Micromechanics of Wave Propagation through Granular Material

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A thesis submitted to Imperial College London in partial fulfilment for the degree of Doctor of Philosophy
That you are here – that life exists and identity,

That the powerful play goes on, and you may contribute

a verse.

Walt Whitman, *Leaves of Grass*
Declaration of Originality

The work presented in this thesis was carried out in the Geotechnics Section of the Department of Civil & Environmental Engineering at Imperial College London. This thesis is the result of my own work and any quotation from, or description of the work of others is acknowledged herein by reference to the sources, whether published or unpublished.

This dissertation is not the same as any that I have submitted for any degree, diploma or other qualification at any university. No part of this thesis has been or is being concurrently submitted for any such degree, diploma or other qualification.

John O’Donovan

London, 20/08/13
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Abstract

The stiffness of soil is an important parameter that has implications on soil-structure interaction, on the response to earthquake motion and on the response of soils to dynamic loadings. Stiffness reduces and behaves plastically at medium to high strains; however, at small-strain the stiffness has been observed to be a constant value and elastic. Small-strain stiffness governs the soil-structure interaction during construction projects and site response during dynamic loading due to earthquakes and man-made operations. Quantifying stiffness, in particular shear stiffness, at small-strain is difficult due to the effect of sample fabric on the values measured and the resolution of the testing equipment that is available. Wave propagation has been used to measure the stiffness of samples by propagating waves in different directions and in different planes. This thesis aims to examine the propagation of stress waves through a granular medium. Samples were created using the numerical discrete element method (DEM) in two- and three-dimensions. Waves, created by a point source, were propagated through the samples and this propagation was measured using micromechanical data. The speed of the propagating wave was assessed using existing techniques and novel methods developed during the research. The effect of macro-scale parameters, such as sample boundary conditions, and the effect of micro-scale parameters, such as interparticle contact laws, on sample stiffness were examined. Randomly packed samples were created with a quantifiable fabric tensor, measured using the contact force network. Wave propagation in different directions was examined to quantify the effect of inherent anisotropy on the sample stiffness. Samples were confined at anisotropic confining pressures to isolate the effect of induced anisotropy on the sample stiffness. Wave propagation results were compared with the results of small amplitude stress probes for a number of simulations and with experimental work carried out in the University of Bristol.
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Figure 7.13: Zoom in on first zero-crossing to better illustrate the effect of increasing the propagation stress, keeping the oscillation stress constant and decreasing the third stress for (a) \( V_{xy} \) shear wave, (b) \( V_{yz} \) shear wave and (c) \( V_{zx} \) shear wave. Results are presented in the time domain. \( f_{\text{trans}} = 30 \text{kHz}, R_d = 4.69 \text{ and } \lambda/d_{50} = 7.68 \).

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Figure 7.19: Zoom in on first zero-crossing to better illustrate the effect of decreasing the propagation stress, increasing the oscillation stress and keeping the third stress constant for (a) $V_{xy}$ shear wave, (b) $V_{yz}$ shear wave and (c) $V_{zx}$ shear wave. Results are presented in the time domain. $f_{\text{trans}} = 30\,\text{kHz}$, $R_d = 4.69$ and $\lambda/d_{50} = 7.68$.

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1 Introduction

1.1 Background

Small-strain soil stiffness is an extremely important parameter in geotechnical engineering. It is used to predict the movement of soil during construction projects and during earthquake motion. Small-strain stiffness is an input to finite element models that capture dynamic soil response. Soils undergo dynamic motion in many everyday situations including road and rail loading and the operation of plant machinery. The importance of small-strain stiffness was highlighted in the Rankine lectures by Atkinson (2000) and Clayton (2011) who outlined the importance of understanding small-strain behaviour to the geotechnical research and industrial communities. The measurement of small-strain soil stiffness is complicated by soil non-linearity, anisotropy and stiffness degradation with increasing shear strain. Two methods of determining small-strain soil stiffness are dynamic wave propagation tests and small amplitude mechanical tests.

Two dynamic tests commonly carried out in geotechnical testing laboratories are resonant column testing and bender element testing. This research focuses on bender element testing. Small amplitude mechanical tests can be stress driven or strain driven depending on the apparatus and this research focuses on the stress driven probes. Bender elements, introduced by Shirley & Hampton (1978), have become ubiquitous in geotechnical testing facilities, both academic and industrial, due to the fact that they are inexpensive and can be fitted to existing soil testing equipment. The interpretation of results from bender elements is complicated by many factors. Near-field effects cloud the arrival of the shear wave, the wave energy is diffused as it spreads through the medium from the point source and dispersion occurs due to the granular nature of the medium. This means that the received wave is of different frequency and amplitude to the transmitted wave and is overlain with a fast moving near-field effect. The difficulty of interpreting bender element tests has been highlighted by Brignoli et al. (1996), Jovičić et al. (1996), Blewett et al. (2000), Arroyo et al. (2003) and Leong et al. (2005) among many others. A number of travel time determination techniques have been developed of which Yamashita et al. (2009) provide a useful summary. In this research, existing and novel travel time determination techniques are rigorously assessed using the numerical simulation.
Small amplitude stress and strain probes were made possible by replacing traditional strain gauges with LVDT’s (linear variable differential transformers) which could measure the strain response of soil at strains below 0.0001%. This approach, developed by Cuccovillo & Coop (1997), was fundamental to allow strains in the small-strain range for soils to be measured. Stress probes are often compared to the results of dynamic bender element tests to provide reassurance that the stiffness measured using bender elements are reasonably accurate such as in Ezaoui & di Benedetto (2009). The numerical simulations presented here allowed very low strains and stresses to be measured.

Wave propagation through granular material has received a large amount of attention from physicists, mathematicians and other engineering communities. Research has been conducted analytically, numerically and experimentally and some of the key studies are summarised in Chapter 2. Much of the research in other communities focuses on frequency domain analysis as a way of characterising a wave, including its speed. This analysis has previously uncovered interesting aspects relating to wave propagation through granular material. These include a non-linear relationship between angular velocity and wavenumber and the existence of a maximum frequency or threshold frequency at which energy does not propagate and a standing wave is formed in the sample. This research attempts to place some of the findings by Mouraille et al. (2006) and Suiker et al. (2001) among others in a geotechnical context to improve our understanding of and ability to interpret dynamic tests.

The numerical discrete element method (DEM) code, Cundall & Strack (1979b), was used to carry out this research as it allowed the grain scale micromechanics of the wave propagation problem to be explored. Wang & Mok (2008), Somfai et al. (2005) and Li & Holt (2002) among others have previously examined wave propagation from a grain scale perspective and made attempts to relate macro-observed behaviour to micromechanical data available in the numerical simulations. In the current study, simulations on a number of different samples, and the sample complexity progressively increased. Initially a two-dimensional regular packing of disks was considered. This was followed by a three-dimensional regular packing of spheres and finally a three-dimensional randomly packed sample of spheres was considered. The computational costs of the regular two- and three-dimensional simulations were relatively low allowing efficient algorithms to be developed and tested before application to the more computationally expensive randomly packed simulation. O’Sullivan et al. (2002), Thornton (1979) and Rowe (1962) have shown that regular, lattice packed simulations can provide useful insight into observed phenomena in more complicated
samples. The simulations of the randomly packed samples are compared with a concurrent study undertaken at the University of Bristol involving bender element and stress probe tests on samples of glass ballotini in a true-triaxial, flexible bounded cubical cell apparatus. The sample size and particle size used in the three-dimensional simulations were comparable with the sample size and particle size used in the physical experiments in the University of Bristol.

