertically shaking a three-dimensional cylinder filled with smaller background particles. Their results indicated that particle density and interstitial air must both be considered in size segregation.

For the binary mixture case, Hong et al. [26] proposed a new condensation driven segregation of binary hard spheres under gravity. They identified the control parameters
and determined the crossover condition from normal BNE to the reverse Brazil nut problem (RBNE). To explain the mechanism, based on experiments and simulation results Rosato et al. [5] proposed that void filling beneath large particles is a mechanism promoting segregation while convection essentially provides a means of mixing. Schröter et al. [55] also studied the segregation of vertically shaken binary mixtures. Brass spheres were used in an experimental study and an event-driven simulation was used in the numerical study. At a shaking frequency of 80 Hz all samples exhibited a strong Brazil-nut effect due to the geometrical mechanism called void filling. The strength of the segregation increases with diameter ratio and decreases weakly with the shaking amplitude. Increasing the number of large particles from a single intruder up to a mixture of equal volumes of large and small particles results only in a slight decrease of the strength of the effect. At a shaking frequency of 15 Hz and shaking amplitudes up to 1.5 large particle diameters, a strong Brazil-nut effect is induced by sidewall-driven convection.
4.3 Simulation Method

The following simulation method was used in the work of Tang et al [78]. The total force and torque on particle $i$ are given by following equations:

\[ F_i = \sum_j \left( F_{ij}^N + F_{ij}^T + F_{ij}^\nu \right) \]
\[ T_i = \sum_j \left( T_{ij}^T + T_{ij}^\nu \right) \]

where $F_{ij}^N$, $F_{ij}^T$, and $F_{ij}^\nu$ respectively represent the normal contact force, tangential contact force, and van der Waals force imposed on particle $i$ by particle $j$. $T_{ij}^T$ and $T_{ij}^\nu$ are the torques on particle $i$ caused by tangential force $F_{ij}^T$ and rolling friction respectively.

The normal contact force consists of two components: an elastic part and a viscous part. The normal force acting on particle $i$, due to the collision with particle $j$ is obtained by using the nonlinear Hertz model as follows:

\[ F_{ij}^N = \left[ \frac{2}{3} E \sqrt{R} \xi_{\text{in}}^{3/2} - \gamma_n E \sqrt{R} \sqrt{\xi_n} (v_{ij} \cdot n_{ij}) \right] n_{ij} \quad (4.1) \]

where $E = Y / (1 - \bar{\sigma}^2)$, $Y$ is the Young modulus and $\bar{\sigma}$ is the Poisson ratio, $n_{ij}$ is a unit vector running from the centre of particle $i$ to the centre of particle $j$, $v_{ij}$ is velocity, $\xi_n$ is the deformation or overlap, and $R = R_i R_j / (R_i + R_j)$. The normal damping constant, $\gamma_n$ is treated as a material property.

The force which opposes the motion of the interacting particles in the tangential direction is given by:

\[ F_{ij}^T = -\text{sgn}(\xi_T) \mu \left| F_{ij}^N \right| \left[ 1 - \left( 1 - \frac{\min(\xi_T, \xi_{T,\text{max}})}{\xi_{T,\text{max}}} \right) \right], \quad (4.2) \]

where $\mu$ is the frictional coefficient, $\xi_T$ is the total tangential displacement of particles during contact, and $\xi_{T,\text{max}} = \mu[(2 - \bar{\sigma})/2(1 - \bar{\sigma})] \xi_n$. 

The torque on particle $i$ due to the tangential force is $T_{ij}^T = R_i \times F_{ij}^T$, where $R_i$ is a vector running from the center of particle $i$ to the contact point with magnitude equal to particle radius $R_i$. In their work, the torque $T_{ij}^r$ caused by the rolling friction is given by:

$$T_{ij}^r = -\mu_r R_i |F_{ij}^N| \omega_i,$$  \hspace{1cm} (4.3)

where $\mu_r$ is the coefficient of rolling friction, and $\omega_i$ is angular velocity of particle $i$. Furthermore, the long-range, noncontact force was considered in their work. That is the van der Waals force denoted by $F_{ij}^\omega$.

A simulation began with the random generation of mono-sized spherical particles with no overlap in a rectangular box with width equal to 12 particle diameters. The particles were allowed to settle down under gravity. Periodic boundary conditions were applied along the two horizontal directions. The vertical position of the bottom of the box at time $t$ is given by

$$x_0(t) = A \sin(2\pi ft),$$ \hspace{1cm} (4.4)

where $f$ is the frequency and $A$ is the amplitude of the vibration. Different combinations of frequencies and amplitudes were used. Table 4.1 shows the physical conditions and parameters for the simulations.
Parameter | Value
--- | ---
Particle density, $\rho$ | $2.5 \times 10^3 \text{kgm}^{-3}$
Young's modulus, $Y$ | $1.1 \times 10^7 \text{Nm}^2$
Poisson's ratio, $\sigma$ | 0.29
Friction coefficient, $\mu$ | 0.3
Rolling friction coefficient, $\mu_r$ | 0.002
Normal damping coefficient, $\gamma_n$ | $2 \times 10^{-5}$

Table 4.1: Simulation parameters for the particle packing

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Mono-sized cases</th>
<th>Binary mixture cases</th>
</tr>
</thead>
<tbody>
<tr>
<td>particle size, $d$</td>
<td>1 mm</td>
<td>1 mm, 2 mm</td>
</tr>
<tr>
<td>number of particles, $N$</td>
<td>2500</td>
<td>1250 small particles, 156 large particles</td>
</tr>
</tbody>
</table>

Table 4.2: Simulation parameters for the particle packing

The particle sizes and the number of particles in each data set are different as presented in Table 4.2.
4.4 Analysis of preliminary data set

The first data set received from UNSW was composed of the $x, y, z$ positions of 2500 particles for 21 time-steps with 0.2s increment of time. The particles are mono-sized of diameter $d$. A 1D vibration along the vertical ($z$) direction was applied of amplitude $0.2d$ and frequency $100 \text{ Hz}$. This vibration results in a final packing fraction of the particles of 0.64.

4.4.1 The visual aid of the simulation: making layers in $Z$ direction

A simulation box with layers

A movie of the flow of the particles was made by using MATLAB in order to examine the particle motion. The program shows movies of 2500 particles in 2D and 3D. In order to understand the motion of the particles, at $t = 0$ the particles are divided into 4 layers in the $Z$ direction: the top layer, the upper middle layer, the lower middle layer and the bottom layer. Figure 4.1(a) shows a schematic diagram of how layers are divided. Firstly, a box is divided into two halves consisting of 1250 particles for each half, then divided again into quarters, consisting of 625 particles for each quarter and finally subdivided the bottom layer and the top layer into two halves, a top-eight and bottom-eight layers consisting of 312 particles. Figure 4.1(b) shows a box in 3 dimensions.
Different colours are used for each layer. Figure 4.2(a) shows a snapshot of the first time step. This consists of 4 views; the top left shows the 3D view, the remaining view shows the projection of the particles on the $(x, y)$, $(x, z)$ and $(y, z)$ planes respectively. The snapshots of time step $3(0.6s)$ and $21(4.2s)$ are shown in Figure 4.2(b) and 4.2(c) respectively.
Figure 4.2: Snapshot pictures illustrating the amount of vertical mixing in the simulation.

As we can see from the movie and also from the snapshot pictures, although there is a small amount of mixing at the boundaries between the layers, to a large extent the particles on the top layer stay at the top, and those in the middle stay in the middle and so on.
4.4.2 The visual aid of the simulation: Making layers in Y direction

In order to observe particle flows in the horizontal \((x,y)\) plane, a movie of particles moving was made. Figure 4.3(a) shows the first time step of flows consisting of four sections in the \((x,y)\) plane. The top left shows all particles and colours according to their position in the \((x,y)\) plane at \(t = 0\). The remaining three pictures show particles in different slices in the \(z\) direction.

In Figure 4.3(b) we show the analogous pictures at time step 21, \(t = 4.2s\). These show that particles in the bottom layer do not mix horizontally as much as those in the top layer: in the top layer some of the dark particles have migrated to the centre of the layer.

![Figure 4.3: Snapshot pictures showing the amount of horizontal movement of the particles during the simulation](image)

The small number of time steps in this preliminary data set did not allow for a more detailed study of the statistics of the time series. Consequently, four different data sets with longer time running were generated: two mono-sized spherical particles data sets and two binary mixture data sets.
4.5 Vibration of mono-sized spherical particles

Two data sets which are the results of the vibration of mono-sized spherical particles are considered here: data set 1 and data set 2. These data sets are similar to the preliminary data set but data are output at every 0.05s instead of 0.2s and there are more time steps, 350 steps instead of 21. Details of each data set are given as follows:

Data set1: The data set was composed of the $x$, $y$, $z$ positions of 2500 particles for each of 350 time steps with a time stepping of 0.05s. The vibration amplitude was $0.2d$, where $d$ was the diameter of a particle, and the vibration frequency was 100 Hz.

Data set2: The second data set was composed of the $x$, $y$, $z$ positions of 2500 particles for each of 99 time steps with a time stepping of 0.2s. The vibration amplitude was $0.008d$ and the vibration frequency was 500 Hz.

Both data sets give the same acceleration applied, $\Gamma = 7.8$. The dimensionless acceleration is given by

$$\Gamma = A(\omega^2)/g,$$

where $\omega = 2\pi f$ and $g$ is the acceleration due to gravity. As described above, the first data set may be called the low frequency high amplitude data set whereas the second data set is at high frequency and low amplitude.

The analysis results are presented as follows. As shown in Figure 4.1 in section 4.4.1, the vibration box is divided into 4 layers at the first step. The mean of particle positions in the $x$, $y$, $z$ directions in each layer are calculated as a function of time. Furthermore, an MRA of mean of particle positions of two different data sets are compared. Also, the fluctuating velocity of particles in both data sets are presented. Later, instead of following the particles that start out in each layer, the layers are fixed and in each time step the particles within the layers are considered. The layers are fixed in the $z$ direction and then the fluctuating velocity, the root mean square velocity of particles are calculated for both data sets.
4.5.1 Mean of particle positions

Note that the simulation uses periodic boundary conditions in the lateral directions. It is important to take this into account since a particle leaving one side of the box and entering the other has a sudden large change in the positions. The following results were calculated with the effect of the periodic boundary condition removed.

The mean of \(x\), \(y\) and \(z\) position of particles in each horizontal layer as shown in Figure 4.1 for both data sets were calculated. Figure 4.4 shows the mean of the \(x\), \(y\) and \(z\) positions of particles as a function of time for the data sets 1 and 2.

As seen in Figure 4.4(a)–(f), the means of the particle positions in these two data sets are different. In the case of low frequency, \(100Hz\) and high amplitude, \(0.2d\), the mean of the \(x\) and \(y\) position move around zero whereas in the high frequency, \(500Hz\) and low amplitude, \(0.008d\) case there is a significant drift of the mean over the course of the simulation indicating bulk movement of the particles. In the \(z\) direction particles seem to remain steady in both cases.

In order to further illustrate the movement in the \(xy\) plane, the mean of the \(x\) position is plotted against the mean of the \(y\) position in each layer for the two data sets: the bottom layer, the lower middle layer, the upper middle layer and the top layer. These plots are presented in Figure 4.5. Also, in order to examine the behaviour close to the very top and very bottom, the mean of the \(x\) position in the top-eighth layer and the bottom-eighth layer are plotted against the mean of the \(y\) position in Figure 4.5(e) and (f).

As seen in Figure 4.5(a)–(d), the motion of particles in horizontal direction in the case of low frequency and high amplitude vibration is different from the one with high frequency and low amplitude. When the particles are subject to high frequency and low amplitude, they tend to move further than those that are subject to low frequency and high amplitude. Furthermore, for the high frequency case there is no significant difference of the particle motion in the different depths of the vibration box.
which is different from the low frequency case. In the low frequency case, the motion of particles in the bottom layer is noticeably different from top layer. Particles at the top tend to show more motion than those at the bottom. Moreover, the difference in particle motion in the two data sets is clearly shown in Figure 4.5(e) and (f), where the figures show the same plots as in Figure 4.5 but in thinner layers: the top-eighth and bottom-eighth layers.
Figure 4.4: Mean of particle positions in $x$, $y$ and $z$ direction (measured in particle diameter)
Figure 4.5: Plotting of the mean of the $x$ against the mean of the $y$ positions in different layers (measured in particle diameter)
Table 4.3: Conversion between wavelet scales and time units

<table>
<thead>
<tr>
<th>Wavelet scale</th>
<th>D1</th>
<th>D2</th>
<th>D3</th>
<th>D4</th>
<th>D5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sampled time unit</td>
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<td>8</td>
<td>16</td>
<td>32</td>
</tr>
<tr>
<td>Time (s)</td>
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<td>0.80</td>
<td>1.60</td>
<td>3.20</td>
<td>6.40</td>
</tr>
<tr>
<td>Space scale (d)</td>
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<td>4.89</td>
<td>9.79</td>
<td>19.59</td>
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</tbody>
</table>

4.5.2 Wavelet analysis

A multiresolution wavelet analysis (MRA) was applied to the means of the $x$, $y$ and $z$ position in each layer for the two data sets. In order to compare results of the two data sets, the first data set is sampled before applying the wavelet analysis. This makes the two data sets have the same time stepping of 0.2s. The number of time steps of the first data set was 350 then reduced to 88. Table 4.3 gives a conversion between the wavelet scale, sampled time unit, real time in seconds and space scale in terms of particle diameters. The space scale is calculated by multiplying the average velocity of the particles in the specimen measured in particle diameter by the time.

The MRA of the mean particle positions of data set 1

Figures 4.6–4.8 show the MRA of the mean of the particle positions in each layer in $x$, $y$ and $z$ directions respectively. In each layer and each direction the MRA of the mean particle position at scale $D_1$–$D_5$ are plotted as a function of time. It can be seen in Figure 4.6–4.8 that the magnitude of the MRA of the mean particle position at scale $D_1$ is very small for all layers except the top and top-eighth layers where the particles freely move. The scale $D_3$ clearly shows significant activity while the scale $D_5$ tends to show overall shape of the signal as it is on quite a long scale. The space scale of scale $D_3$ is 4.89$d$. This means that in order to see the significant events the particles have to travel about 4.89 particle diameters. The MRA can clearly identify the difference of the particle motion in different layers, particularly the bottom eighth and the top eighth layers. The MRA of the mean particle positions at scale $D_3$ of this data set will be compared with the MRA of the mean particle positions of data set 2 in section 4.5.3.
Figure 4.6: MRA of the mean of particle position in $z$ direction (Data set 1).
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Figure 4.7: MRA of the mean of particle position in $y$ direction (Data set 1).
Figure 4.8: MRA of the mean of particle position in z direction (Data set 1).
Table 4.4: Conversion between wavelet scales and time units

<table>
<thead>
<tr>
<th>Wavelet scale</th>
<th>D1</th>
<th>D2</th>
<th>D3</th>
<th>D4</th>
<th>D5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sampled time unit</td>
<td>2</td>
<td>4</td>
<td>8</td>
<td>16</td>
<td>32</td>
</tr>
<tr>
<td>Time (s)</td>
<td>0.40</td>
<td>0.80</td>
<td>1.60</td>
<td>3.20</td>
<td>6.40</td>
</tr>
<tr>
<td>Space scale (d)</td>
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<td>0.4</td>
<td>0.8</td>
<td>1.6</td>
<td>3.2</td>
</tr>
</tbody>
</table>

The MRA of the mean particle positions of data set 2

A similar analysis was performed on the second data set. Figure 4.9-4.11 shows the MRA of mean of particle positions in each layer in $x$, $y$, and $z$ directions respectively. In each layer and each direction the MRA of mean particle position at scale D1-D5 are plotted as a function of time. Again, the scale D3 clearly shows significant activity while the scale D1 is very small. The scale D5 seems to show overall shape of the signal. These results will be compared with the results from the data set 1 in section 4.5.3.

Table 4.4 gives a conversion between wavelet scale, sampled time unit, real time in seconds and space scale in term of particle diameter. The space scale of scale D3 is 0.8d. This means that in order to see the significant events the particles have to travel about 0.8 particle diameters.
Figure 4.9: MRA of the mean of particle position in z direction (Data set 2).
Figure 4.10: MRA of the mean of particle position in y direction (Data set 2).
Figure 4.11: MRA of the mean of particle position in z direction (Data set 2).
4.5.3 The MRA of the mean of particle positions at scale D3

According to Figure 4.6-4.11, the scale that clearly shows activity is scale D3. The MRA of the mean of particle position in x, y and z direction at scale D3 of the two data sets are plotted side by side in this section. Respectively, Figure 4.12-4.14 compares the MRA of the mean of particle positions in x, y and z directions in 4 layers: the bottom layer, the lower middle layer, the upper middle layer and the top layer for the two data sets.

![Graphs showing MRA of the mean of particle position in x direction for two data sets](image)

Figure 4.12: MRA of the mean of particle position in x direction.

Firstly, we consider the MRA of the mean of particle position in x direction. It clearly reveals the difference of particle motions of these two data sets. In the low frequency and high amplitude vibration box (data set 1), particles in the bottom, lower middle and upper middle layer move forth and back at the first few seconds after starting vibration and then they only show small movements. Particles in the top layer show different phenomenon due to the free upper surface at the top of the layer. This
allows particles to move freely. For the high frequency and low amplitude vibration case (data set 2), there is no significant differences in the mean of the $x$ position of particles in any layers.

![Figure 4.13: MRA of the mean of particle position in y direction.](image)

We now consider the MRA of the mean of particle position in the $y$ direction. For the data set 1, the low frequency and high amplitude vibration data, as for the $x$ direction there is significantly more change in the mean for particles in the top layer than in the other layers. This is shown in Figure 4.13(a). Again, as for the mean in $x$ direction, the wavelet analysis shows little variation in drift of scale $D3$ for the mean in $y$ direction for the high frequency and low amplitude case (data set 2). This is shown in Figure 4.13(b).
Figure 4.14: MRA of the mean of particle position in z direction.

With regarding to scale D3, for the MRA of the mean particle position in the z direction, the particles subject to low frequency and high amplitude (data set 1) tend to move further than those that are subject to high frequency and low amplitude (data set 2). This motion is in the same direction as the vibration, Figure 4.14. In the low frequency and high amplitude case, 100Hz and 0.2d, we can see clearly that the mean moves up and down while in the high frequency and low amplitude case, 500Hz and 0.008d, the particles move up and down after first few seconds when the vibration applied and then they only stay steady. In both cases, the particles at top layer move more than those in the other layers as they are in the free surface.
The MRA of the mean of particle position in $x$, $y$ and $z$ direction for the particles in the top-eighth layer and the bottom-eighth layer were also calculated. The result at scale $D3$ is shown in Figure 4.15.

Figure 4.15: MRA of mean of particle position in $x$ and $y$ directions for top and bottom eighth layer.

Figure 4.15 clearly shows the same points: for data set 1 there is a strong dependence of behaviour with depth with little variation with time in the mean of scale $D3$ in the bottom layer whereas the means at the scale $D3$ vary significantly with time in the top layer where there is a free surface. In contrast, for data set 2 there is very little depth dependence with the mean at scale $D3$ showing very similar time dependence both in the top layer and the very bottom layer.
4.5.4 The Fluctuating velocity

From the particle positions at successive time steps the velocity of the particles in the \( x, y \) and \( z \) direction were calculated. According to the layers in the \( z \) direction in figure 4.1, the instantaneous mean velocity in layer \( k \) at time \( t \) is given by [88]

\[
\mu(k, t) = \frac{\sum_{i \in k} v_i(t)}{n}
\]  \hspace{1cm} (4.6)

where \( v_i(t) \) is the velocity of particle \( i \) staying in layer \( k \), \( n \) is the number of particle in the layer \( k \). The instantaneous fluctuating velocity, \( C_i(t) \) of particle \( i \) in layer \( k \) is then calculated from,

\[
C_i(t) = v_i(t) - \mu(k, t),
\]  \hspace{1cm} (4.7)

and the instantaneous root mean square (RMS) of the fluctuating velocity of particles in the layer \( k \) is given by

\[
C(k) = \left( \frac{\sum_i [\sum_{i \in k} C_i(t)^2]}{\sum_i n_i(t)} \right)^{1/2}
\]  \hspace{1cm} (4.8)

The granular temperature, \( T \) of layer \( k \) is defined by

\[
T(k) = \frac{m}{3} \cdot (C(k))^2
\]  \hspace{1cm} (4.9)

where \( m \) is the particle mass.

The fluctuating velocity for both data sets was calculated in two different ways. In the first way particles from the layer are traced and in the second way particles occupying the layer at particular time point are considered. Both these approaches are explained in more detail below.
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The fluctuating velocity of particles when tracing the particles

According to Figure 4.1, layers in the z direction were made at $t = 0$ and then particles that originated in these layers were traced. The fluctuating velocity in each layer was calculated. Figures 4.16 and 4.17 shows fluctuating velocity in $x$, $y$ and $z$ directions in each layer for the data sets 1 and 2 respectively.
As we can see from Figure 4.16(a)–(d), most of the fluctuation in velocity comes from the fluctuation in the vertical direction, while in the case of high frequency and low amplitude vibration, Figure 4.17, most velocity fluctuation is due to fluctuations horizontally. Also, Figure 4.16 shows that there is a dependence of fluctuating velocity with depth.
4.5.5 Root mean square of fluctuating velocity of particles in fixed layers

As well as calculating the fluctuating velocity of particles that originated in a particular layer at \( t = 0 \) we also looked at the fluctuating velocity of particles when the layers are fixed. This allows us to study the behavior of particles in different parts of the box. The vibration box is partitioned into layers of thickness equal to the particle diameter, \( d \). Layers are assigned by the \( z \)-coordination. At each time step the fluctuating velocity of particles staying in the layer are calculated. Figure 4.18 shows fluctuating velocity of particles in the selected fixed layers for the two data sets.

As it is clearly seen in Figure 4.18, the fluctuating velocity of particles from data set 1 is higher than those from data set 2. For the data set 1, the fluctuating velocity of particles occupying near the top surface is higher than those occupying near the bottom as revealed in Figure 4.18(a). There is little difference of the fluctuation of velocity in different zones in the high frequency and low amplitude vibration box, Figure 4.18(b). The results agree the results in section 4.5.4 where the particles are traced.

![Figure 4.18: Fluctuating velocity of particles in the fixed layers](image-url)
Root mean square of fluctuating velocity

We now compare the granular temperature of the two data sets by considering the RMS of the fluctuating velocity. In this case, the fixed layers are considered as we are interested in the dependence with the position of the particles within bed. According to equation (4.7), the instantaneous RMS of fluctuating velocity of particles in each layer was computed. Figure 4.19 shows the RMS of the fluctuating velocity of particles in the fixed layers.

![Figure 4.19: the RMS of fluctuating velocity of particles](image)

As shown in the Figure 4.19, the root mean square of fluctuating velocity of particles in the low frequency and high amplitude vibration box is higher than the one in the
high frequency and low amplitude.

4.5.6 Packing fraction

As the layers are fixed, the packing fraction of each layer was calculated. At each time step, the volume occupied by particles staying in the layer were calculated. If particles were partly in the layers, only parts of particles occupying in the layers were taken into account. Figure 4.20 gives comparisons of the packing fraction of the two data sets at some instantaneous times. As seen in Figure 4.20, the high frequency low amplitude (data set 2) vibration gives a higher packing fraction than the low frequency, high amplitude (data set 1).

Figure 4.20: The particle packing
4.6 Vibration of a binary granular mixture

Two data sets are considered here for the binary mixture case: data set 3 and data set 4. Details of each data set are given as follows:

**Data set 3**: The data set was composed of the \(x, y, z\) positions of 1250 small particles and of 156 large particles. The diameter of the small and large particles are \(d_s\) and \(d_L\), respectively. The diameter of the large particle is double of the small one, so the diameter ratio, \(d_L/d_s\), is 2. The ratio of the total volume of large to small particles in a box, \(V_L/V_s\), is 1. The particles are shaken in box with a square base of side length \(12d_s\) with a height of \(15d_s\). The simulation runs for 48 time steps with a time step of 0.2s in the output. The vibration amplitude was 0.2\(d_s\), and the vibration frequency was 100 \(Hz\).

**Data set 4**: The second binary data set was generated using the same conditions as the first one but running with a different vibration amplitude and frequency. The vibration amplitude was 0.008\(d\), and the vibration frequency was 500 \(Hz\).

As described above, the first data set may be called low frequency high amplitude data set while the second data set is at high frequency and low amplitude. The acceleration of the both data sets is 7.8.

The same calculations as performed in the mono-sized case were done for this case. The results are presented as follows. Mean of particle positions in \(x, y, z\) directions are plotted as a function of time in section 4.6.1. Furthermore, in section 4.6.2 – 4.6.4 the MRA of the mean of the particle positions of the two different data sets are compared. Later, in section 4.6.5 the layers are fixed in the \(z\) direction and then the fluctuating velocity, root mean square of the fluctuating velocity of the particles in fixed layers for both data sets are calculated. The granular temperature for the mono-sized and the binary mixture cases are compared at the end of this section.
4.6.1 Mean of particle positions

In the analysis of the binary mixture cases, four layers are made at $t = 0$ according to Figure 4.1 and then particles that originated in these layers were traced. Each layer contains small and large particles. The mean of the particle positions that started out in each layer was calculated as a function of time for both types of particles. Figure 4.21 and 4.22 show the mean of the particle positions in the $x$ and $y$ directions for the large and small particles subject to different frequency vibrations.

Figure 4.21: Mean of particle positions in the $x$ direction (measured in particle diameter)
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Figure 4.22: Mean of particle positions in the $y$ direction (measured in particle diameter)

The mean of the particle positions in these two data sets are different when they are vibrated with different frequencies and amplitude. In the case of low frequency, $100Hz$ and high amplitude, $0.2dg$, the mean of the $x$ and $y$ position move further in the horizontal direction than the one with high frequency, $500Hz$ and low amplitude, $0.008dg$. There are very small differences in the mean particle positions between large and small particles in both cases. Figure 4.23(a)–(d) shows the same plots as in Figure 4.21 but in the $z$ directions. Furthermore, Figure 4.23(e) and (f) show the difference of the mean particle position in $z$ direction between the large particle and
the small particles in each layer for low and high frequency vibration respectively.
The differences between the mean of particle position in z direction for the two data sets are clearly revealed in Figure 4.23(a)-(d). Both type of particles in the low frequency vibration box move up and down. For the high frequency vibration box, the particles tend to stay where they are.

As can be seen in Figure 4.23(a) and (c), the large and small particles move up and down when they are subject to low frequency, 100Hz and high amplitude, 0.2d_s vibration. In order to compare the motion of the small and large particles, the difference of mean particle position between the large and small particles at time t are calculated as follows:

$$z_{\text{different}}(t) = \bar{z}_{\text{large}}(t) - \bar{z}_{\text{small}}(t). \quad (4.10)$$

If the difference of mean is greater than zero, this means the large particles are going up relative to the small particles but if the difference of mean is less than zero, this means the large particles are moving down. Figure 4.23(e) show results of the calculations. Also, the same calculations are performed in the high frequency vibration case as in Figure 4.23(f).

As is clearly shown in Figure 4.23(e), the difference of the mean particle position between the large and small particles in the lower middle, upper middle and top layers increases while in the bottom layer the difference remains steady. This shows that the large particles tend to move up to the top while the small particles move down as also can be seen in Figure 4.23(a) and (c). This is called the Brazil-nut effect (BNE).
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(a) The mean of the small particle position subject to low frequency vibration (data set 3)

(b) The mean of the small particle position subject to high frequency vibration (data set 4)

(c) The mean of the large particle position subject to low frequency vibration (data set 3)

(d) The mean of the large particle position subject to high frequency vibration (data set 4)

(e) low frequency vibration case (data set 3)

(f) high frequency vibration case (data set 4)

Figure 4.23: Mean of particle positions in the z direction (measured in particle diameter)
The Mean of the particle positions in the horizontal directions

In order to see the motion of particles in the horizontal direction, the mean of $x$ position is plotted against the mean of $y$ position in every layer for the two types of particles in both data sets: the bottom layer, the lower middle layer, the upper middle layer and the top layer. These plots are presented in Figure 4.24 and 4.25.