1.2 Aims and objectives

The scope of this research is to gain a better understanding of the small-strain stiffness of granular packings using the numerical discrete element method (DEM). The aims of this current study are to quantify the small-strain stiffness of a granular packing and to model existing methods to determine this stiffness such as wave propagation and small amplitude stress probes. It is hoped that comparisons could be made between the numerical research carried out here and the experimental research carried out simultaneously at the University of Bristol on the same sample sizes and same sample material. An important aim is to examine the mechanism by which stress waves propagate through granular material at the micro-scale and the relationship to sample scale stiffness. The effect of wave propagation on micro-scale parameters is identified as a key research area. Also important is to assess how these micro-scale parameters, such as the interparticle contact model, influence wave propagation mechanism and speed. To accomplish these aims a number of research objectives are identified.

The main objectives of the research are as follows:

1. To develop two- and three-dimensional models of both regularly and randomly packed granular material using the discrete element method and quantify the stiffness of these packings using a variety of methods.
2. Model the propagation of small amplitude stress waves through a discrete element simulation of granular material.
3. Model the application of small amplitude stress probes on a granular packing.
4. Use the micromechanical DEM data to explain the source of some of the macro-scale observations during bender element testing.
5. Critically assess existing analytical methods used to determine the effective elastic moduli of granular material using grain-scale inputs.
6. Critically assess existing travel time determination methods used in bender element testing on both laboratory and numerical samples.
7. Examine the effect of interparticle contact models on the small-strain sample stiffness. The contact models considered were Hertz-Mindlin, Hertz-Mindlin-Deresiewicz and the rough surface Cavarretta-Mindlin.

8. Quantitatively compare the test results from laboratory experiments with DEM simulations on samples containing the same particles, similarly prepared and of similar sample size.

9. Relate the rich information obtained by time and frequency domain analysis of the wave propagation to sample scale parameters such as the sample stiffness.

1.3 Thesis layout

The work presented in this thesis has been divided into eight chapters.

Chapter 1 (the current Chapter) provides the background, aims and objectives of this research.

Chapter 2 contains a literature review on wave propagation through granular material and the relationship to soil stiffness. Section 2.2 briefly describes the discrete element method, which was the numerical method used in this study. Section 2.3 outlines small-strain stiffness of granular material, including soil, and the relationship between small-strain stiffness and sample anisotropy. A review of methods to quantify small-strain stiffness in both laboratory and numerical studies is presented. Section 2.4 describes how stress waves propagate through granular material and includes the relevant theory that is used to interpret the stress wave motion. There is a review of analytical, experimental and numerical tests examining wave propagation. Section 2.5 reviews bender element testing including methods of travel time determination. Previous key experimental and numerical studies on bender element testing are presented. Section 2.6 outlines how small-strain and small-stress probes can be used to measure small-strain stiffness and some studies compare bender element test results with probe results.

Chapter 3 describes the interparticle contact models that were implemented in this study. Section 3.2 describes the default Hertz-Mindlin model that is implemented in many DEM codes. Section 3.3 outlines the Cavarretta-Mindlin model while Section 3.4 outlines the Hertz-Mindlin-Deresiewicz model. Section 3.5 discusses the implementation of these models in PFC3D, the discrete element method software used in this research and the verification
exercises that were carried out on each model. Section 3.6 reviews multi-particle simulations and the effect of the contact models on these simulations.

Chapter 4 outlines the two-dimensional wave propagation simulations that were carried out in this research. Section 4.2 outlines the simulation approach used in these simulations. Section 4.3 illustrates the analysis of the received signal while Section 4.4 presents an overview of the system response to the inputted stress wave. Section 4.5 explains how sample stiffness was calculated using different travel time determination techniques and small strain probes. Section 4.6 illustrates the effect of varying model parameters on the results.

Chapter 5 describes the regularly packed three-dimensional wave propagation simulations with isotropic confining pressures. Section 5.2 reviews the regularly packed samples and how they were created including how a stress wave was transmitted. Section 5.3 illustrates the waves that are formed from a point source input and Section 5.4 shows the propagation of the stress wave through the sample using micromechanical measures. Section 5.5 reviews the analytical solutions that were implemented during the course of this study to calculate effective sample moduli using particle scale inputs. Section 5.6 reviews the methods used in this study to analyse the received signal and determine wave speed or travel time of the wave. Section 5.7 compares the sample stiffness over different confining pressures and how it varies as the interparticle contact model varies, the boundary conditions vary and the input wave type, whether point-source or plane, varies. There is a discussion on the differences between transmitted compressional waves and transmitted shear waves.

Chapter 6 describes the randomly packed three-dimensional wave propagation simulations with isotropic confining pressures. Section 6.2 describes the randomly packed sample, how it was prepared and how the stress waves were transmitted. Section 6.3 illustrates the propagation of the wave through the sample using particle-scale measures. Section 6.4 outlines the analytical methods that can be applied to the sample under consideration here to calculate effective sample moduli. Section 6.5 reviews the analysis methods that were used to determine the wave speed or wave travel time. Section 6.6 presents the results for sample stiffness calculated on different planes and using different methods. There is also a review of parametric studies carried out. The results of small-stress probes carried out on the sample are presented here also.

Chapter 7 outlines the regularly packed and randomly packed three-dimensional wave propagation simulations with anisotropic confining pressures. Section 7.2 deals with the
regularly packed sample and Section 7.3 deals with the randomly packed sample. The effect of anisotropy on the received signal traces, micromechanical behaviour and sample stiffness was explored for both samples for a number of loading cases.

Chapter 8 summarises and discusses the major findings of this research. Recommendations for future research on this topic are made.
2 Literature review

2.1 Introduction

This Chapter provides the reader with the necessary background information for this thesis. The discrete element method is introduced in Section 2.2. The overall aim of the research is to aid interpretation of bender element tests to determine small-strain stiffness of soil and small-strain stiffness is considered in Section 2.3. The mechanics of stress wave propagation are discussed in Section 2.4. The final two Sections of this Chapter consider experimental determination of small-strain stiffness using bender element tests (Section 2.5) or small-strain probes (Section 2.6).

2.2 Discrete element method

Use of the discrete element method (DEM) to provide insight into granular material is now well established and only a brief introduction is presented here. Cundall (2011) and Potyondy & Cundall (2004) provide useful overviews of the theory and application of DEM. The primary software packages used in this research were PFC2D Version 3.1 and PFC3D Version 4.0 (Particle Flow Code). Some of the samples were created using the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) code. More information on PFC, which is a commercial code, can be found in Itasca Consulting Group (2007), while more information on LAMMPS, which is an open source code, can be found in Plimpton (1995).

2.2.1 General introduction to the discrete element method

The DEM algorithm is outlined in Cundall & Strack (1979a) and Cundall & Strack (1979b). DEM uses a time-stepping algorithm where particle accelerations are updated at discrete time intervals. Particle accelerations are calculated based on the resultant forces acting on particles. Those forces arise due to contacts with neighbouring particles and external forces, such as gravity, acting on the system of particles. From the accelerations the particle velocities and displacements can be updated using Verlet time integration over each time-step. The time-step is a function of the particle mass and contact stiffness as outlined in Itasca Consulting Group (2007) and Cundall & Strack (1979a). Particles can come into contact and lose contact; they can also slide relative to each other.
The interaction between two particles is summarised in Figure 2.1. Particle contacts are modelled as a set of orthogonal springs, one in the normal direction and one in the tangential direction. Particles are modelled in PFC using a soft particle approach. This means that particles are allowed to overlap when they come into contact. The spring’s resistive force increases in proportion to the overlap in the normal direction or the relative tangential displacement in the tangential direction. For sphere-sphere interactions the contacts occur at points. Different contact models have been proposed to relate spring displacement to contact force and these are discussed in more detail in Chapter 3. The most commonly used models are the linear elastic contact model and Hertz-Mindlin contact model.