![Graphs showing particle motion](image)

Figure 4.24: The motion of particles in horizontal direction (measured in particle diameter) subject to low frequency vibration (data set 3)

Particles staying in the bottom layer tend to show further motion in horizontal direction than those staying in the layers, especially in the top layer. The large particles tend to show slightly more movement than the small ones.
For the high frequency vibration case, there is very little different in the horizontal motion of the two types of particle as shown in Figure 4.25. There are small differences in each layer.
4.6.2 Wavelet analysis

Similar to a mono-sized spherical case, a multi-resolution wavelet analysis (MRA) was applied to the mean of the \( x, y \) and \( z \) position of particles for the small and large particles in each layer for the two data sets. Due to the large number of figures of the MRA analysis, the MRA of the mean position in the \( z \) direction of the small particles and large particles are selected to show the analysis results. Respectively, Figure 4.26 and 4.27 show the MRA of mean of the \( x \) position of small particle and of the large particle in four layers.

The first case: low frequency and high amplitude vibration (data set 3 )

![Wavelet analysis figures](image)

Figure 4.26: The MRA of the mean of the \( x \) position of the small particles
Figure 4.27: The MRA of the mean of the $x$ position of the large particles
The second case: high frequency and low amplitude vibration (data set 4)

For the second case, the MRA of the mean of the \( x \) position of the small particles and of the large particles in the four layers are presented in Figure 4.28 and 4.29.

Figure 4.28: The MRA of the mean of the \( x \) position of the small particles
As we can see from the Figure 4.28 and 4.29, scale $D_1$ and $D_2$ clearly show activity.
Table 4.5: Conversion between wavelet scales and time units of the data set 3

<table>
<thead>
<tr>
<th>Wavelet scale</th>
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<th>D2</th>
<th>D3</th>
<th>D4</th>
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</thead>
<tbody>
<tr>
<td>Sampled time unit</td>
<td>2</td>
<td>4</td>
<td>8</td>
<td>16</td>
</tr>
<tr>
<td>Time (s)</td>
<td>0.40</td>
<td>0.80</td>
<td>1.60</td>
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<tr>
<td>Space scale (d)</td>
<td>2.68</td>
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Table 4.6: Conversion between wavelet scales and time units of the data set 4

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<tbody>
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<td>Sampled time unit</td>
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</tr>
<tr>
<td>Time (s)</td>
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<td>2.10</td>
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4.6.3 The MRA of mean particle positions at scale D1 and D2

In order to show the conversion between wavelet scales, time unit and space scales, the velocity of small and large particles in each data set averaged over time were calculated. Table 4.5 and 4.6 give a conversion between wavelet scale, sampled time unit, real time in seconds and space scale in term of particle diameter for the data sets. Note that the differences in table 4.5 and 4.6 are a result of the different mean velocities.

The MRA of mean particle position in x, y and z directions at scales D1 and D2 for the two data sets are plotted together as presented in Figure 4.30 and 4.31. As can be seen in Figure 4.30 and 4.31, the MRA of the mean particle positions in a box subject to low frequency and high amplitude vibration (data set 3) have larger absolute values than those subject to high frequency and low amplitude vibration (data set 4) in both scales, D1 and D2. For the low frequency vibration box, the large particles seem to be slightly more excited than the small ones but there is little difference between large and small particles for the high frequency vibration box.
Figure 4.30: The MRA of mean position at scale D1
Figure 4.31: The MRA of mean position at scale D2
4.6.4 The MRA of the difference of mean of $z$ position between the large and small particles

As seen in Figure 4.23, there is some evidence of the Brazil-nut effect in the case of low frequency case from the difference of mean of the $z$ position between the large and small particles. The wavelet transform is applied to the difference of the mean for both data sets. Figure 4.32 and 4.33 show the analysis results for the case of low and high frequency vibration respectively.

Figure 4.32: The MRA of the difference of mean of $z$ position between large and small particles when particles are subject to low frequency vibration.
Figure 4.33: The MRA of the difference of mean of z position between large and small particles when particles are subject to high frequency vibration.
Figure 4.34: The MRA of the difference of mean of $z$ position between large and small particles for scale D1 and D2. In each case, the MRA is given for both low frequency, high amplitude vibration and for high frequency, low amplitude vibration.

The MRA of difference of mean of the $z$ position between large and small particles does not seem to indicate the Brazil-nut effect. The analysis results only show the motion of particles with different fluctuations for the two vibration boxes.

4.6.5 Fluctuating velocity

The fluctuating velocity of the small and large particles in the two data sets were calculated separately using the equation (4.7) in section 4.5.4. In this calculation the layers are fixed with a thickness layer of $2d_S$ or $d_S$, where $d_S$ and $d_L$ are the particle diameter of the small and large particles respectively. Figure 4.35 shows the fluctuating velocity of small and large particles for these two data sets in each layer.

As can be seen in Figure 4.35, the magnitude of the fluctuating velocity of particles under the low frequency and high amplitude vibration is typically higher than that under the high frequency and low amplitude vibration. It does not seem to depend on the depth in both cases.
4.6.6 Root mean square of fluctuating velocity

In order to see the magnitude of fluctuation, the root mean square of fluctuating velocity of small and large particles in fixed layers were also calculated using equation (4.8) in section 4.5.4. Figure 4.36 shows root mean square velocity of small and large particles for these two data sets in each layer. These diagrams clearly show that the velocity of particles subject to low frequency and high amplitude vibration is more fluctuating than that for particles under the opposite scenario. Also, there is little difference of the root mean square of fluctuating velocity between the large and small particles in the case of high frequency vibration. There is dependence on the depth in the case of low frequency and high amplitude vibration.

Figure 4.35: The Fluctuating velocity
4.6.7 The granular temperature

The granular temperature of particles in the 4 data sets was calculated. Figure 4.37 shows 6 different series of the granular temperature along the bed depth: the granular temperature of the particles in 2 mono-sized cases and in 2 binary mixture cases is separately presented for the large and small particles.

The larger granular temperature indicates that the vibration bed is more excited.
4.6.8 Packing fraction

The packing fractions of the fixed layers for the two data sets were calculated. Figure 4.38 shows the packing fraction of particles in these two data sets at 4 intervals of time.

As can be seen in Figure 4.38, the packing fractions of the particles subject to high frequency and low amplitude vibration tend to be higher than that for particles subject to low frequency and high amplitude. A large vibration amplitude (> d/10) leads to a crystallization of the system whereas a small vibration amplitude (< d/40) induces an efficient compaction of the packing [72].
(a) Packing fraction at $t = 0.7s$

(b) Packing fraction at $t = 2.3s$

(c) Packing fraction at $t = 4.3s$

(d) Packing fraction at $t = 8.3s$

Figure 4.38: Packing fraction
4.7 Summary and conclusion

The data sets which result from a simulation study of packing by the application of vertical vibration of spherical particles were analysed. The analysis results of four data sets were presented: two mono-size spherical cases and two binary mixture cases. In each group, different frequencies and amplitudes were applied. In order to see the behaviour of particles in different regions in the box, the box was divided into layers. The MRA was applied to the mean of the particle positions in each layer.

When the particles are subject to different frequencies and amplitude, they show different motions. For the mono-sized case when the particles are subject to low frequency and high amplitude, they tend to move in vertical direction rather than in the horizontal direction which is the same direction of the vibration applied. The particles in the top layer show movement more than particles in the other layers due to a free surface. The motion of particles depends on the bed depth. In contrast, there is very little depth dependence when the particles are subject to high frequency and low amplitude. Furthermore, the particles show the motion in horizontal direction rather than vertical direction. Evidence can be seen in plots of the mean of particle positions, especially plot of the mean of $x$ against the mean of the $y$ positions. The results of the MRA of the mean of the particle positions also strongly support these phenomenon.

Similar calculations were applied to the two binary mixture data sets. For both data sets, the particle movements do not depend on the bed depth but depend on the frequency and amplitude of vibration. The particles subject to low frequency and high amplitude show more movement than those that subject to high frequency and low amplitude in all directions, $x, y$ and $z$ directions.

The fluctuating velocity, the granular temperature were calculated in all cases. Also, the packing fraction was calculated. It can be seen that in the mono-sized case, the high frequency and low amplitude vibration induces an efficient packing of the particles.
Chapter 5

DEM biaxial compression test

5.1 Introduction

This chapter will show results of the analysis of data sets received from Dr. O’Sullivan [10], Imperial College London. These data sets are a result of a discrete element simulation of a biaxial compression test on a dense, two dimensional specimen of discs. There are two equivalent specimens with different numbers of particles: specimen A and specimen B. Three data sets were analysed, one from specimen A and two from specimen B.

This chapter begins with a summary of the phenomena investigated in biaxial compression tests both in experiments and simulations. Subsequently, the results of an analysis of data from specimen A are presented, followed by results of an analysis of data from specimen B in section 5.4. The results of the analysis of the second data set generated from specimen B, made in order to test the robustness of our tool, are presented in section 5.6. Finally, in the last section a summary of the main findings is presented.
5.2 Overview of work in plane strain

Microscale deformations in granular material have been studied experimentally and numerically. Various experimental techniques have been used to investigate the evolution of the internal state. Drescher et al. [1] used the photo-elasticity techniques to verify the flow rules developed for granular assemblies. By averaging forces over a small region called a representative area, ranging from 4-10 particles diameter in the interior of the assembly, it was possible to assign an average stress tensor for that region. From the photographs of successive stages during a deformation cycle it was possible to determine the relative displacement of the individual discs. The flow of granular materials in bunkers was investigated by using the X-ray technique by Bransby et al. [9, 65]. The X-ray technique allowed measurements to be taken of the displacements and strain inside the flowing material.

The stress-strain behaviour and failure patterns of a granular assembly have received a great deal of attention, especially for plane strain (biaxial) compression. Generally, the stress-strain behaviour of a sample under plane-strain compression can be illustrated by stress-strain curves as in Figure 5.1. The figure shows plots of stress ratio against the global axial strain for the responses of two tests: test 1 and test 2. The samples respond differently as displayed by the stress ratio curves. The stress ratio of test 1 is indicated by a dashed-line.

For both tests, during the loading state, the specimens are deformed in a homogeneous way, as illustrated by the increase of stress ratio from point A to B1 in test 1 and to B2 in test 2. The stress ratio increases up to a maximum, when the specimen undergoes incipient failure. As a result of the failure, the stress ratio drops considerably. At failure, the particles slip and rotate against each other along ‘shear bands’ (slip planes). So that the particles can slip and rotate, the sample first undergoes dilation along the slip plane. For test 1, the specimen reaches a critical consolidation level and sustained slip after the initial peak occurs at a constant stress level. Unlike test 1, specimen 2 exhibits oscillations between over-dilation at E2 and G2 and over-consolidation at points D2 and F2 resulting in successive cycles of shearing followed
Desrues and Viggiani [32] experimentally investigated and provided insight into the phenomenon of shear banding in sand using stereophotogrammetry. A number of features of shear banding in plane strain compression of sand were summarised. Stereophotogrammetry indicated that, for all tests, shear banding initiates at, or shortly before, the peak in the stress ratio. As soon as a band traverses the entire specimen, the stress ratio essentially levels off, or slightly increases with increasing global axial strain.

An investigation of the stress fluctuations along the shear band formation was numerically studied by Pena et al. [63]. He performed molecular dynamics simulations of a biaxial test to investigate the behaviour of granular materials under monotonic loading. The micro-structural arrangement of the granular sample was studied by following two internal variables: the co-ordination number and the fraction of sliding contacts. He showed that at large strains the samples reach the critical state independent to their initial density, and they deform at a constant void ratio, volume and
mechanical coordination number. In this state the system approaches and retreats from an unstable behaviour leading to strong fluctuations of stress, as for test 2 in Figure 5.1. The stress drops were correlated to the evolution of the coordination number and to the fraction of sliding contacts. Stress collapses remove the contacts from sliding condition. The characterization of the critical state in terms of a critical coordination number was shown to depend on interparticle friction by Rothenburg and Kruyt [41]. Using the DEM simulation they generated several biaxial tests with varying interparticle friction to confirm that the critical coordination number depends on interparticle friction.

Oda et al. [59] showed how anisotropy is inherently related to the development of shear bands in granular soils. Anisotropy induced by the formation of columns is a common feature in the strain-hardening process. After the peak stress, buckling of the columns becomes apparent. Buckling first takes place at random locations, but then tends to concentrate in conjugate shear bands where strain is localized. The columns collapse by buckling and a new micro-structure is then developed. In the shear bands, large voids appear between the buckling columns. Increase of the shear band thickness results from the growth of large voids between adjacent columns. Rolling, rather than sliding, take place at contacts in parallel with the buckling of columns.

A well-developed column-like structure in the DEM simulation was presented by Iwashita and Oda [39]. The development of shear bands can be simulated well only when the rolling resistance is considered in the DEM. Their result supports strongly the idea that the development of columns is a common feature in the strain hardening process of granular soils. In the strain softening process, buckling of the columns takes place parallel to the development of shear bands. The generation of large voids and particle rotation are produced as a result of the buckling of columns. Their simulation results compare well with the plain strain test which was carried out using natural sands (Toyoura sand), where very large voids appeared in the shear band.

Furthermore, Iwashita and Oda [53] proposed a modified version of distinct element
method (MDEM) to study the micro-deformation mechanism leading to the development of shear bands. The MDEM version is capable of dealing with the rolling resistance at contact points. According to their numerical work, in the hardening process up to failure, particles are arranged in chains to form column-like structures whose elongation directions are more or less parallel to the major principal stress axis. During the process, pre-existing contacts are lost in the minor principal stress direction. As a result of this, an elongated void is generated between two neighboring columns. This is the micro-mechanism leading to dilatancy before failure. The micro-structure becomes more and more anisotropic due not only to the column-like structure but also to the elongated void parallel to the major principal stress direction. Such anisotropic structure becomes gradually unstable because of the loss of surrounding contact points, and is finally collapsed around at the peak stress. A new micro-structure is re-constructed during the following strain softening process. The main micro-process is a kind of buckling of the column-like structure in some limited bands (shear bands). This, leading to the high rotation gradient, makes it possible to continue further concentration of the shear strain and to form large voids between buckling columns. The microstructure reaches a dynamically stable state at the so-called residual state. This means the generation of the newly developed microstructure is balanced with the collapse of the pre-existing structure, leading to a constant void ratio.