Frictional sliding dissipates energy in the system. Additional sources of energy dissipation present in real granular materials are simulated using damping. Itasca Consulting Group (2007) and Potyondy & Cundall (2004) show a number of damping options that are available in DEM simulations and two, namely local damping and viscous damping, are briefly outlined here. Local damping applies a reduction to the resultant force causing motion. This reduction is proportional to a local damping ratio specified by the user. The second method is viscous damping that acts at contacts. Viscous damping reduces the contact force in proportion to the relative particle velocities and is proportional to the viscous damping ratio which is specified by the user. A different viscous damping ratio can be applied to the normal and shear directions. The coefficient of restitution for impacts occurring in a DEM simulation has been shown by Cleary (1998) to be influenced by the choice of viscous damping ratio. A desired coefficient of restitution can be achieved by varying the viscous dashpot parameters.

2.3 Small-strain stiffness and anisotropy of granular material

The small-strain stiffness of granular material is a very important parameter that is hard to quantify. In soil, stiffness can be influenced by a number of factors including confining stress level, fabric, structure, induced anisotropy and loading history. Whether or not the stiffness value measured is a true elastic stiffness can be hard to discern. The stiffness is elastic if the work done in deformation is recoverable and there is no permanent loss of energy. It is generally assumed that the stiffness measured at small strain levels is an elastic stiffness but this elastic stiffness is much harder to quantify and more likely to be influenced by the inherent anisotropy of the sample. This Section explores some attempts to quantify
small-strain soil stiffness, small-strain stiffness of analogue soils and the small-strain stiffness of numerical granular materials. Stiffness anisotropy is also considered. There are analytical solutions for predicting the stiffness of granular materials but these are dealt with in Section 2.4.1 as their primary use in this research has been to predict the wave speed in granular packings.

### 2.3.1 Small-strain soil stiffness

Soil stiffness can be used to predict the movement of the ground during construction and the response of a soil to an earthquake. The interaction between structures and soil is also governed by the soil stiffness. It is, however, a difficult parameter to quantify due to its non-linearity, as highlighted in the 40th Rankine lecture by Atkinson (2000). Soil shear stiffness decreases with increasing shear strain as illustrated on Figure 2.2 taken from Atkinson’s Rankine lecture. DEM can capture this behaviour as illustrated on Figure 2.3 where a DEM model of Castlegate sand is compared with experimental results for that sand. Both sets of data show a decrease in soil stiffness with increasing shear strain. The importance of small strain soil stiffness to engineering design was highlighted by Burland (1989) in his Bjerrum lecture. Clayton (2011), in the 50th Rankine lecture, also highlighted the importance of small strain stiffness for the prediction of ground movements during construction. Shear strains that can be considered to lie within the small-strain zone vary with the type of material, however, the following approximations hold. Jardine (1992) found that for sand shear strains lower than $10^{-3}\%$, for till shear strains lower than $10^{-2}\%$ and for clays shear strains lower than $10^{-1}\%$ can be considered to be small-strain values.

Jardine (1992) and Kuwano & Jardine (2007) proposed breaking the non-linearity of soil stiffness using sub-yield surfaces or zones. These zones were defined by changes in the slope of the stiffness versus strain curves. These zones are illustrated on $q – p’$ space on Figure 2.4, where $q$ is the deviatoric stress, $p’$ is the mean effective stress and $p’_e$ is the Hvorslev equivalent $p’$. $p’_e$ is defined as the mean effective pressure on the normal consolidation line corresponding to the specific volume at failure. Zone 1 is the region that corresponds to perfectly linear elastic behaviour. Zone 2 corresponds to a region of non-linear stress-strain behaviour; however fully recoverable behaviour during complete load-unload cycles is observed. The development of irrecoverable strains is observed in Zone 3. Large scale changes in particle packing are observed when the stress path reaches the initial Boundary
Surface. The small-strain stiffness considered in this study restricts us to considering strains in the Zone 1 and Zone 2 regions.

Attempts to accurately model small-strain stiffness have attracted much attention in both industry and academia. Simpson et al. (1979) modelled London clay by dividing the stress-strain response into three zones: elastic, intermediate and plastic. Small-strain behaviour occurs in the elastic zone at strains frequently encountered in the field. Laboratory tests, at the time, measured stress-strain response in the intermediate zone. The stiffness of London clay in the elastic zone is much higher than in the intermediate zone which meant that the predictions of ground movement during construction based on the results of laboratory tests were inaccurate. This difference in stiffness is highlighted on Figure 2 for shear modulus against shear strain. Puzrin & Burland (1998) modelled the small-strain behaviour of Bothkenner clay by creating a linear elastic region (LER) and small-strain region (SSR) which correspond to the Zone 1 and Zone 2 regions in Jardine (1992). The constitutive model presented in Puzrin & Burland (1998) accurately predicted the stress-strain behaviour of undisturbed Bothkenner clay for a range of stress probe directions in triaxial stress space.

The anisotropy of soil stiffness is an important aspect to consider. Inherent anisotropy depends on the method of deposition or laboratory sample preparation conditions. Inherent anisotropy is usually cross-anisotropic as most soils are deposited vertically under gravity. This means that their vertical properties are different to their horizontal properties and the compliance tensor contains 5 independent parameters. Lings et al. (2000) provided the following compliance tensor for a cross-anisotropic soil.

\[
\begin{pmatrix}
\frac{1}{E_h} & -\frac{\nu_{hh}}{E_h} & -\frac{\nu_{hv}}{E_h} & 0 & 0 \\
-\frac{\nu_{hh}}{E_h} & \frac{1}{E_h} & -\frac{\nu_{vh}}{E_h} & 0 & 0 \\
-\frac{\nu_{hv}}{E_h} & -\frac{\nu_{vh}}{E_h} & \frac{1}{E_v} & 0 & 0 \\
0 & 0 & 0 & G_{hv} & 0 \\
0 & 0 & 0 & 0 & G_{hh}
\end{pmatrix}
\times
\begin{pmatrix}
\delta\sigma'_{xx} \\
\delta\sigma'_{yy} \\
\delta\sigma'_{zz} \\
\delta\tau'_{yz} \\
\delta\tau'_{xz} \\
\delta\gamma_{xy}
\end{pmatrix}
\]

where the z-axis is vertical, \(E_v, E_h\) are the Young’s moduli, \(\nu_{vh}, \nu_{hv}, \nu_{hh}\) are the Poisson’s ratios and \(G_{hv}, G_{vh}, G_{hh}\), are the shear moduli. Figure 2.5 shows two elements subjected to stresses in the xy-plane and the xz-plane. The elastic moduli describe relationships between
stress and strains and between two different strains. The Young’s modulus governs the relationship between stress and strain in each of the principal directions. The Poisson’s ratio describes the relationship between strains in two different principal directions. The shear modulus describes the relationship between shear stress and shear strain in a particular plane. The subscript $v$ refers to the $xz$- or $yz$-plane and the subscript $h$ refers to the $xy$-plane. Jung & Chung (2008) link micromechanical features with the cross-anisotropic elastic moduli in granular soils. Particle size, contact stiffness, and degree of contact anisotropy under isotropic confining pressure influence the magnitude of the elastic moduli calculated from the analytical work in Jung & Chung. A unique relationship between the degree of fabric anisotropy with stress ratio, $q/p$, was proposed where $q$ is the deviatoric stress and $p$ is the mean confining pressure. The derivation of the degree of fabric anisotropy is outlined in Barreto (2009). This improves the analytical model’s ability to model tests where there is increasingly anisotropic confining pressure such as the triaxial test.

Stress induced anisotropy depends on the confining stress acting on the soil. Induced anisotropy causes the stiffness measured in the direction of highest stress to increase. Roesler (1979) experimentally investigated the effect of anisotropic stress conditions on the speed of a stress wave propagating through a soil sample. As is discussed further in Section 2.4 the velocity of stress wave propagation is directly linked to stiffness. Roesler found that the shear wave velocity, which is indicative, of the shear modulus was dependent on the stresses in the direction of propagation and in the direction of oscillation but independent of the stress normal to the plane of shear. Using analytical methods Hardin & Blandford (1989) expanded on this observation to calculate a stress-compliance tensor that models the Roesler observation that elastic shear stiffness is independent of the stress normal to the plane of shear. The constitutive equations presented in Hardin & Blandford include, in addition to the stress-compliance tensor, a reference fabric tensor, a Poisson’s ratio tensor and two scalar functions representing effects of void ratio and stress history. As well as accounting for the effects of stress induced anisotropy using the stress-compliance tensor, the reference fabric tensor accounts for the effect of inherent anisotropy.

2.3.2 Studying stiffness using analogue soils

The stiffness of idealised granular materials has been analysed to improve insight into soil stiffness. Researchers have often linked the non-linearity observed at the macro-level with grain scale responses such as particle rotations and contact force chain changes. Force chains
are links of contacting particles that behave like “columns” in the sample. The chains can indicate the effects of induced or inherent anisotropy. Force chains indicate the direction of major principal stress when the sample is anisotropically loaded or can indicate the direction of major principal fabric when the sample is anisotropically packed.

Rothenburg & Bathurst (1989) showed, using DEM simulations, how contact force chains appear as a response to induced anisotropy. Figure 2.6 shows the initial state of the contact force network and the initial distribution of contact normals on a polar histogram. On (a) the contact forces appear randomly orientated and this is confirmed on (b). The stress acting on the sample in the vertical direction is increased producing a different contact force chain network shown on (c). It is orientated in the vertical direction, i.e. the direction of increasing stress, and this is confirmed by plot (d) which is the contact normal distribution. The stiffness of a sample under anisotropic stress conditions is increased in the direction of major principal stress and the plots on Figure 2.6 confirm that this is linked to the evolution of contact chains in the numerical sample.

Behringer et al. (1999) used photoelastic disk experiments to examine the predictability with which these contact force chains form, further improving the understanding of how stiffness is related to the formation of contact force chain networks. The source of stiffness was explored through examining the force chains present in two-dimensional photo-elastic disks. Majmudar & Behringer (2005) explored the evolution of contact forces using a biaxial test. An image from their work, shown in Figure 2.7, shows the evolution of contact force chains in the direction of major principal stress, it is easy to argue that such evolution must influence the stiffness of the sample.

2.3.3 Quasi-static particle-scale simulations examining stiffness

Yimsiri & Soga (2000) examined the effect of interparticle contact models on the stiffness moduli of an assembly of spheres using an analytical model. The three models considered were linear, Hertz-Mindlin and rough-surface. Yimsiri & Soga found that the linear contact model was not suitable to model soil as it showed no dependence on confining stress as is seen in real soil. The Hertz-Mindlin contact model showed a dependence on confining stress but the form of the relationship differs from that seen in experiments as noted by Goddard (1990). Hertz-Mindlin predicts a dependence of $p^{1/3}$ for the elastic moduli, whereas a dependence of approximately $p^{1/2}$ is observed in the lab where $p$ is the confining stress. McDowell & Bolton (2001) investigated the two plausible reasons behind the differences in
predicted and measured relationships between shear modulus and confining pressure. Firstly they proposed that conical contacts can occur instead of circular Hertzian contacts due to surface asperities and secondly that new contacts form without any change in void ratio. McDowell & Bolton found that if one of those is true then approximately $p^{1/2}$ dependence is observed; however, if both are true it would be lost. The rough-surface contact model, which was inspired by the work done by Greenwood & Tripp (1967), resulted in moduli with a dependence on pressure closer to that observed in experiments as it models conical contacts.

Using the rough-surface contact model Yimsiri & Soga (2000) observed a transition between low pressure and high pressure behaviour and a dependence on the inherent anisotropy as observed in Figure 2.8 where $a$ is the degree of fabric anisotropy. Yimsiri & Soga also observed the effect of anisotropic stress conditions on the sample where the Young’s modulus was found to be influenced mostly by the principal stress in its direction and the shear modulus was found to be influenced by the principal stresses in the in-plane directions, confirming the earlier Roesler observations.

Chang & Liao (1990) considered the effect of accounting for particle rotation on constitutive relationships and hence on sample stiffness by comparing analytical solutions that predict stiffness with two-dimensional DEM simulations. Fourth-order stiffness tensors were obtained for granular assemblies. A randomly packed sample of 276 monodisperse circular disks was created by digitizing a photograph of an assembly of aluminium rods randomly placed in a box. The researchers carried out a discrete element method analysis and compared with the results predicted from their microstructural continuum model. Two loading cases were considered in the analysis; loading case 1 is a combination of symmetrical shear stress and normal stress in one principal direction, loading case 2 is a polar or moment stress. Excellent agreement was found for the particle displacement and particle rotation fields between the two methods of analysis (Figure 2.9). Understanding of small-strain stiffness which governs the continuum model at these strain levels is improved by considering the behaviour of particle scale properties.

Kruyt et al. (2010) used analytical methods to calculate constitutive relationships for a two-dimensional packing of disks and examined the effect of how these constitutive models are calculated. Kruyt et al. considered the elastic moduli calculated using energy-based and stress-based methods. The energy-based moduli were calculated by evaluating the energy density of a displacement and rotation field and gave an upper bound for the moduli. The stress-based prediction was found by evaluating a stress tensor from the contact force field.
and since the strain tensor is prescribed the moduli can be calculated. Similar to Chang & Liao (1990), Kruyt et al. compared analytical results with DEM simulations. The stress-based predictions were closer to the true value than the energy-based predictions (Figure 2.10). The value $m$ refers to the sub-assembly orders where $m = 1$ is a sub-assembly consisting of all the particles that contact a single, chosen particle. The sub-assembly where $m = 2$ is a sub-assembly consisting of all the particles that contact the particles which are in contact with the single, chosen particle. The predictions made by both the stress-based and energy-based methods improved in accuracy as the sample size increased and the sample size increased when $m$ was increased.

In the study by Wang & Mok (2008), the influence of contact force magnitude and distribution on sample stiffness was examined using DEM simulations. Isotropic and anisotropic packings (inherent anisotropy) and isotropic and anisotropic stress states (induced anisotropy) were examined. The relationships between shear moduli and confining pressures were examined for these different set-ups. The relationships varied with packing and with imposed stress state. The contribution of contact forces to the stiffness of the sample was examined in the DEM simulations. The variation of the stiffness in different packings under different anisotropic confining pressures was attributed to the variation of the contact forces in the sample. Figure 2.11 shows the change in contact force distributions when the stress conditions became increasingly anisotropic. There is a decrease in the number of contact forces in the xy-plane and an increase in the number of contacts in the z-direction.

In an effort to improve constitutive relationships, Magnanimo & Luding (2011) accounted for the influence of anisotropy in granular material in a micro-mechanics based constitutive model. This analytical model was compared with DEM simulations. The structural anisotropy of a granular packing is described by a tensor, $A$, and the rate of change of anisotropy, $\beta_A$. The influence of $\beta_A$ on structural anisotropy, deviatoric stress ratio and volumetric strain are shown on Figure 2.12 during isobaric (constant pressure) axial-symmetric deformation. The stress-strain response predicted by this model evolved with increasing strain to achieve a critical state where the volume, the stresses and the anisotropy modulus remained constant as the axial strain increased.

### 2.4 Wave propagation through granular material

Information about the propagation of stress waves through an infinite elastic medium can be used to investigate the elastic properties of that medium. Kramer (1996) explained that using
the theory of plane wave propagation two types of body waves can be identified namely primary (P) waves and secondary (S) waves. Figure 2.13 shows that primary waves have an oscillatory motion in the same direction as the direction of wave propagation while secondary waves have an oscillatory motion that is orthogonal to the direction of wave propagation. Primary waves, also known as compression waves, have a speed, $V_p$, that is a function of the constrained modulus of the sample, $M$, while secondary waves, also known as shear waves, have a speed, $V_s$, that is a function of the shear modulus of the sample, $G$.

$$V_p = \sqrt{\frac{M}{\rho}} \tag{2.2}$$

$$V_s = \sqrt{\frac{G}{\rho}} \tag{2.3}$$

where $\rho$ is the sample density.