The deformation of a large two-dimensional assembly of discs subjected to quasi-static biaxial loading at low and moderate strains was investigated by Kuhn [58, 57]. Numerical DEM experiments were used. The experiments involved the slow biaxial compression of the assembly at pre-failure load levels. Deformation within individual voids were computed from the relative motions of surrounding particles. Evolution of the local fabric was measured in term of void-base parameters. Deformation was very nonuniform at the microscale of individual voids. The microbands, bands of void cells within intense slip deformation, ranged in thickness between one and four particle diameters.
Parameter | Value  
---|---
Density | $20 \times 10^9 \text{kg/m}^3$
Spring Stiffness | $5 \times 10^7 \text{N/m}$
Damping parameter | 0.2
Coefficient of contact friction | 0.3

Table 5.1: Simulation parameters for specimen A

### 5.3 Specimen A

Specimen A consisted of 5728 discs in an initially rectangular domain that is 90 mm wide and 180 mm high. During the simulation the lateral boundaries were modelled as a stress-controlled membrane. The particle radii were uniformly distributed between 0.75 mm and 1.0 mm. The initial porosity was 0.1. The parameters of the simulations are shown in Table 5.1. Further details of simulations are described in O’Sullivan [12].

The simulation of specimen A was run for a total analysis time of 72.64 s corresponding to a total axial strain of 12%. Data was saved at strain intervals of $8.1152 \times 10^{-6}$. Specimen A was subdivided into 23 measurement circles with the radii of 14.36 mm, approximately 14–19 particle diameters as the shear bands observed in experiments in the experiments are shown to be around 4–10 particle diameters across [58, 57]. Each measurement circle roughly contains 230 particles. The measurement circles are illustrated in Figure 5.2(a). For each measurement circle the coordination number, porosity and stress components were recorded along with the analysis time and axial strain. The measurement circles remain in the same position during loading. Figure 5.2 shows the specimen at the first and last time step.

The coordination number, $N$ was calculated using

$$N = \frac{2N_c}{N_p}, \quad (5.1)$$

where $N_c$ is the number of contacts within the measurement circle and $N_p$ is the
CHAPTER 5. DEM BIAXIAL COMPRESSION TEST

Figure 5.2: Specimen A showing the position of the 23 measurement circles.

number of particles. The average stress tensor \( \bar{\sigma}_{ij} \) was calculated from

\[
\bar{\sigma}_{ij} = \frac{1}{V} \sum_{c=1}^{N_c} f_j^c \quad (i, j = x, y)
\]

(5.2)

where \( V \) is the \( i \) component of the area of the measurement circle, \( f_j^c \) is the \( j \) component of the contact force vector at contact \( c \), \( l_i^c = x_i^b - x_i^a \) is the branch vector connecting two contacting particles, \( a \) and \( b \), with centroids \( x_i^a \) and \( x_i^b \). From the stress tensor the principal stress ratio

\[
\frac{\sigma_1 - \sigma_3}{\sigma_1 + \sigma_3}
\]

was constructed, where \( \sigma_1 \) and \( \sigma_3 \) are the principal stresses calculated from the eigenvalues of the stress tensor.

The biaxial simulations considered in this study are analogous to strain controlled triaxial tests typically used in experimental soil mechanics to analyse soil response characteristics. In a physical test the specimen is subject to an all round confining pressure, \( \sigma_r \) and the deviator stress, \( \sigma_d - \sigma_r \), is measured using a load cell placed between the specimen and the loading frame. Since the stress ratio, \( \frac{\sigma_d - \sigma_r}{\sigma_d + \sigma_r} \), versus strain is a common way of representing laboratory data, the analogous quantity was
also computed from the simulation. In the simulation, $\sigma_r$ is equivalent to the stress imposed along the vertical boundaries, and the axial stress $\sigma_a$ is determined by integrating the contact forces along the rigid horizontal boundaries.

5.3.1 Preliminary plots

As shown in Figure 5.2, the circles lie in 10 diagonal planes: plane 1 composed of circles 12, 21, 3, plane 2 composed of circles 11, 20, 2, 17, 8, plane 3 composed of circles 14, 22, 1, 16, 7, plane 4 composed of circles 15, 23, 4, 18, 6, plane 5 composed of circles 5, 19, 9, plane 6 composed of circles 3, 17, 7, plane 7 composed of circles 13, 21, 2, 16, 6, plane 8 composed of circles 12, 20, 1, 18, 9, plane 9 composed of circles 11, 22, 1, 18, 9 and plane 10 composed of circles 14, 23 and 5.

![Diagram of the specimen with planes](image)

(a) Plane 1-5  (b) Plane 6-10

Figure 5.3: Specimen A.

5.3.2 Stress ratio at the boundary

We first consider the simulation results for the axial stress ratio $\frac{\sigma_a - \sigma_r}{\sigma_a + \sigma_r}$ as a function of axial strain. Figure 5.4 shows a plot of stress ratio at the boundary as a function of axial strain. As can be seen in Figure 5.4, the response of the specimen is analogous to the response of a slightly dense sand, the stress ratio increases up to a peak value.
of 0.376 at an axial strain of 1.2%. Post-peak, there is a decrease in the mobilised stresses, with a residual stress ratio of about 0.25 being attained between 6% and 12% strain.

Figure 5.4: Stress ratio, $\frac{\sigma_n - \sigma_v}{\sigma_n + \sigma_v}$, versus axial strain.

Stress ratio, porosity and coordination number

The stress ratio, porosity and coordination number of the measurement circles lying in each diagonal plane of Figure 5.3(b) were plotted as a function of the axial strain. For planes 6–10 the results are shown in Figure 5.5–5.9. As we can see from Figure 5.5–5.9, most circles along each plane achieved a peak stress ratio at different values, mainly between 3.5 and 4.5% and then softened to a state of constant stress with fluctuations. The porosity first decreases slightly with applied axial strain and then dilation occurs. This is also shown by a first increase and then decrease of the coordination number.

So we see that while the behaviour of the principal stress ratio, porosity and coordination number are qualitatively similar in all regions, they can differ quantitatively.
For example, the final porosity varies from 0.155 to 0.175 as seen in Figure 5.5(b).
Figure 5.5: Plot of stress ratio, porosity and coordination number of measurement circles lying in plane 6 as a function of time: (a) stress ratio, (b) porosity and (c) coordination number.
Figure 5.6: Plot of stress ratio, porosity and coordination number of measurement circles lying in plane 7 as a function of time: (a) stress ratio, (b) porosity and (c) coordination number.
Figure 5.7: Plot of stress ratio, porosity and coordination number of measurement circles lying in plane 8 as a function of time: (a) stress ratio, (b) porosity and (c) coordination number.
Figure 5.8: Plot of stress ratio, porosity and coordination number of measurement circles lying in plane 9 as a function of time: (a) stress ratio, (b) porosity and (c) coordination number.
Figure 5.9: Plot of stress ratio, porosity and coordination number of measurement circles lying in plane 10 as a function of time: (a) stress ratio, (b) porosity and (c) coordination number.
5.3.3 Wavelet analysis

A multiresolution wavelet analysis (MRA) was applied to the stress ratio, porosity and coordination number of the 23 measurement circles and also to the stress ratio at the boundary of the specimen. A member of Daubechies, $db2$ was selected as the mother wavelet as discussed in Chapter 3.

**MRA of stress ratio at boundary**

Figure 5.10 presents plots of the stress ratio as well as the detail at each resolution. As can be seen in the figure, the sudden increase in size of $D2$, $D3$, and $D4$ coincides with the peak of the stress ratio.

![Figure 5.10: MRA of the stress ratio, $\frac{\sigma_a - \sigma_c}{\sigma_a + \sigma_c}$, of specimen A at the boundary.](image-url)

Figure 5.10: MRA of the stress ratio, $\frac{\sigma_a - \sigma_c}{\sigma_a + \sigma_c}$, of specimen A at the boundary.
MRA of the stress ratio

In order to investigate if any spatial structure was visible using the MRA technique, the MRA was applied to the principal stress ratio data for each measurement circle. The measurement circle 21 was selected as an example to show this result. Typical results in this case for measurement circle 21 are shown in Figure 5.11.

The graph in Figure 5.11(a) shows the principal stress ratio versus the axial strain for circle 21. This data shows similar characteristics to the stress ratio from the bulk response (as illustrated in Figure 5.4) with a relatively smooth increase to a local maximum value of 0.3435 at an axial strain value of 1.17% before levelling off to an approximately constant level.

Figure 5.11(b)–(h) show the MRA detail coefficients D2 through to D8. Note that the maximum value of the magnitude of the coefficients for the lower detail coefficients is small suggesting that principal stress ratio changes on the scale of D2, D3
### Table 5.2: Strain and space scales related to the detail coefficients for specimen A.

The space scale in mean particle diameters is calculated by dividing the space scale measured in centimetres by the mean particle diameter, 0.0875 cm.

<table>
<thead>
<tr>
<th>Detail</th>
<th>Sample Unit</th>
<th>Strain Scale (%)</th>
<th>Space Scale (cm)</th>
<th>Space Scale (mean particle diameters)</th>
</tr>
</thead>
<tbody>
<tr>
<td>D1</td>
<td>2</td>
<td>0.0016</td>
<td>0.000292</td>
<td>0.0033</td>
</tr>
<tr>
<td>D2</td>
<td>4</td>
<td>0.0032</td>
<td>0.000584</td>
<td>0.0067</td>
</tr>
<tr>
<td>D3</td>
<td>8</td>
<td>0.0065</td>
<td>0.001168</td>
<td>0.0134</td>
</tr>
<tr>
<td>D4</td>
<td>16</td>
<td>0.0130</td>
<td>0.002337</td>
<td>0.0267</td>
</tr>
<tr>
<td>D5</td>
<td>32</td>
<td>0.0260</td>
<td>0.004674</td>
<td>0.0534</td>
</tr>
<tr>
<td>D6</td>
<td>64</td>
<td>0.0519</td>
<td>0.009349</td>
<td>0.1068</td>
</tr>
<tr>
<td>D7</td>
<td>128</td>
<td>0.1030</td>
<td>0.018698</td>
<td>0.2136</td>
</tr>
<tr>
<td>D8</td>
<td>256</td>
<td>0.2060</td>
<td>0.037396</td>
<td>0.4272</td>
</tr>
</tbody>
</table>

and D4 are small. As is particularly clear in D7, there are a number of peaks events that are localized in strain. Each detail corresponds to a different strain scale. Using the strain and the height of the specimen one can also relate the strain to a space scale, as summarised in Table 5.2.

The MRA detail coefficients for all circles were considered. All showed qualitatively similar behaviour with small values for the details D2, D3 and D4 and noticeable peak events in D7. As an example, Figure 5.12 shows D7 from the MRA of the stress ratio of the measurement circles along plane 7. Note that peaks at approximately regular intervals appear to occur: this is particularly clear around an axial strain of 6%.
Similar peaks were seen in the wavelet analysis for the other circles. In order to systematically identify if the peaks in the details correlated to a particular spatial structure/time structure, for each circle, each detail $D_j$, was divided into 25 equal intervals in axial strain. For each interval, the maximum absolute value of the MRA detail coefficient was evaluated. Each circle was then shaded according to this value. Typical examples are shown in Figure 5.13 for $D3$, $D7$ and $D8$ for the axial strain interval of 5.80%-6.28%.

In scale $D3$, the sample appears fairly homogeneous with little variation in the shading in the main part of the specimen but noticeably activity in the corners. For the same strain interval at scale $D7$, Figure 5.13(b), the shading indicates the maximum value of the detail coefficient $D7$ is relatively large along a line from the top left sloping down to the middle at the right. At scale $D8$, the sample also shows high values of the detail coefficient, but less than at scale $D7$, Figure 5.13(c).
Figure 5.13: Measurement circles shaded according to the magnitude of the MRA detail coefficients for the principal stress ratio (The maximum value of the MRA is 0.016).

According to Figure 5.11(b)-(h) and Figure 5.13 the scale that clearly shows important events is scale D7. Figure 5.14 and Figure 5.15 shows measurement circles shaded according to the maximum of the magnitude of the absolute value of the MRA of the stress ratio at scale D7 for the same intervals of axial strain. As seen in Figure 5.14 and 5.15, the maximum value of the MRA of measurement circles along plane 7 are comparatively large at the axial strain interval of 5.80%-6.28%, Figure 5.14(l). The plane 7 is a line that passing through circles 13, 21, 2, 16 and 6.
Figure 5.14: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale D7 for strain interval starting at 0.485% and ending at 6.28% (The maximum absolute value of the MRA is 0.016).
Figure 5.15: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale D7 for strain interval starting at 6.28% and ending at 12.09% (The maximum absolute value of the MRA is 0.016).
MRA of porosity

A similar analysis was also carried out for the porosity. The MRA of the porosity of the 23 measurement circles were calculated. Again, the measurement circle 21 was selected as an example to show this result. Typical results in this case for measurement circle 21 are shown in Figure 5.16. Figure 5.16(b)–(h) show the MRA detail coefficients $D_2$ through to $D_8$. Note that the maximum value of the magnitude of the coefficients for the lower detail coefficients is small suggesting that coordination number changes on the scale of $D_2$, $D_3$ and $D_4$ are very small. As is particularly clear in $D_7$, there are a number of peaks events that are localized in strain.

Figure 5.16: MRA of the porosity for circle 21.
The results of the MRA analysis of the 23 measurement circles are shown in Figure 5.17 and Figure 5.18. The measurement circles are again shaded according to the maximum absolute value of the MRA detail coefficients of porosity at scale D7 in a given axial strain interval. The same intervals of axial strain were used as those used in the MRA of the stress ratio.