The compressional wave speed is related to the shear wave speed by the following equation using $\nu$, the Poisson’s ratio of the sample:

$$\frac{V_p}{V_s} = \sqrt{\frac{2(1-\nu)}{(1-2\nu)}} \tag{2.4}$$

As can be seen from Equation 2.4 the compressional wave will be faster than the shear wave speed as generally $0 < \nu < 0.5$.

The theory behind these relationships was developed by considering waves travelling through an infinite, isotropic, elastic medium. For the one-dimensional case of a compressional wave travelling through a rod, the constrained modulus in Equation 2.2 is replaced by the Young’s modulus, $E$. A free body analysis of an element of the rod of length $dx$ at a distance $x$ with a uniform cross-section $A$ and mass density $\rho$ sustaining a P-wave vibration, $\delta \sigma_x$, gives force, $F$, equal to:

$$F = \frac{\delta \sigma_x}{\delta x} dx A \tag{2.5}$$

provided that the cross-section remains plane during wave motion. For clarity, $\delta \sigma_x$ is an incremental normal stress induced by the perturbation causing the compressive wave.
Newton’s second law of motion offers an alternative method of determining the force, $F$, acting on $dx$ and is given by:

$$F = \rho dx A \frac{\delta^2 u}{\partial t^2}$$

where $u$ is the displacement in the direction of $\delta \sigma_x$. Combining the two above equations provides the following:

$$\frac{\delta \sigma_x}{\partial x} = \rho \frac{\delta^2 u}{\partial t^2}$$

The stress term, $\sigma_x$, in Equation 2.7 can be replaced with the following:

$$\sigma_x = E \frac{\delta u}{\partial x}$$

Differentiating Equation 2.8 with respect to $x$ and placing in Equation 2.7 results in:

$$\frac{\delta^2 u}{\partial t^2} = \rho \frac{\delta^2 u}{\partial x^2}$$

Comparing the above result with the general one-dimensional wave equation results in a value for speed:

$$v_p^2 = \frac{E}{\rho}$$

Equation 2.3 can be obtained in a similar manner using $\delta \tau_{xy}$ as the S-wave vibration. Granular materials, both real and simulated, challenge this existing framework as they are frequently contained in boundaries, anisotropically packed (usually deposited under gravity) and able to change their packing as the wave propagates by slippage of contacts. They are, therefore, unlikely to be truly infinite, homogenous or elastic.

### 2.4.1 Analytical work on wave propagation through granular material

Due to the small-strains involved wave propagation results for stiffness are frequently compared with the results predicted by effective medium theory, EMT. EMT is an approximate model that describes the macroscopic properties of a composite material from
averaging the multiple values of the discrete elements that make up composite material. In a pioneering study relating experiments to EMT Duffy & Mindlin (1957) showed how a stress-strain relationship can be obtained for a granular medium. The analytical solution, EMT, considered monosized spheres in a regular packing and compared their results to experimental results on steel ball bearings and found good agreement at higher confining pressures. Digby (1981) and Walton (1987) explored randomly packed granular particles and developed effective elastic moduli for these packings. Digby (1981) examined porous granular rocks while Walton (1987) investigated the elastic moduli of monosized spheres. Santamarina & Cascante (1996) list the EMT solutions for different regular packings, including face-centred cubic packing, to calculate shear modulus, $G_{FCC}$, and Poisson’s ratio, $\nu_{FCC}$. The face-centred cubic packing formulations are shown below.

\[
G_{FCC} = \frac{(4 - 3\nu) \left[ \frac{3\sigma_0 G_{\text{particle}}}{2(1 - \nu_{\text{particle}})^2} \right]^{1/3}}{2(2 - \nu_{\text{particle}})}
\]  

\[
\nu_{FCC} = \frac{\nu_{\text{particle}}}{8 - 5\nu_{\text{particle}}}
\]

where $\nu_{\text{particle}}$ and $G_{\text{particle}}$ are the particle Poisson’s ratio and shear modulus respectively and $\sigma_0$ is the sample confining pressure.

Chang et al. (1991) derived analytically, using the principal of virtual work, the EMT solutions for the elastic moduli of randomly packed samples of monosized particles. Although the condition for equal contact forces between the particles is not violated much with regular packings it is less likely to hold true for randomly packed samples.

\[
G_p = \frac{1}{5} \left( \frac{\sqrt{3}}{\sqrt{2\pi(1 - \nu_{\text{particle}})}} \right)^{2/3} \frac{5 - 4\nu_{\text{particle}}}{2 - \nu_{\text{particle}}} \left( \frac{n}{1 + e} \right)^{2/3} G_{\text{particle}}^{2/3} \sigma_0^{1/3}
\]

\[
\nu_p = \frac{\nu_{\text{particle}}}{2(5 - 3\nu_{\text{particle}})}
\]

where $G_p$ is the shear modulus of the packing, $\nu_p$ is the Poisson’s ratio of the packing, $\sigma_0$ is the mean isotropic confining pressure, $e$ is the sample void ratio and $n$ is the coordination number respectively.
Duffaut et al. (2010) explored the influence of micro-slip on the shear modulus using an analytical model. Figure 2.14 illustrates the influence of contact slippage on shear modulus on the left and wave velocity on the right. A bulk modulus, $K$, of a packing was calculated that was independent of the stick/slip ratio, $f(\mu)$, and a shear modulus, $G$, of the packing was calculated that was dependent on $f(\mu)$. If $f(\mu)$ is 1 the contact area is stuck and if $f(\mu)$ is 0 the contact area is sliding. The variation of $f(\mu)$ produces the variation of $G$ on Figure 2.14 (a). The compressional wave speed, $V_P$, and the shear wave speed, $V_S$, were calculated using the values of $K$ and $G$ so there is a variation of $V_P$ and $V_S$ with $f(\mu)$ that is shown on Figure 2.14 (b).

The principle of virtual displacements can be used to calculate a fourth order stiffness tensor for frictional and frictionless granular materials in a regular lattice. The formulation can be found in de Mol (2013) and in Mouraille et al. (2006) for a unit cell which is representative of the packing as a whole. In a face-centred cubic packed sample this is a single particle with twelve contacts. The derivation presented below is for a frictionless packing. The potential energy at the contact is calculated by considering the strain energy at contact, $u$, and this can be expressed per unit volume by dividing by the Voronoi volume, $V$, of the particle as shown in Equation 2.15.

$$u = \frac{1}{2V}(k_n \Delta^2)$$

2.15

where $k_n$ is the normal contact stiffness and $\Delta$ is the interparticle overlap. The first derivative of the potential energy density with respect to the second order strain tensor, $\varepsilon_{\alpha\beta}$, gives a second order stress tensor, $\sigma_{\alpha\beta}$, and the derivative of the second order stress tensor with respect to strain gives a fourth order stiffness tensor, $C_{\alpha\beta\gamma\phi}$.

$$\sigma_{\alpha\beta} = \frac{\partial u}{\partial \varepsilon_{\alpha\beta}}$$

2.16

$$C_{\alpha\beta\gamma\phi} = \frac{\partial \sigma_{\alpha\beta}}{\partial \varepsilon_{\gamma\phi}}$$

2.17

For a single contact the stiffness tensor can be expressed as
where $l$ is the magnitude of the branch vector between two particle centroids and $n$ is the unit vector in the direction of normal force. The branch vector is the straight line between two particle centroids.