It is clearly seen that there are no very high peak events in the MRA of the porosity until the axial strain reaches 1.45%, as in Figure 5.17(c). After that, there are occasional changes as seen in Figure 5.17(f)–(i). At the axial strain interval of 5.80% to 6.28%, the measurement circles along plane 7 show a high magnitude of MRA of porosity, Figure 5.17(l).
Figure 5.17: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for porosity at scale D7 for strain interval starting at 0.485% and ending at 6.28%.
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Figure 5.18: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for porosity at scale D7 for strain interval starting at 6.28% and ending at 12.09%.
Finally, the MRA was applied to the coordination number data from the 23 measurement circles. The measurement circle 21 was again selected as an example to show this result. Figure 5.19(a) shows the coordination number versus the axial strain and Figure 5.19(b)–(h) show the MRA detail coefficients $D_2$ through to $D_8$. As is particularly clear in $D_7$, there are a number of peaks events that are localized in strain.

The results of MRA analysis of the 23 measurement circles are shown in Figure 5.20 and Figure 5.21. The 23 measurement circles are shaded according to the maximum absolute value of the MRA at scale $D_7$ for a given strain interval. The same intervals of axial strain were used as for the porosity and the stress ratio. It can be seen that there are no peak events in the coordination number until at the axial strain interval of 0.967% to 1.45%. Also, the measurement circles along plane 7 show high magnitude of MRA of coordination number at the axial strain interval of 5.80% to 6.28% as in Figure 5.20(i).
Figure 5.20: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for coordination number at scale D7 for strain interval starting at 0.485% and ending at 6.28%.
Figure 5.21: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for porosity at scale D7 for strain interval starting at 6.28% and ending at 12.09%.
Figure 5.22: Particles shaded according to the absolute value of their cumulative rotation.

5.3.4 Cumulative rotation plot

The results of the MRA suggests that there is a shear band onsetting at an axial strain of 5.8% along plane 7. For comparison the cumulative rotation for each of the strain intervals was calculated. This is a common method for visualising shear banding in 2 space dimensions. Cumulative rotation plots for three successive strain intervals are shown in Figure 5.22.

It can be seen in Figure 5.22, the cumulative rotations indicate that there is a clear localization of rotational activity indicative of a shear band along plane 7 in a position consistent with results from MRA technique. These can be compared with Figure 5.14(l), Figure 5.17(l) and Figure 5.20(l).

As is evident both from the MRA and the cumulative rotation plots the amount of activity can vary significantly from one strain interval to the next: in strain interval 5.8%–6.28% the shear band is clearly visible, but it is less visible in the following interval 6.28%–6.77%.
5.3.5 Wavelet cross-correlation

As we know, the wavelet transform can pick up local fluctuations at different scales of strain. The MRA results in a number of series of wavelet coefficients of different scales of strain for each circle. We will make use of cross correlation in order to see if a change in the stress ratio in one circle correlates with any changes in porosity or coordination number in the other circles.

Cross-correlation between stress ratio and porosity

Cross-correlation calculations between the absolute values of the detail coefficients for the stress ratio and porosity for each circle for scale $D_1$–$D_6$ and for all reasonable lags were carried out. As presented in chapter 3, the cross-correlation between the absolute value of the wavelet coefficients of two signals over time delay $\tau$ at scale $j$ is defined as

$$
 r(|d|) = \frac{\sum_k (|d_x(j,k)| - |\tilde{d}_x(j,k)|)(|d_y(j,k+\tau)| - |\tilde{d}_y(j,k)|)}{\sqrt{\sum_k (|d_x^2(j,k)| - n|\tilde{d}_x(j,k)|)(\sum_k (|d_y^2(j,k+\tau)| - n|\tilde{d}_y(j,k)|)}}
$$

where $d_x(j,k)$ and $d_y(j,k)$ are respectively the wavelet coefficients of signal $x$ and $y$ at scale $j$ and $\tau$ denotes the delay between two signals or time lagging. The values of the cross-correlation coefficients were investigated to confirm whether or not they were statistically significant. In order to do this, a student $t$-test was applied to test the hypothesis that there was no cross-correlation. In order to apply this test we consider the value of

$$
 t = \frac{r(|d|)\sqrt{n-2}}{\sqrt{1 - r(|d|)^2}},
$$

where $n$ is the number of data points in the time series. For specimen A and detail $D_7$ the $n = 117$. If, for example, $r(|d|) = 0.422$, then this gives a value of $t = 4.99$ and we can reject the hypothesis that there is no cross-correlation with a certainty of more than 99%.
Each measurement circle was then shaded according to the magnitude of the cross-correlation coefficient, as shown for D1-D6 in Figure 5.23.

Figure 5.23: Measurement circles shaded according to cross-correlation coefficient between the absolute values of the wavelet detail coefficients of stress ratio and porosity for scale D1-D6 at lag 0.
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### Table 5.3: Cross-correlation coefficient between the absolute values of the detail coefficients of stress ratio and porosity along plane 7 at scale D4

<table>
<thead>
<tr>
<th>Measurement circle</th>
<th>Lag</th>
<th>Correlation coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0</td>
<td>0.464</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>0.343</td>
</tr>
<tr>
<td>13</td>
<td>0</td>
<td>0.572</td>
</tr>
<tr>
<td>16</td>
<td>0</td>
<td>0.2649</td>
</tr>
<tr>
<td>21</td>
<td>0</td>
<td>0.2690</td>
</tr>
</tbody>
</table>

### Table 5.4: Cross-correlation coefficient between the absolute values of the detail coefficients of stress ratio and porosity along plane 7 at scale D5

<table>
<thead>
<tr>
<th>Measurement circle</th>
<th>Lag</th>
<th>Correlation coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0</td>
<td>0.461</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>0.274</td>
</tr>
<tr>
<td>13</td>
<td>0</td>
<td>0.542</td>
</tr>
<tr>
<td>16</td>
<td>0</td>
<td>0.475</td>
</tr>
<tr>
<td>21</td>
<td>0</td>
<td>0.434</td>
</tr>
</tbody>
</table>

It can be seen in Figure 5.23(a)-(c), only cross-correlation coefficients of some measurement circles at boundary are significance but the coefficients are not high. However, at scale D4 and D5 the measurement circles along plane 7 seem to show significance as well as some measurement circles at the boundary.

As previously seen in results of MRA analysis, the highest peaks occur along the plane 7. The cross-correlation coefficient between the absolute values of the wavelet detail coefficients of stress ratio and porosity was calculated for each circle. The most significant results were found for circles in plane 7. Significant values for the cross-correlation coefficients were only found for a lag of 0. Table 5.3 and 5.4 reveal the cross-correlation coefficient between the absolute values of the detail coefficients of stress ratio and porosity for the measurement circles along plane 7 at scale D4 and D5 respectively.
Cross-correlation between stress ratio and coordination number

Cross-correlation coefficients between the absolute values of the wavelet detail coefficients for the stress ratio and coordination number for each circle for scale D1–D6 and for all reasonable lags were also calculated. Each circle was then shaded according to the magnitude of the cross-correlation coefficient, as shown for D1–D6 in Figure 5.24.

![Measurement circles shaded according to cross-correlation coefficient between the absolute values of the detail coefficients of stress ratio and coordination number for scale D1-D6 at lag 0.](image)

Figure 5.24: Measurement circles shaded according to cross-correlation coefficient between the absolute values of the detail coefficients of stress ratio and coordination number for scale D1-D6 at lag 0.

It can be seen in Figure 5.24 that the cross-correlation coefficients are largest in the corners.
5.4 Specimen B

Specimen B, a larger specimen, was considered in order to further test the wavelet technique. The data sets were generated using the same conditions as in specimen A. Specimen B had the same aspect ratio as specimen A but 12512 particles as compared with 5728 particles for specimen A. As for specimen A the particles were uniformly distributed between 0.75 mm. and 1.0 mm. The particle properties are given in Table 5.1. The simulation of this specimen has a longer running time. The simulation of specimen was run for a total analysis time of 187.48s corresponding to a total axial strain of 15.5%. The data was output at axial strain intervals of $5.4374 \times 10^{-6}$.

Similar to specimen A, the specimen was subdivided into 23 measurement circles with the radii of 28.72 mm, approximately 28–38 particles diameter. There are around 900 particles in each measurement circle. For each measurement circle the coordination number, porosity and stress components were recorded with the analysis time and axial strain. The measurement circles remain in the same position during loading. The location of the measurement circles is relative to the specimen at the beginning of loading. Two data sets were generated from specimen B. For the second data set the initial conditions for all the particles were identical to the first so that the behaviour of the sample was identical in both cases. However, in the second data set, the 23 measurement circles were slightly moved downward. Figure 5.25 shows the positions of the 23 measurement circles of the first run and the second run.
5.4.1 Preliminary plots

**Stress ratio at the boundary of specimen**

Figure 5.26(a) shows plots of the stress ratio at the boundary of specimen B as a function of axial strain. The stress ratio increases up to a peak value of 0.369 at the axial strain of 1.21%. The similarities between this behaviour and that for specimen A can be seen in Figure 5.26(b) where the stress ratio for both specimen A and B are shown. Both specimens show qualitatively similar behaviour. The characteristic contact loading followed by slippage is visible.
Figure 5.26: Stress ratio at the boundary of specimen A and B.
Stress ratio, porosity and coordination number

The measurement circles were positioned into 10 diagonal planes as shown in Figure 5.3 in section 5.3.1. The stress ratio, porosity and coordination number of measurement circles lying on each diagonal plane were plotted as a function of the axial strain. Planes 2 and 7 were selected to show these plots and are shown in Figure 5.27 and 5.28 respectively.
Figure 5.27: Plot of stress ratio, porosity and coordination number of measurement circles lying in plane 2 as a function of time: (a) stress ratio, (b) porosity and (c) coordination number.
Figure 5.28: Plot of stress ratio, porosity and coordination number of measurement circles lying in plane 7 as a function of time: (a) stress ratio, (b) porosity and (c) coordination number.
5.4.2 Wavelet analysis

Similar to specimen A, a multiresolution wavelet analysis (MRA) was applied to the stress ratio, porosity and coordination number of the 23 measurement circles and also to the stress ratio at the boundary of specimen. A member of Daubechies, \( db2 \) was again selected as a mother wavelet.

MRA of stress ratio at boundary

Figure 5.29 shows the results of a MRA of the stress ratio at the boundary: plot of stress ratio and the details at each scale.

![Wavelet Analysis Graphs]

Figure 5.29: MRA of the stress ratio of specimen B.
MRA of stress ratio

A similar analysis using the MRA technique was applied to this data set. The principal stress ratio data for each measurement circle was wavelet transformed. Again, the measurement circle 21 was selected to illustrate the typical effect of applying an MRA to the stress ratio. Figure 5.30 presents the MRA of measurement circle 21. The graph in figure 5.30(a) shows the local stress ratio versus the axial strain. Figures 5.30(b)–(h) show the MRA detail coefficients D2 through to D8.

Figure 5.30: MRA of the stress ratio of measurement circle 21 of specimen B.

Figure 5.30(a) shows similar characteristics to the stress ratio from the bulk response with a relatively smooth increase to a local maximum value of 0.4124 at an axial strain value of 1.18% before leveling off to an approximately constant level. Similar to specimen A, high peak events are clearly seen at the scale D7. There are very small changes at scale D2–D4.

The MRA was applied to the stress ratio data for each measurement sphere and
Table 5.5: Space and strain scales related to detail coefficients for specimen B. The space scale in mean particle diameters is calculated by dividing the space scale in centimetres by the mean particle diameter, 0.0875 cm.

then the total strain interval was divided into 25 equal intervals and the circles were shaded according to the maximum absolute value of the MRA detail coefficient for each interval. Since again most activity was at the larger details, only D7 is shown. The relation between the different detail coefficients and strain/space scales is given in table 5.5.

Figures 5.31 and 5.32 present measurement circles shaded according to the maximum absolute value of MRA of the stress ratio in the given strain interval at scale D7.

As seen in Figures 5.31 and 5.32, the shading shows that D7 is not homogeneous in either strain or space. There are measurement circles that show high magnitudes of absolute MRA of stress ratio at various intervals of axial strain. Firstly, we can see measurement circles showing up high magnitudes along a line from the top right down to the middle left at the axial strain interval of 2.48%-3.11%, Figure 5.31(e). This pattern can be seen again at the axial strain interval of 3.73%-4.35%, Figure 5.31(g). According to Figure 5.3(a), this line is plane 2 consisting of measurement circles 2, 8,
11, 17 and 21.

As the axial strain increases to the interval of 6.83%–7.45%, Figure 5.31(l), different measurement circles show high magnitudes of absolute MRA. There are measurement circles along plane 7 rather than plane 2. Again, it can be seen at the axial strain interval of 11.2%–11.8%, Figure 5.32(g).
Figure 5.31: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale D7 for strain interval starting at 0.108% and ending at 7.45% (The maximum absolute value of the MRA is 0.016).
Figure 5.32: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale D7 for strain interval starting at 7.45% and ending at 15.5% (The maximum absolute value of the MRA is 0.016).
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MRA of porosity

A similar analysis was also carried out on the porosity data. The MRA of the porosity of the 23 measurement circles was performed. Scale D\textsubscript{7} again revealed a number of peak events. The results of MRA analysis are shown in Figure 5.33 and Figure 5.34. The measurement circles were shaded according maximum absolute value of the MRA detail coefficient at scale D\textsubscript{7} for the same intervals of axial strain as shown for the MRA of stress.

It is clearly seen that there are no significant changes in the maximum absolute value of the MRA detail coefficient at scale D\textsubscript{7} for the porosity until the axial strain reaches the interval of 1.24\%–1.87\% as in Figure 5.33(c). The same pattern as seen in the MRA of stress ratio can be seen at the axial strain of 1.87\%–2.48\%, Figure 5.33(d).
Figure 5.33: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for porosity at scale D7 for strain interval starting at 0.108% and ending at 7.45% (The maximum absolute value of the MRA is 0.0004).
Figure 5.34: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for porosity at scale $D_7$ for strain interval starting at $7.45\%$ and ending at $15.5\%$ (The maximum absolute value of the MRA is 0.0004).
MRA of the coordination number

The MRA was applied to the coordination number of the 23 measurement circles. Again, scale D7 reveals a number of peak events. The results of MRA analysis are shown in Figure 5.35 and Figure 5.36. The 23 measurement circles were shaded according to the maximum absolute value of MRA of the coordination number in the given strain interval at scale D7.