Suitable averaging can be used to obtain the stiffness tensor for a unit cell containing a single particle.

\[ C_{\alpha\beta\phi} = \frac{l^2}{V} \left( k_n n_\alpha n_\beta n_\phi \right) \tag{2.18} \]

Mouraille et al. (2006) and de Mol (2013) also investigated dispersion relations as an analytical solution to the wave speed travelling through a granular sample. Dispersion occurs when the phase velocity varies with frequency and the phase velocity and group velocity are different. The phase velocity is the velocity of a wave component with a particular frequency whereas the group velocity is calculated by considering an average velocity for a group of waves propagating at different frequencies. Solving the dispersion relation involves solving the eigenvalue problem

\[ \left[ K - \omega^2 M \right] U_0 = 0 \tag{2.20} \]

where $M$ is a diagonal mass matrix for the particles in the system, $\omega$ are the eigenvalues corresponding to the angular velocity of response and $U_0$ are the eigenvectors corresponding to each eigenvalue. $K$ is not the interparticle stiffness matrix but it is related to it and it is derived below. The starting point is Newton’s second law which can be expressed discretely as

\[ M \ddot{U} = \sum_{c=1}^{C} F^c \tag{2.21} \]

The terms in Equation 2.21 are explained below. Using the harmonic wave equation $U$ is

\[ U = U_0 e^{i(k \cdot r')} \tag{2.22} \]
\[ \ddot{U} = -\omega^2 U_0 e^{i(\omega t - k \cdot r^p)} \]  

2.23

where \( k \) is the wavenumber and \( \mathbf{r}^p \) is the particle position. \( F^c \) is the contact force and

\[ F^c = S^c \Delta^c \]  

2.24

where \( \Delta^c \) is the relative displacement between two particles, \( p \) and \( q \) and \( S^c \) is the second order particle stiffness tensor.

\[ S^c = k_n I^3 + (k_n - k_t) n^c n^c \]  

2.25

where \( k_n \) is the interparticle contact stiffness normal to the contact plane, \( k_t \) is the interparticle contact stiffness parallel to the contact plane, \( n^c \) is the vector normal to the contact plane and \( I^3 \) is the 3x3 identity matrix.

Using Equation 2.22 for particle \( p \) and \( q \) where \( \mathbf{r}^q = \mathbf{r}^p + 2an^c \) (\( a \) is the particle radius) we can obtain an expression for \( \Delta^c \) which is

\[ \Delta^c = -D^c U_0 e^{i(\omega t - k \cdot r^p)} \]  

2.26

where \( D^c \) is

\[ D^c = (1 - e^{-2ak \cdot n^c}) I^3 \]  

2.27

where \( I^3 \) is the 3x3 identity matrix. Inserting the above equations into Equation 2.21 leads to

\[ M(-\omega^2 U_0) = -\sum_{c=1}^{C} [S^c D^c] U_0 \]  

2.28

Substituting \( K = \sum_{c=1}^{C} [S^c D^c] \) into Equation 2.28 leads to the eigenvalue problem in Equation 2.20. By inputting different wavenumbers and calculating the associated angular velocities the dispersion relation can be solved. Example dispersion relations for a frictionless particle system with different tangential contact stiffness are shown in Figure 2.15 for a face-centred cubic packing.

Marketos & O’Sullivan (2013) also examined dynamic response by solving an eigenvalue problem for a granular material. It takes a similar form to Equation 2.20. \( K \), the stiffness matrix of the sample in this case, was created by considering all the contacts in the chosen
system and could account for boundary conditions. The researchers examined a two-dimensional regular assembly of disks. The mass matrix, $M$, was a diagonal matrix containing all the masses in the system. These two inputs were used to analytically solve for eigenvalues, which are the response frequencies, and eigenvectors, which are the displacements. This allows a transmitted signal to be input into the sample and received signals to be obtained analytically. An example is shown in Figure 2.16 to illustrate the horizontal and vertical displacement produced by a sine pulse propagating through the system. Using this analytical solution the effect of sample aspect ratio, lateral boundary conditions and input frequency were investigated as all of these affect the solution of the analytical solution. This analytical solution can be used to obtain the transfer function for the granular material that determines how the medium responds to an inputted stress wave.

In most analyses performed on wave propagation the influence of reflected and refracted waves are ignored. Sanchez-Salinero et al. (1986) used Fourier superposition to create a received signal for a wave propagating through a linearly elastic medium that was created by a point source. By assuming the medium is isotropic, homogenous and elastic the Green’s function for waves propagating in the medium can be calculated. The response of a medium to an excitation is defined by the Green’s function. The Green’s function can be convoluted in the frequency domain with the Fourier transform of the transmitted signal to obtain a received signal. The Green’s function, $GR$, contains a near-field term ($N$), a far-field compressional wave term ($F_p$) and a far-field shear wave term ($F_s$)

$$GR = N(r,t)[3A - 1] + F_p(r,t)A - F_s(r,t)[A - 1]$$

$$A = \nabla r \otimes \nabla r = \hat{r} \otimes \hat{r}$$

$$\|\hat{r}\| = 1$$

where $r$ is the position vector of the particle relative to the source of the wave.

The effect of this near-field term on the received signal can be observed in Figure 2.17 where there is displacement of the received signal before the arrival of the shear wave. Researchers in bender elements have observed near-field effect in the laboratory such as Jovičić et al. (1996), in continuum analysis such as Arroyo et al. (2003) and in discrete analysis such as O’Donovan et al. (2012).
2.4.2 Experimental research on wave propagation through granular material

A considerable amount of research on wave propagation through granular material has focused on the discrepancy between the observed wave speed and the speed predicted by Hertzian contact mechanics as discussed in Section 2.3.3. Goddard (1990) examined this difference in detail. Goddard proposed two reasons for this discrepancy, (1) departures at the single-contact level from the Hertzian contact, due to conical asphericity and (2) variation in the number density of Hertzian contacts due to buckling of particle chains. These two methods would obtain a power law relationship between wave speed and confining pressure of the value of 1/4 which is closer to the experimental observations than the Hertzian power law relationship between wave speed and confining pressure of 1/6.

In an extensive study involving experimental, numerical and theoretical work, Makse et al. (2004) sought to explain the deficiencies of effective medium theory for describing the stiffness of granular materials. They examined similar packings under different confining pressures and propagated waves using transducers. It was found that effective medium theory was insufficient for describing grain relaxation after an infinitesimal affine strain transformation. Affine strain is where all particles move in the same direction as the applied strain to the sample and there is no motion against the imposed strain field. This does not always happen in the case of granular material. Makse et al. found that relaxation of the grains was an essential component of the shear modulus but not the bulk modulus. When comparing values of $G$ and $K$ at different confining pressure it was found that the simulations and experiments would match but that the effective medium theory did not match these values (Figure 2.18).

Although not concerned with modulus determination, Jia et al. (1999) performed experiments on confined samples of glass beads in an oedometer apparatus to improve the interpretation of results from wave propagation experiments. High frequency signals were propagated through the samples. The received signals were split into a low frequency initial oscillation, marked ‘E’ on Figure 2.19, and a high frequency coda-like response, marked ‘S’ on Figure 2.19. They found that the initial low frequency response, ‘E’, was often similar for different samples; however, the following coda-like response, ‘S’, was not. They recommend that this initial response be used in determining arrival time as it is less susceptible to change than the high frequency ‘S’ region. Figure 2.19 shows the similarity between the points ‘E’ marked
for a sample undergoing initial loading and reloading and the differences between the ‘S’ regions marked on the same sample. The ability of the high frequency wave to propagate through the system appears to contradict the frequency filtering observations of Yang & Gu (2013) and Mouraille (2009); however, the fact that Jia et al. recommend to use the low frequency wave and not consider the higher frequency component indicates that the higher frequency component may be a function of the apparatus. The large plate transducers may act as broad band receivers and produce a higher frequency response when disturbed by the arriving waves.