The MRA of coordination number seems to show a change first at the axial strain interval of 1.87–2.48%. Measurement circles showing high magnitudes can be seen along a line from the top right down to the middle left.
FIGURE 5.35: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for coordination number at scale D7 for strain interval starting at 0.108% and ending at 7.45%.
Figure 5.36: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for coordination number at scale D7 for strain interval starting at 7.45% and ending at 15.5%.
5.4.3 Wavelet cross-correlation

Cross-correlation between the absolute values of the wavelet coefficients of the stress ratio and porosity and between the stress ratio and the coordination number for scale D1–D8 and for all reasonable lags were calculated.

**Cross-correlation between the stress ratio and the porosity**

Cross-correlation calculations between the absolute values of the detail coefficients for the stress ratio and porosity at lag 0 for each circle for scale D1–D8 were carried out. Each circle was then shaded according to the magnitude of the cross-correlation coefficient, as shown for D1–D8 in Figure 5.37.

**Cross-correlation between the stress ratio and the coordination number**

Cross-correlation between the absolute values of the detail coefficients for the stress ratio and coordination number at lag 0 for each circle for scale D1–D8 were also calculated and then each circle was shaded according to the magnitude of the cross-correlation coefficient, as shown for D1–D8 in Figure 5.38.

After applying the student’s t-test, there are some measurement circles, mainly at the boundary that show statistically significant cross-correlation between the absolute values of the detail coefficients for the stress ratio and porosity and cross-correlation between the absolute values of the detail coefficients for the stress ratio and coordination number, but the magnitude of the coefficients are not high.

Cross-correlation between the absolute values of the detail coefficients for the stress ratio and porosity of specimen B is not as high as of specimen A. This is possibly because of large measurement circles. Consequently, it may be that, although peak events in a circle are identifiable, some of the detail required for cross-correlation is averaged out.
Figure 5.37: Measurement circles shaded according to cross-correlation coefficient between the absolute value of the detail coefficients of stress ratio and porosity for scale D1–D8 at lag 0.
Figure 5.38: Measurement circles shaded according to cross-correlation coefficient between the absolute value of the detail coefficients of stress ratio and coordination number for scale D1-D8 at lag 0.
CHAPTER 5. DEM BIAXIAL COMPRESSION TEST

5.5 Specimen B with measurement circles moved down

The second data set of specimen B was generated with different positions of the measurement circles, as shown in Figure 5.25(b). This was in order to see if moving the measurement circles significantly changes the results. The same analysis was repeated. The MRA of the stress ratio, the MRA of the porosity and the MRA of the coordination number of each measurement circles are shown as in section 5.5.1. In section 5.5.2 the results of a cross-correlation study are presented.

5.5.1 MRA of the stress ratio, the porosity and the coordination number

The MRA was applied to the stress ratio, porosity and coordination number and then the total strain interval was divided into 25 equal intervals and the circles were shaded according to the maximum absolute value of the MRA detail coefficient for each interval. Since again most activity was at the larger details, only scale D7 is shown. Figure 5.39 and Figure 5.40 present the MRA of the stress ratio. Figure 5.41 and Figure 5.42 present the MRA of the porosity. Finally, Figure 5.43 and Figure 5.44 show the MRA of the coordination number.

As can be seen in Figure 5.39–Figure 5.44, lines of changes of magnitude of MRA are still clear as seen in Figure 5.31–5.35 at the same intervals of axial strain. For example, the MRA of the stress ratio we can firstly see a line of dark measurement circles along the top right down to the middle left at the interval of axial strain of 2.48–3.11%, Figure 5.39(e).
Figure 5.39: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale D7 when circles moved down for strain interval starting at 0.108% and ending at 7.45% (The maximum absolute value of the MRA is 0.016).
Figure 5.40: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale D7 when circles moved down for strain interval starting at 7.45% and ending at 15.5% (The maximum absolute value of the MRA is 0.016).
Figure 5.41: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for porosity at scale D7 when circles moved down for strain interval starting at 0.108% and ending at 7.45% (The maximum absolute value of the MRA is 0.0004).
Figure 5.42: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for porosity at scale D7 when circles moved down for strain interval starting at 7.45% and ending at 15.5% (The maximum absolute value of the MRA is 0.0004).
Figure 5.43: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for coordination number at scale D7 when circles moved down for strain interval starting at 0.108% and ending at 7.45%.
Figure 5.44: Measurement circles shaded according to the maximum absolute value of the MRA detail coefficients for coordination number at scale D7 when circles moved down for strain interval starting at 0.108% and ending at 7.45%.
Table 5.6: Cross correlation between absolute wavelet coefficients of stress ratio and porosity for measurement circles along plane 7 at scale D7 when measurement circles moved down.

5.5.2 Wavelet cross-correlation

Cross-correlation between the absolute values of the detail coefficients for the stress ratio and porosity at lag 0 for each circle for scale D1–D8 were calculated and then each circle was shaded according to the magnitude of the cross-correlation coefficient, as shown for D1–D8 in Figure 5.45.

Cross-correlation between stress ratio and porosity

As explained in section 5.4.3, the cross-correlation results were not very conclusive for specimen B, possibly because the size of the measurement circles is too large. There are only measurement circle at the boundary showing significant cross-correlation coefficients but the magnitude of the coefficients are not high.

Cross-correlation between stress ratio and coordination number

Figure 5.46(a)–(h) show measurement circles shaded according to the cross-correlation coefficient between the absolute values of the detail coefficients of stress ratio and coordination number for scale D1–D8 at lag 0. Similar to the results of the cross-correlation between absolute wavelet coefficients of stress ratio and porosity, there are only measurement circle at the boundary showing significant cross-correlation coefficients but the magnitude of the coefficients are not high.
Figure 5.45: Measurement circles shaded according to cross-correlation coefficient between the absolute values of the detail coefficients of stress ratio and porosity for scale D1–D8 at lag of specimen B when the measurement circles are moved down.
Figure 5.46: Measurement circles shaded according to the cross-correlation coefficient between the absolute values of the detail coefficients of stress ratio and coordination number for scale D1–D8 at lag 0 of specimen B when the measurement circles are moved down.
Cumulative rotation plot

Similar to specimen A, the results of the MRA analysis of the local stress ratio, porosity and coordination number of specimen B were compared with the cumulative rotation. According to the analysis results in section 5.4.2 and section 5.5.1, three intervals of axial strain are selected to show plots of the cumulative increment rotation. Figure 5.47 shows cumulative rotation plots of 3 intervals of axial strain: 0.62%–1.24%, 1.87%–2.48% and 2.48%–3.11% for specimen B. In order to see the position of the measurement circles relative to the slip plane, the position of measurement circles is also shown and Figure 5.48 shows the similar plot when measurement circles are moved down.

It can be seen in Figure 5.47 and Figure 5.48, the cumulative rotations indicates that there is a clear localization of rotational activity indicative of a shear band along a line that passes through measurement circles 8, 17, 2, 20 and 11, plane 2, in a position consistent with the results from the MRA technique.

![Figure 5.47: Particles shaded according to the absolute value of their cumulative rotation.](image-url)
5.6 Summary and conclusions

An MRA analysis of data from a DEM simulation of two different specimens subject to a planar biaxial strain were presented in this chapter. Three data sets were analysed. In each specimen, the specimen was sub-divided into 23 small regions, measurement circles, in space. Three quantities are focused on in each small region: the stress ratio, the porosity and the coordination number. By applying the MRA to the stress ratio, the porosity and the coordination number of each measurement circle and considering intervals in axial strain, the MRA coefficients can identify where and when the significant events occur. The wavelet analysis indicates that most activity occurs along a line, plane 7 for specimen A and plane 2 for specimen B. This line coincides with lines along which there is maximal cumulative rotation of the particles.
Chapter 6

Triaxial compression test

6.1 Introduction

This chapter shows results of the analysis of data sets which are results of a discrete element simulation of a triaxial compression test. These data sets were provided by Geraldine Cheung, a PhD student from Imperial College. Three data sets were analysed.

The chapter begins with a brief summary of work in triaxial compression testing. The details of the contact model are described in section 6.3. A similar analysis to the case of biaxial test were carried out. The results of an analysis of the first 3D data set are presented as a preliminary result in section 6.4 and then followed by the results of two further data sets in section 6.5 and 6.6 respectively.
6.2 Overview of work in triaxial compression test

A triaxial compression test is a common procedure used to study behaviour of soil. The structure responses of specimens under triaxial compression have been numerically studied, e.g. by using the finite element simulations [27, 50] and DEM simulations [20, 17]. Huang et al. [27] have shown that the failure mode in triaxial tests do not depend on the initial imperfections. Softening behaviour of specimens has been examined also.

An experimental investigation of the localisation phenomena in sands under very low-confining pressure was studied using F-75 Ottawa sand by Alshibli et al. [4]. He used computed tomography and other digital image techniques to study the development and evolution of shear bands under very low-confining pressure (0.05–1.3kPa). He also compared the development and evolution of shear bands in the triaxial case with the biaxial case. Experimental findings show that the failure of specimens subjected to plain strain loading conditions are characterized by distinct shear bands accompanied by softening in the stress response depending on the specimen density and confining pressure, as discussed in section 5.2. In contrast, specimens in triaxial compression experiments dilate uniformly in the locality of peak stress and can develop either complex multiple symmetrical radial shear bands at higher axial strain levels or a few large shear bands. Based on this work, it is quite clear that the deformation processes and the stability behaviour are quite different for triaxial and plane strain tests.

The fact that multiple shear bands can form in triaxial tests was also found by Desrues et al. [18, 31]. The evolution of global and local densities during the test in terms of the void ratio ($e$) was monitored by Desrues et al. [18, 31] by using computer tomography. The numerical image of the cross sections recorded during the test not only gives qualitative but also provides quantitative information. The global and local void ratios were plotted in term of the axial strain. Here, the term global means averaged cross section of specimen while local means averaged over a zone identified as a localized shear zone. Local curves depart from the global ones as soon as a localized
zone is detected for the specimen considered. The slope of the local curve is higher indicating that the void ratio averaged over the localised zone changes faster than the global one. The major result is that all these local curves tend to reach the same plateau whose level is significantly higher than the level of global curves. The void ratio corresponding to the ultimate part (plateau) of the local curve is approximately 0.85 ± 0.02.

Furthermore, an X-ray computed tomography (CT) was used to investigate the three dimensional (3D) microstructure of a shear band by Oda et al. [60]. The sample that they used was solidified before observing the particle-scale microstructure. This showed the structure called columns which is commonly observed around large voids in the shear band. The direction of the columns is parallel, on average, to the maximum principal stress direction. When the sample is stressed beyond a peak, the columns start buckling in shear bands, thus forming inclined columns. More importantly, large voids are generated between such buckling columns as discussed in the biaxial test, section 5.2.
6.3 Simulation Model

6.3.1 Triaxial test simulation: Sample generation

The sample is a cylinder initially of 20 mm radius and 80 mm high filled with 12622 particles. The particles radii were uniformly distributed between 0.88 mm and 1.32 mm. The simulation was initialised by first placing the particles at random within the specimen. The isotropic confining pressure was set up to be 10MPa. This was done by moving the walls to provide an appropriate force on the specimen. The axial force was then applied by moving the top platen slowly downwards. The test is carried out to 12% of the axial strain.

6.3.2 Contact models

Three data sets were generated from a simulation of a triaxial test using DEM. In this simulation, the simulation model is different from that used for the biaxial test discussed in Chapter 5. The discrete element model with bonding model were used. For the discrete element method, the following assumptions are used:

- The particles are rigid.
- The particles are allowed to overlap at the small area of contact.
- The particles interact only at the contact area.
- The contact constitutive model relates to the contact force and overlap.

Two main models are included: the contact stiffness model and the parallel-bond model.

Contact stiffness model

The force-displacement law for the grain behavior at each contact is described by contact normal force and contact tangential force. The normal force is calculated by

\[ F = KU, \]  \hspace{1cm} (6.1)
where $U$ is the overlap and $K$ is the contact stiffness. The shear force is given by the cumulative tangential displacement at the contact point.

Parallel-bond model

The parallel-bond model is a model used to describe a cement-based portion of force-displacement behaviour [19]. At each cemented contact, a parallel bond is defined by three parameters: the stiffness consisting of normal and shear stiffness, the strength consisting of tensile and shear strength and the parallel-bond radius.

Parallel bonds can transmit both force and moment between particles. The total force and moment carried by the parallel bond are denoted by $F_{pb}^n$ and $M_{pb}$. The maximum tensile and shear stress acting on the parallel-bond are calculated from

$$\sigma_{\text{max},pb} = \frac{-F_{pb}^n}{A_{pb}} + \frac{|M_{pb}|}{I_{pb}} R_{\text{bond}}$$  \hspace{1cm} (6.2)$$

$$\tau_{\text{max},pb} = \frac{|F_{pb}^s|}{A_{pb}}$$  \hspace{1cm} (6.3)$$

where $R_{pb}$ is the radius bond, $I_{pb}$ is the moment of inertia of parallel-bond, $A_{pb}$ is the area of parallel bond, $M_{pb}$ is the computed moment at the parallel-bond and $F_{pb}^n$ and $F_{pb}^s$ are the computed normal and shear force at the parallel-bond respectively.