Liu & Nagel (1993) and Liu (1994) examined the spatial propagation of a wave travelling through an experimental granular sample of spherical glass beads. By placing receivers within the sample during preparation they were able to examine the propagation of the wave through the system and determine preferential paths for the propagation. The variation in the wave with spatial location is illustrated on Figure 2.20 for detectors placed at three different locations. These detectors will have disturbed the fabric surrounding them. As the wave propagates through the system both diffusion and dispersion are observed as the wave reduces in amplitude and frequency. The researchers were able to correlate the preferential paths of propagation to strong force chains in the sample.

Research on wave propagation through photo-elastic disks was carried out by Zhu et al. (1996) where the photoelastic disks were used to measure wavelength (Figure 2.21). The orientation of the photoelastic disks is seen to affect the wavelength. Whether a wave will propagate through a contact is observed to be a function of the contact normals and branch vectors in the system. If either of those angles is greater than 90° then the wave will propagate to that contacting particle. This is related to the load transfer path between contacting particles through which the wave propagates and the load will not transfer if one of the angles is not greater than 90°. The shape of the propagating wavefront was seen to be a function of the particle packing (Figure 2.22). This provides an indication of how packing (inherent) anisotropy affects the speed of wave propagation and therefore the stiffness of the sample.

A more fundamental exploration on wave propagation through a curved chain of particles is found in Cai et al. (2013) who experimentally propagated compressional waves through curve chains of steel spheres varying deflection angle, θ, and radius of curvature, R_c. Cai et al. found good agreement between their experimental results and numerical DEM simulations
which are summarised on Figure 2.23. The results are compared in terms of transmission ratio which is the peak amplitude of the received signal divided by the peak amplitude of the transmitted signal.

In an important fundamental study Santamarina & Aloufi (1999) considered a point source wave propagating from the centre of a two-dimensional grid of photoelastic disks. The effect of induced anisotropy on wave propagation is observed on Figure 2.24 where the wave travels faster in the direction of increased loading. The researchers also investigated wave propagation for particles in different regular packings and found that the packing affected the wave parameters. The wave propagation was visualised using photoelastic disks where changes in contact forces and contacting particles could be observed during wave propagation through the regular packings.

2.4.3 Numerical research on wave propagation through granular material

Discrete element modelling of wave propagation through a granular medium has been the focus of a number of research groups. While the material is not always considered to be an analogue to soil and therefore the focus is not always on geotechnical applications the findings are still applicable for a discrete model of a granular medium. As with experimental research into wave propagation, much of the numerical research is concerned with examining why wave speeds in numerical models that adopt Hertzian contact mechanics do not produce the same behaviour as experimental wave propagation studies. Using DEM Somfai et al. (2005) examined wave propagation through a granular system consisting of particles with a Hertz-Mindlin contact model. Somfai et al. found that the initial coherent wavefront was insensitive to the details of the packing such as the force chains. The coherent wave has a constant velocity that is comparable with macroscopic elasticity predictions. The speed of this wavefront scaled with confining pressure, $p$, as $p^{1/6}$; however, experimental data from granular systems did not match this scaling. A summary of the scaling laws found in this investigation and in other tests, both numerical and experimental, is shown in Figure 2.25 where the two scaling laws of $1/4$ and $1/6$ are clearly observed.

Sadd et al. (1993) investigated wave propagation using a two-dimensional DEM model and examined the effect of contact model employed on the wave propagation. Sadd et al. considered the effect of linear, non-linear and non-linear hysteretic force-deformation contact
laws along with damping proportional to relative particle velocity at the contact, i.e. viscous damping. The behaviour of the wave in terms of its attenuation and dispersion was examined. These numerical results were compared with the observations from previous photoelastic experiments. Sadd et al. found that the contact model employed did affect the wave attenuation and dispersion as did the presence of viscous damping. The new hysteretic contact model without viscous damping, proposed by Sadd et al, was found to best match the existing experimental data for attenuation and dispersion.

Mouraille et al. (2006) numerically investigated a plane wave propagating through a face-centred cubically packed column of particles in three-dimensions using DEM. The system is illustrated on Figure 2.26 and the darkly shaded region of particles was used to input the plane wave. The samples were varied in their polydispersity and in whether they were frictional or frictionless particles. Compressional (P-) and shear (S-) waves were propagated through this medium. The attenuation of the waves was measured by recording the stress acting on the particles as the wave passed through the system. The stiffness of the sample was calculated using a fourth order material tensor, principle of virtual displacement (PVD), and compared with the results of the wave propagation simulations. The frequency dependency of the waves was illustrated using dispersion relations which illustrate the wave propagation through the simulation in the frequency domain. The propagating wave was found to vary both temporally and spatially in the time domain. By obtaining a two-dimensional fast Fourier transform of this information the variation of the wave in angular velocity and wavenumber can be obtained. Typical dispersion relations for the P-waves and S-waves are shown in Figure 2.27 and these relations can be compared with theoretical solutions, dispersion relation theory (DRT), based on particle stiffness tensor and the harmonic wave solution. The wave velocity and thus sample stiffness can be measured from measuring the slope of these dispersion relation plots as angular velocity divided by wavenumber equals the wave speed. As both plots are non-linear, wave speed is a function of the wave frequency. A group wave velocity can be obtained from the tangent slope of the curve and phase velocities can be obtained from the secant slopes of the curve at specific frequencies.

The frequency behaviour of the system was analysed in Mouraille & Luding (2008) and they found evidence that the granular medium was acting as a filter to limit the frequencies which were allowed to propagate through the system. When the frequency-space diagram was plotted for both monodisperse and polydisperse packings the maximum frequency observed
at the receiver end is less than that which is inputted at the transmitter end. This is shown in Figure 2.28 with the monodisperse sample on the left and the polydisperse sample on the right. These plots were created by carrying out fast Fourier transforms on the received signal versus time at different positions on the direction of propagation. The amplitude of the frequency domain plots was used to colour the plots where darker regions have higher amplitude than lighter regions. The frequency filtering, due to the observation of the maximum frequency, is more pronounced for the polydisperse sample than for the monodisperse sample. The researchers propose that this could be due to attenuation or scattering of the wave. Increasing disorder in the packing by increasing polydispersity led to increased filtering of the frequency by removing the ability of higher frequency waves to propagate through the system. Granular material was found by Suiker et al. (2001) to naturally behave as a frequency filter and exhibit dispersion compared to a truly linear elastic system.

Using an analytical approach, Lawney & Luding (2013) further investigated the observation of frequency filtering in a one-dimensional chain of particles. The interaction law was varied between linear and Hertz and the researchers examined disorder in the packing chain. The authors found that disordered systems behave like a low-pass frequency filter that causes higher frequency components to decay with distance from the source.

Anderson (1958) noted the localization of waves in the presence of sufficiently strong random potentials in the context of quantum mechanical particles. Leibig (1994) and Rosenstock & McGill (1962) confirmed that this “Anderson localization” is found in disordered mechanical systems of vibrating masses. The particles in the DEM simulation are considered to be vibrating masses during the propagation of the stress wave. Hu et al. (2008) link the peaks observed on an amplitude versus frequency plot of a received wave with the presence of Anderson localisations. The amplitude versus frequency plot with resonant frequency localisations from Hu et al. is shown on Figure 2.29. These resonant frequencies may be linked with Anderson localisations.

Zamani & El Shamy (2011) simulated wave propagation through a dry granular soil column simulated in DEM and an equivalent linear method programme called SHAKE and found good agreement between the DEM simulation and SHAKE for all frequencies except those close to the resonant frequency of the column. Dynamic properties for the soil were
measured in the DEM simulation directly and were inputted into SHAKE. Samples with different porosity were created and could be compared.