Parameters used in the sample generation are shown in Table 6.1. Three data sets were generated from this simulation. The analysis results of these data sets is shown in the next sections.
<table>
<thead>
<tr>
<th>Sphere properties</th>
<th>Parallel bond properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radius = 0.00088 – 0.00132m</td>
<td>strength = $5.2 \times 10^4$ kPa</td>
</tr>
<tr>
<td>Young's modulus(Ec) = $1.43 \times 10^6$ kPa</td>
<td>Young's modulus(Epb) = $1.82 \times 10^6$ kPa</td>
</tr>
<tr>
<td>friction coefficient ($\mu$) = 0.25</td>
<td></td>
</tr>
</tbody>
</table>

Table 6.1: Parameters using in sample generation for the triaxial compression test.
6.4 Preliminary 3D data set

As mentioned in the section 6.3.1, the cylinder which was 20 mm radius and 80 mm high was filled with 12622 particles. The particle radii were uniformly distributed between 0.88 mm and 1.32 mm. In this data set, the sample was subdivided into 59 (numbered 101 to 159) measurement spheres which were 10 mm in diameter, approximately 3-5 particles diameter. The confining pressure was controlled by a servo-control. For each sphere the coordination number, and stress components were recorded with the analysis time and axial strain. The test was carried out to 12% of the axial strain and data was output at increments of $3.7659 \times 10^{-3}\%$, giving a total number of 3187 data points. The measurement spheres remain in the same position during loading. The location of the measurement spheres is relative to the specimen at the beginning of loading. Figure 6.1 shows the cylinder with the 59 measurement spheres. Figure 6.1(a) shows 59 spheres and cross-section with the portion of the overlapping spheres in (d). Non-overlapping measurement spheres are shown in (b), (c), (e) and (f) with their cross sections.

![Figure 6.1: A cylinder with measurement spheres.](image-url)
6.4.1 Preliminary plots

The overall stress ratio from boundary measurements was plotted as a function of axial strain as shown in figure 6.2. The stress ratio increases up to a peak value of 0.763 at the axial strain of 3.24%.

![Stress Ratio from boundary measurements](image)

**Figure 6.2:** Stress ratio of bulk versus axial strain

In order to look inside the cylinder, different cross-sections were considered as shown in Figure 6.3. Figure 6.3(a) shows a cylinder with non-overlapping measurement spheres. Figure 6.3(b) and (c) show cross-sections in 2D when column 1 and 2 are taken out respectively.
The principal stress ratio and coordination number of measurement spheres along the middle column are plotted as a function of axial strain as shown in Figure 6.4.

As we can see from Figure 6.4(a), the graphs of the principal stress ratio against strain within each measurement sphere show similar trends: a relatively smooth increase in the principal stress ratio while the contacts are loaded, with the principal stress ratio taking a similar value for each sphere. Once past 3.5% in axial strain the principal stress ratio tends to vary significantly both with strain and with position.

The coordination number for the middle column of measurement spheres is shown in Figure 6.4(b). These show that, during the initial loading the coordination number increases, but then drops significantly once the bonds start to break. For the following analysis, events happening in the interval of axial strain of 3.5 - 5% are the main focus.

Figure 6.3: schematic of cross sections
Figure 6.4: Principal stress ratio and coordination of measurement spheres along the middle column.
6.4.2 Wavelet analysis

A multiresolution analysis was applied to the stress ratio of the 59 measurement spheres. The measurement sphere number 121, the measurement sphere on the right hand side in the YZ plane in Figure 6.3(c), is selected to show the result of the MRA of the stress ratio and of the coordination number. Figure 6.5(a) and (b) show the MRA of the stress ratio and of coordination number of the measurement sphere 121 at scale D1–D7 respectively.

As seen in figure 6.5(a), on scales D1 up to D5 the transition from loading to slipping is clearly visible at around 3.5%. The wavelet coefficients for D1 up to D4 show that there are many small events at these small scales. At the scale of D5 there are a number of larger peaks. These can be directly related to points where there is a sudden change in the principal stress ratio and are characteristic of the fact that after the first failure frequently granular materials exhibit repeated smaller peaks in the stress ratio followed by smaller failures.

In order to see if the other measurement spheres show significant events at the same scale and at the same interval of axial strain, the non-overlapping measurement spheres are shaded according to their magnitude of absolute value of the MRA at scale D4 and D5 for the strain increment of 0.5% starting at the axial strain of 3.5% and ending at 5% as high peak events clearly seen in these intervals. Each detail corresponds to a different strain scale. Using the strain and the height of the specimen one can also related the strain to a space scale, as summarised in Table 6.2.
Table 6.2: Strain and space scales related to the detail coefficients. The space scale in mean particle diameters is calculated by dividing the space scale measured in millimetres by the mean particle diameter, 1.1mm.

Figure 6.6 and 6.7 respectively show measurement spheres shaded according to the maximum absolute value of the MRA of the stress ratio at scale D4 and D5 for the strain interval starting at 3.5% and ending at 5%. Figure 6.8 and 6.9 show the same kind of plot but with the magnitude of the MRA of the coordination number at scale D4 and D5 respectively.

As can be seen, in Figure 6.7 and 6.9 although the large measurement spheres do indicate that there are specific regions within the assembly where the largest changes in the detail coefficients at scale D5 occur, the spheres are too large to enable much spatial structure to be seen.
Figure 6.5: MRA of measurement sphere number 121
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MRA of the stress ratio at scale D4

Figure 6.6: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for the stress ratio at scale D4 for the strain interval starting at 3.5% and ending at 5% (The maximum absolute value of the MRA is 0.06).
MRA of the stress ratio at scale D5

Figure 6.7: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for the stress ratio at scale D5 for the strain interval starting at 3.5% and ending at 5% (The maximum absolute value of the MRA is 0.06).
MRA of the coordination number at scale D4

Figure 6.8: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for the coordination number at scale D4 for the strain interval starting at 3.5% and ending at 5%.
MRA of the coordination number at scale D5

Figure 6.9: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for the coordination number at scale D5 for the strain interval starting at 3.5% and ending at 5%.
6.4.3 Plot of parallel-bond failure

The parallel-bond model describes a cement-based portion of the force displacement. Once the cemented bonds are broken, they cannot re-form. This means that one can look at which parts of material have undergone most stress by looking at where most of the parallel bonds have been broken. Only broken bonds occurring in a cross-sectional slice are plotted. This slice passes through the centre of the cylinder and has a thickness of 10 mm. Two cross-sections are plotted: XZ and YZ planes. Three intervals of the axial strain were selected as being used to compare to the results of the MRA analysis. The broken bonds are depicted as bi-coloured lines. The red line represents a failure of parallel-bond because the maximum tensile stress exceeds the tensile strength while the blue line represents a failure because the maximum shear stress exceeds the shear strength.

Failures of parallel bonds for three intervals of axial strain between 3.5 and 5% were plotted. Figure 6.10(a)-(c) show plots of parallel bonds broken when the axial strain increases from 3.5 to 4%, 4 to 4.5% and from 3.5 to 5% respectively.

The MRA seems to pick up some changes of the stress ratio and the coordination number if we compare the results of the MRA with the failure of the parallel bonds but it is not very clear. This is possibly because the measurement spheres are large. In order to investigate this, the same simulation was run again with smaller measurement spheres. The results are shown in section 6.5.
Figure 6.10: Failures of parallel bonds for the strain interval starting at 3.5% and ending at 5%. Red lines represent a failure of parallel-bonds because the maximum tensile stress exceeds the tensile strength while blue lines represent a failure because the maximum shear stress exceeds the shear strength.
6.5 The second data set: the 3D data set rerun with small measurement spheres

The second data set is a re-run of the first data set with smaller measurement spheres. There were 196 measurement spheres which were of 6 mm in diameter, approximately 2-3 particles diameter. For each sphere the coordination number and the stress component were recorded with the analysis time and the axial strain. The test was carried out to 12% of the axial strain and data was output at increments of $2.242 \times 10^{-3}\%$, giving a total number of 5352 data points. Figure 6.11 shows the cylinder with the measurement spheres. As shown in Figure 6.11, four different planes were considered as illustrated in Figure 6.12: XZ plane, YZ plane, plane 3 and plane 4.
6.5.1 Preliminary plots

The stress ratio and coordination number of the measurement spheres of the middle column consisting of measurement sphere number 1, 18, 35, 52, 69, 86, 103, 120, 137, 154, 171 and 188 are plotted. Respectively, Figure 6.13(a) and (b) show these plots. As can be seen from Figure 6.13(a), most spheres achieved a peak stress ratio at the axial strain interval of 3.5% to 5%. The stress ratio plots show qualitatively similar features to the preliminary plots in section 6.4.1, Figure 6.4(a). Also, a decrease of the coordination number is seen at the same interval of the axial strain as revealed in Figure 6.13(b). There are small differences in the coordination number plot, flat parts in Figure 6.13(b). This is possibly because of a technique of calculation of the coordination number. For the following analysis, the events happened at the interval of axial strain of 3.5–5% were the main focus, in order to compare with section 6.4.
Figure 6.13: Stress ratio and Coordination of measurement spheres along the middle column
6.5.2 Wavelet analysis

A multiresolution wavelet analysis (MRA) was applied to the stress ratio and coordination number of the 196 measurement spheres. The measurement sphere number 75 was selected to show typical results of this analysis as it lies inside the region that was covered by the large measurement sphere 121 in section 6.4.2. The measurement sphere number 75 can be seen to the right hand side of the YZ plane in Figure 6.12. Respectively, Figure 6.14(a) and 6.14(b) show MRA of the stress ratio and coordination number at scale D1–D7.

The MRA of the small sphere shows similar features to the MRA of the large one, with again scale D5 picking out both the transition from loading to contact breaking at 3.5% axial strain and a number of further sudden changes in the principal stress ratio.
Figure 6.14: MRA of data from measurement sphere 75.
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The MRA of the stress ratio

According to Figure 6.14 the peak events can be seen at scale D1–D5. For each measurement sphere, each detail Dj was divided at every 0.5% of the axial strain. For each interval, the maximum absolute value of MRA detail coefficients was calculated. Each measurement sphere was shaded according to this value. Figure 6.15–Figure 6.19 show these results for the stress ratio at scale D1–D5 respectively. Only intervals of the axial strain starting at 3.50% and ending at 5.0% are shown in order to compare with the results in section 6.4 and because this is the region where the peak stress occurs and bonds start to break.

As the spheres were shaded according to the maximum absolute value of the MRA detail coefficients for the stress ratio, the dark sphere indicates that there is a significant change of the principal stress ratio at the scale and the interval of axial strain considered.

For the scale D1–D4, Figure 6.15–6.18, there are a few measurement spheres at different parts in the cylinder showing the peak events, at different interval of the axial strains, mainly at the interval of axial strain of 3.5–5%. However, zones, rather than just individual measurement spheres, of significant activity are clearly seen in scale D5 as illustrated in Figure 6.19(a)–(c). Most peak events primarily occur during the strain increment from 3.5 to 4.5%. If we consider Figure 6.19(a) in the YZ plane, we see a zone showing peak events that occur at the bottom half of the cylinder starting at the sphere near the boundary on the right going down to the bottom left. The measurement spheres in the XZ plane also show significant change, mainly at the middle of the bottom half of the cylinder.

For the XZ plane, Figure 6.19(b), shows a zone of peak event. It shows that the MRA detail coefficients are relatively large along line from the top right to the left of the upper half of the cylinder.
Figure 6.15: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale D1 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.06).
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Figure 6.16: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale D2 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.06).
Figure 6.17: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale D3 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.06).
Figure 6.18: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale $D_4$ for strain interval starting at 3.502% and ending at 5.002% (The maximum absolute value of the MRA is 0.06).
Figure 6.19: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale D5 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.06).
The MRA of the coordination number

A similar analysis was also performed for the coordination number. The MRA of the coordination number of the 196 measurement spheres were calculated. As seen in Figure 6.14(b), the peak events can be seen at scale D1–D5. Again, the measurement spheres are shaded according to the maximum absolute value of the MRA of the coordination number for each scale D1–D5 in the same axial strain intervals as those used in the MRA of the stress ratio.

As shown in Figure 6.20–6.23, there are a few measurement spheres revealing the peak event at scale D1–D4 but it can be more clearly seen at scale D5 as illustrated in Figure 6.24.

The MRA of coordination number seems to pick up significant changes in only some measurement spheres as it does not clearly show a zone of significant changes which is different from the results of the MRA of the stress ratio.
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Figure 6.20: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for coordination number at scale D1 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.25).
Figure 6.21: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for coordination number at scale D2 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.25).
Figure 6.22: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for coordination number at scale D3 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.25).
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Figure 6.23: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for coordination number at scale $D_4$ for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.25).
Figure 6.24: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for coordination number at scale D5 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.25).
6.5.3 Plot of parallel-bond failure

The broken bonds of 4 planes are plotted: XZ plane, YZ plane, plane 3 and plane 4. The thickness of the plane is 6 mm which is equal to the measurement sphere diameter. As in section 6.4.3, the broken bonds are depicted as bi-colored lines. The red line represents a failure of the parallel-bond because the maximum tensile stress exceeds the tensile strength while the blue line also represents a failure because the maximum shear stress exceeds the shear strength.

In order to compare the results of the MRA technique with plots of parallel-bond failure, results involving axial strain between 3.5-5% are focused on. The broken bonds of three intervals of axial strain were plotted. Figure 6.25(a)-(c) show plots of parallel bonds broken when the axial strain increases from 3.5 to 4%, 4 to 4.5% and from 4.5 to 5% respectively.

As the MRA of the stress ratio and coordination number at scale D5 clearly show peak events, we will only compare the results of the MRA at scale D5 with a plot of broken bonds. As it can be seen in Figure 6.19(a) and (b), the MRA of the stress ratio can be compared well with a plot of parallel-bond failure in Figure 6.25(a) and (b). Figure 6.19(a) and Figure 6.25 show similar diagonal lines originating from the top left to the middle right and the middle right to the bottom left in YZ plane in the axial strain of 3.5-4%. Also, the horizontal line can be seen in XZ plane.

The plot of parallel-bond failure in Figure 6.25(a) and (b) indicate that there are clear localisation at the regions agreeing with the results from the MRA technique, Figure 6.19(a) and (b).
Figure 6.25: Failures of parallel bonds for the strain interval starting at 3.5% and ending at 5%. Red lines represent a failure of parallel-bonds because the maximum tensile stress exceeds the tensile strength while blue lines represent a failure because the maximum shear stress exceeds the shear strength.
6.6 The 3D data set with different configuration

The third data set for the triaxial testing was generated using the same parameters as the second data set but with a different random number generator. There were 196 measurement spheres which were 3 mm in radius. For each sphere the coordination number and the stress component were recorded with the analysis time and the axial strain. The test was carried out to 12% of the axial strain and data was output at increments of $2.193 \times 10^{-3}\%$, giving a total number of 5474 data points. Similar analysis was carried out on this data set.

6.6.1 Preliminary plots

The stress ratio of the boundary for this data set is plotted with the one from the second data set as a function of the axial strain as illustrated in Figure 6.26.

![Stress Ratio Versus Axial Strain](image)

Figure 6.26: Stress ratio of bulk versus axial strain

The stress ratio for both data sets increase up to roughly the same value of 0.76 at the axial strain of 3.24%. After that, there is a decrease with small fluctuations in
CHAPTER 6. TRIAXIAL COMPRESSION TEST

Stress Ratio Versus Axial Strain

Figure 6.2: Principal stress ratio of measurement spheres along the middle column versus axial strain.

both data sets as illustrated in Figure 6.26.

Similar to the second data set, the stress ratio and coordination number of the measurement spheres of the middle column consisting of measurement sphere number 1, 18, 35, 52, 69, 86, 103, 120, 137, 154, 171 and 188 were plotted. Respectively, Figure 6.27 and 6.28 show these plots.

As seen in Figure 6.27, the principal stress ratio of every measurement spheres increases with increasing strain up to roughly 3-4% and then drops. At the axial strain greater than 5% the stress goes up and down with fluctuation.

The coordination number of the most measurement spheres is level with some fluctuations at the beginning and then drops when the axial strain increases up to 3%. After the axial strain goes up to 5%, the coordination number fluctuates around a new lower value as shown in Figure 6.28.
6.6.2 Wavelet analysis

A multiresolution wavelet analysis (MRA) was again applied to the principal stress ratio and coordination number of the 196 measurement spheres. As in section 6.5.2, the measurement sphere number 75 was selected to show typical results of this analysis. Respectively, Figure 6.29(a) and 6.29(b) show the MRA of the stress ratio and the coordination number at scale \(D_1 - D_7\).

The MRA detail coefficients of the stress ratio at scale \(D_1 - D_5\) reveal significant changes of the stress ratio at some intervals of axial strain as shown in Figure 6.29(a). At the same scale of the MRA of the stress ratio, the MRA detail coefficients of the coordination number are also high, showing peak events as seen in Figure 6.29(b). For this data set, the sphere 75 seems to show peak events at different strain intervals, e.g. showing high peak event at around 5% at scale \(D_5\). This possibly suggests that the sphere 75 is not in the significant zones.
Figure 6.29: MRA of data from measurement sphere 75.
The MRA of the stress ratio

Similar to the analysis results of the second data set, the peak events can be seen at scale D1–D5. For each measurement sphere, each detail coefficients Dj was divided at every 0.5% of the axial strain. For each strain interval, the maximum absolute value of MRA detail coefficients was calculated and each measurement sphere was again shaded according to this value. Figure 6.30–Figure 6.34 show these results for stress ratio at scale D1–D5 respectively. Only intervals of the axial strain starting at 3.5002% and ending at 5.002% are shown as these intervals are the main focus.

A dark sphere indicates that there is a significant change of the principal stress ratio at the detail scale and the interval of axial strain considered. As it can be seen in Figure 6.30–6.34, zones of significant activity are clearly seen in scale, D1–D5. Most peak events primarily occur during the strain increment from 3.5 to 4.5%. If we consider at Figure 6.34(a) at the XZ planes, we see measurement spheres showing the peak events that happen at the region of a top half of the cylinder starting at the sphere near the boundary on the top right down to the left. At the bottom half of the cylinder, the measurement spheres seem to show a zone starting from the left down to the bottom right.
Figure 6.30: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale D1 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.06).
Figure 6.31: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale D2 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.06).
Figure 6.32: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale D3 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.06).
Figure 6.33: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale D4 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.06).
Figure 6.34: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for stress ratio at scale $D_5$ for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.06).
The MRA of the coordination number

The MRA of the coordination number was calculated for of the 196 measurement spheres. As seen in Figure 6.29(b), the peak events can be seen at scale D1–D5. Again, the measurement spheres are shaded according to the maximum absolute value of the MRA of the coordination number for each scale D1–D5 in a given axial strain interval as those used in the MRA of the stress ratio.

As shown in Figure 6.35–6.39, there are a few measurement spheres revealing peak events at scale D1–D5, mainly at the interval of axial strain of 3.5–4%. It seems that the MRA of coordination number can pick up vital changes in measurement spheres in the same zones as the MRA of the stress ratio does, but the position of planes of broken bonds are less clearly seen with the coordination number than with the stress ratio.
Figure 6.35: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for coordination number at scale D1 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.25).
Figure 6.36: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for coordination number at scale D2 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.25).
Figure 6.37: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for coordination number at scale D3 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.25).
Figure 6.38: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for coordination number at scale D4 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.25).
Figure 6.39: Measurement spheres shaded according to the maximum absolute value of the MRA detail coefficients for coordination number at scale D5 for strain interval starting at 3.5002% and ending at 5.002% (The maximum absolute value of the MRA is 0.25).
6.6.3 Plot of parallel-bond failure

Similar to the first two data sets, the broken bonds of 4 planes are plotted: XZ plane, YZ planes, plane 3 and plane 4. The broken bonds are depicted as bi-colored lines. The red line represents a failure of parallel-bond because the maximum tensile stress exceeds the tensile strength while the blue line represents a failure because the maximum shear stress exceeds the shear strength.

As focused on before the interval of the axial strain between 3.5–5% is considered. Figure 6.40(a)-(c) show plots of parallel bonds broken when the axial strain increases from 3.5 to 4%, 4 to 4.5% and from 3.5 to 5 % respectively.

As it can be seen in Figure 6.34(a) and (b), the MRA of the stress ratio can be compared with a plot of parallel-bond failure in Figure 6.40(a) and (b). The plot of parallel-bond failure in Figure 6.40(a) and (b) indicate that there are clear localization at the regions agreeing with the results from the MRA technique, Figure 6.34(a) and (b).
Figures 6.40: Failures of parallel bonds for the strain interval starting at 3.5% and ending at 5%. Red lines represent a failure of parallel-bonds because the maximum tensile stress exceeds the tensile strength while blue lines represent a failure because the maximum shear stress exceeds the shear strength.
Summary and conclusion

In this chapter, we extended the use of wavelet analysis to examine data from a DEM simulation of a three-dimensional sample under triaxial compression. We show that the wavelet analysis can identify regions in space and strain when the localisation in the sample appeared. The results of the MRA of the stress ratio and coordination number were again used to identify the localised zones.

In the first data set, the MRA technique does not show significant event zones clearly. This is possibly because of large local measurement spheres. Therefore, the simulation was re-run again with smaller measurement spheres.

Again, the MRA was applied to the second data set, the re-run data set. The MRA of the stress ratio at scale $D_5$ clearly revealed zones of peak events. This result is consistent with a plot of broken bond.

In order to test the robustness of the technique, the third data set was identically generated except for the initial position of the particles. Again, the MRA analysis of the stress ratio at scale $D_5$ compares well with the regions in the sample where most broken bonds occur.

The MRA of the coordination number for the triaxial test data were more inconclusive. This was unlike the biaxial test analysis, where the MRA of the coordination number clearly show the localised zones.
Chapter 7

Summary and conclusions

This thesis uses wavelet transforms to explore the dynamic evolution of granular material by post-processing data from DEM simulations. As the techniques efficiently work with non-stationary signals, the wavelet transforms are used as an alternative to time-frequency analysis. How wavelets are superior to Fourier transforms in this case was illustrated in chapter 3.

A number of data sets generated from two different physical scenarios were analysed: particles in vibration cells and samples under compression. Two different situations were considered in the case of the compression test: biaxial and triaxial tests. A member of Daubechies wavelet, db2 was used as a mother wavelet in all cases.

For the particles in vibration cells, four data sets were analysed: two data sets of mono-sized spheres and two of a binary mixture. The particles in each case, i.e. mono-sized sphere and binary mixture, were subject to a combination of different frequencies and amplitudes of vibrations: a vibration frequency of 100 Hz with amplitude of 0.2d or a vibration frequency of 500 Hz with amplitude of 0.008d. For both cases, $\Gamma = 7.89$ where $\Gamma$ is the acceleration of the bottom of the cell measured in $g$. The vibration cell was subdivided into horizontal layers in order to see how the particles act when they are in different parts of the box.

For the mono-sized cases, when the particles were subject to low frequency and high
amplitude vibration, they tend to show different motions when they are in the different parts of the box. The particles mainly move in a vertical direction rather than in horizontal direction and the particles at the top layer tend to show more movement than those in the bottom layer. These can be seen in plots of the mean of particle positions, especially plot of the mean of $x$ against the mean of the $y$ positions as illustrated in Figure 4.5. The results of the MRA of the mean of the particle positions strongly supports this phenomenon. The MRA of the mean particle positions at scale $D_3$ clearly reveal the difference of particle motions. However, when the particles are subject to high frequency and low amplitude vibration, particles move mainly in the horizontal direction and there is little difference between movements of particles in one part of the box and another. Again evidence for this can be seen in plots of the mean of $x$ against the mean of the $y$ positions and the MRA of the mean particle positions at scale $D_3$. This is evidence of bulk movement.

The root mean square of the fluctuating velocity and the packing fraction of the two data sets are also consistent with the analysis results of the wavelets technique. The root mean square of the fluctuating velocity of particles in the low frequency and high amplitude vibration box is higher than the one in the high frequency and low amplitude, and the maximum of the RMS of the fluctuating velocity occurs near the top surface, where the packing fraction is low. In the high frequency and low amplitude vibration box, the RMS of the fluctuating velocity showed very little differences in depth. These results agree with the work of Lan et al. [88] when low vibration accelerations were applied.

For the case of a binary mixture, in the case of low frequency and high amplitude vibration evidence of the Brazil Nut Effect is seen in the plot of the difference of the mean particle position in the $z$ direction between large and small particles. The particles in the bottom layer show more movements in horizontal direction than those in the top layer as depicted in the MRA of the mean particle positions at scale $D_2$. There is no evidence of different movements in depth when particles subjected to high frequency and low amplitude and there is little difference of particle motions between
large and small particles.

The granular temperature of particles in the low frequency and high amplitude box is higher than the one under high frequency and low amplitude. Again, the maximum of the granular temperature is near the surface.

Next, data sets from simulations of biaxial compression tests were analysed. Three data sets from two analogous specimens with different sizes were analysed: one data set from specimen A and two data sets from specimen B. The specimen was subdivided into local zones. The MRA were applied to the stress ratio, porosity and coordination number for these zones. The robustness of the wavelet technique was shown by the analysis result of the third data set where the position of the local zones was changed.

It is shown how the MRA of data from a DEM simulation of two different specimens can aid in finding the time/strain scales on which significant events occur. This information could be used to determine how frequently to output data. For example, for Specimen A, key scales for cross-correlation and for peak events were on the detail scale of D5 and above, suggesting that data could have been reduced by a factor of 32 without losing significant information. Furthermore, by dividing the specimen down into regions in space and considering intervals in strain we were able to find both when and where peak events occur. These matched well with results from a study of the incremental rotation. Using cross-correlation it was shown that the geometric property of porosity correlates with the principal stress ratio along the slip plane for specimen A. Cross-correlation results were less successful in specimen B, perhaps because the measurement circles were too big [82, 58, 57], 28-38 particle diameters. This makes it difficult to find significant cross-correlations between geometric property of porosity and the principal stress ratio along the slip plane.

Finally, the wavelet technique was extended to analyse the three dimensional data sets, samples under triaxial compression. The sample is a cylinder. Again, the sample was subdivided into small zones called measurement spheres. Three data sets were
analysed. In the first data set, the MRA technique could not clearly show the localised zones as the measurement spheres were too large. Consequently, the simulation was re-run with smaller measurement spheres. With the re-run data set, the MRA of the stress ratio at scale D5 clearly reveals zones of peak events. This result is consistent with the plots of broken bonds as in Figure 6.25. The MRA of the coordination number was inconclusive. The third data set was generated in order to test the robustness of the technique. The data set was generated using the same parameters except for the initial position of the particles. The MRA of the stress ratio again compares well with a plot of the broken bonds. The MRA analysis of the coordination number for the triaxial test data was more inconclusive. This was unlike the biaxial test analysis, where the MRA of the coordination number clearly show the peak events.

As illustrated in the two main analysis results by the wavelet techniques, post-processing data sets from DEM simulation is still a major challenge for future investigations. In the case of vibration cells, vertical vibrations have been studied under various conditions. The behaviour of granular particles depends on a number of factors, e.g. the frequency and amplitude of vibration. The strength of the applied floor acceleration, $F$, also plays a major role in the bed character [89]. Work focused on two combinations of amplitude and frequency which give the same acceleration of $7.89g$, a scope of investigation of different acceleration amplitudes can be possibly extended in both cases: mono-sized spheres and a binary mixture. In particular, in the case of a binary mixture, the transition state between BNE and RBNE is an interesting phenomenon.

Furthermore, there is scope to investigate the different properties of different binary mixtures and possibly to extend to ternary and other mixtures.

For the case of samples under compression, the size of small regions, e.g. measurement circles in biaxial compression, is an important factor for the analysis. The cross-correlation of wavelet detail coefficients may be considered with appropriate small regions [58, 57] in order to possibly find significant relationships between vari-
ables. Further investigation of void ratio is also an interesting phenomenon as the void ratio plays an important role in the triaxial compression [18, 31].

Moreover, the wavelet technique should be considered for applications involving quantitative analysis of experimental data generated by the other advanced experimental techniques such as photo-elasticity and X-ray computed tomography techniques.
Bibliography


[80] Tkacz E., Kostka P. and Komorowski D. An application of wavelet transform and adaptive filters for decomposition of the HRV signal in the case of patients with


[90] Yousefia S., Weinreichb I. and Reinartz D. Wavelet-based prediction of oil prices. 