### 2.5 Bender element testing

Dynamic testing of soil, utilising seismic waves, relies on the theory of body wave propagation through a medium. This theory makes two major assumptions 1) that the medium is elastic and 2) that the domain is infinite as outlined in Section 2.4. Bender elements are thin pieces of piezoceramic material that deflect when a voltage is sent through them and produce a voltage when they are deflected. A schematic cross-section of a bender element is illustrated in Figure 2.30. A bender element consists of two oppositely polarised piezoceramic plates bonded together and usually insulated by a layer of epoxy resin. When voltage is applied to a piezoceramic material it will either contract or extend depending on its polarisation. When oppositely polarised plates receive the same voltage they will bend as one contracts and the other extends. When the voltage is reversed the bender element will bend in the opposite direction. The motion of a “transmitter” bender element generates a stress wave that moves through the sample and is detected when the “receiver” element moves in response to this disturbance. By carefully controlling the voltage applied signals of different shapes, frequencies and amplitudes can be produced using the transmitting bender element. The receiving bender element is sensitive enough to record the corresponding small deflections that arise as the perturbation propagates through the system. An oscilloscope can be used to record the transmitted and received signals and from these a travel time for a wave could be found. Knowing the travel distance as a constant in the experiment a wave speed can be found and the speed of the wave can be used to obtain a parameter of the medium using the theory of body wave propagation outlined in Section 2.4. Figure 2.31 is a schematic of a triaxial bender element test. Usually bender elements are fitted to triaxial cells in soil mechanics laboratories. They are commonly used to measure $G_{max}$ under different isotropic and anisotropic confining pressures. Originally bender elements were restricted to measuring $G_{max}$ in the vertical direction until Pennington (1999), Pennington et al. (2001) and Kuwano (1999) used horizontally embedded bender elements in a triaxial cell. By combining horizontally-mounted bender elements with monotonic shear probes researchers have been able to measure the full-suite of elastic parameters for cross-anisotropic materials illustrated in Equation 2.1.
2.5.1 Experimental method

Bender elements were introduced to geotechnical engineering by Shirley & Hampton (1978) and later by Horn (1980). Dyvik & Madshus (1985) compared their results from bender element testing to the results from resonant column testing and obtained a good agreement between the two methods. This led to their acceptance worldwide as a laboratory method of obtaining soil parameters such as the shear modulus and constrained modulus and their use has increased since then. Bender elements were found to be an inexpensive way of obtaining soil properties and were believed to be reasonably accurate. As their use in research and industry increased, however, problems in signal interpretation began to be reported, for example in Viggiani & Atkinson (1995), Brignoli et al. (1996) and Blewett et al. (2000). Due to the effects of geometric spreading of the wave, reflections off the boundaries and dispersion of the wave the signal recorded by the receiver often looked very different to the signal recorded by the transmitter (Figure 2.32) taken from Leong et al. (2009). As can be observed in the signals presented there is dispersion of the signal as the receiver oscillates with a lower frequency than the transmitter. There is attenuation as the received signal is measured in mV and the transmitted in V. There is a change in shape of the signals and none are similar in shape to the transmitted signal. Different travel time determination techniques in both the time and frequency domains have been proposed by different researchers to overcome these uncertainties as discussed below. The time and frequency domains are linked by Fourier transforms. Examples of different travel time determination techniques can be found in Arulnathan et al. (1998), Jovičić et al. (1996), Alvarado & Coop (2012), Wang et al. (2007) and Greening & Nash (2004). An overview of the more popular travel time determination techniques is presented later in Section 2.5.2.

The Japanese domestic committee for TC29 (Technical Committee 29 – Laboratory Stress Strain Strength Testing of Geomaterials) organised a comparative study using the same soil in different laboratories around the world implementing different travel time determination techniques described by Yamashita et al. (2009). The set-up for a bender element test has been varied by many researchers in efforts to improve the interpretation of the test. However TC29 illustrates some common specifications in bender element testing. In general, the thickness of the bender elements used is typically between 0.5mm and 1.0mm and they were typically rectangular in shape with an aspect ratio of 1.5 to 2.0. The length of the bender elements tended to vary between 15mm and 20mm and the width was 10mm. The average penetration length into the sample was 6mm. The TC29 report details the specifications for
the tests considered in the report. The wiring of the bender element can produce different deflections of the bender element. A parallel wiring can produce a translational deflection and thus a shear wave is produced. A series wiring can produce a longitudinal deflection and thus a compressional wave is produced. Lings & Greening (2001) illustrated how the control that is obtained by varying the wiring configuration can be used to create bender/extender elements that can both produce and receive shear and compressional waves along the same travel paths without the need to alter the installation of the bender/extender element. A schematic of the bender/extender element from Lings & Greening (2001) is shown in Figure 2.33. In their study, Lee & Santamarina (2005) outline how the wiring of the bender elements can affect the test and which wiring should be used for transmitting and receiving shear and compressional waves.

2.5.2 Interpreting bender element signals

There are a variety of techniques available to determine the stress-wave travel time in a bender element test. The two broad categories are time domain methods and frequency domain methods. A number of these time domain techniques are illustrated on Figure 2.34, reproduced here from Viggiani & Atkinson (1995). The time domain methods involve attempting to match two characteristic points on the transmitted and received signals, such as peak-peak. The frequency domain methods involve obtaining the wave velocities of particular frequencies contained within the received signal. When the time domain methods are used the time measured considers popular characteristic points such as the start of the transmitted signal to the point of first local minimum on the received signal, the start of the transmitted signal to the point of first zero crossing on the received signal and the peak of the transmitted signal to either the first peak on the transmitted signal or the maximum peak on the transmitted signal.

In the cross-correlation method a fast Fourier transform (FFT) is taken of both the transmitted and received signals and the resulting FFT’s are convoluted by multiplying one by the conjugate of the other to give a resulting cross-correlation function which can be transformed back to the time domain. In the method outlined by Viggiani & Atkinson (1995) and Arulnathan et al. (1998) the arrival time is taken as the time at which the maximum peak on the cross-correlation function occurs. In more recent work Mohsin & Airey (2003) demonstrate that taking the maximum peak does not always produce a satisfactory result. They propose picking the peak on the cross-correlation that occurs near the arrival time.
calculated using an existing first arrival method. The maximum peak choice implies confidence that the received shear wave is propagating with the frequency it was transmitted with, however, as dispersion occurs in granular materials the frequency of the shear wave will change as it propagates through the system. Therefore the peak of the cross-correlation, which will correspond to the arrival of a wave propagating at the frequency of the transmitted wave, may not be the shear wave. A typical transmitted signal, received signal and cross-correlation function using the Mohsin & Airey (2003) technique for establishing arrival time are plotted on Figure 2.35. The peak corresponding with first arrival is marked to illustrate the difference that and the maximum peak. Yang & Gu (2013), in their experimental work, also adopted this approach to interpreting cross-correlation functions.

The frequency domain travel time determination methods involve transforming the received signal using FFT. The FFT can be used to calculate the stacked phase of the different frequencies contained in the received signal. Stacked or unwrapped phase is when phase angles are corrected to produce smoother curves. The radian phase angles are corrected by adding multiples of \( \pm 2\pi \) when absolute jumps between consecutive elements of the phase vector are greater than or equal to a tolerance of \( \pi \) radians. The stacked phase is then plotted against the frequency and the gradient of that line is a measure of the travel time of the wave. The secant of the curve gives the travel time at a particular frequency that is used to calculate phase velocity, while the tangent of the curve gives the travel time for a number of frequencies that can be used to calculate the group velocity. Figure 2.36 illustrates this method which was outlined in Greening & Nash (2004) and is a plot of stacked phase versus frequency. The researchers found that this method underestimated wave velocity compared to other methods.

An extension to existing travel time determination techniques is the wavelet analysis suggested by Bonal et al. (2012) who compared their wavelet analysis technique with various existing travel time determination techniques. A schematic of their technique is shown in Figure 2.37 and by selecting different windowed FT’s the user can obtain different travel time values. The most commonly occurring values are deemed to be the arrival of the shear wave.

Lee & Santamarina (2005) illustrate clearly the shape of the shear and compressional waves produced by a bender element test. The shear wave produced was demonstrated to be a spherical frontal lobe that travels through the centre of the sample. The compressional waves
produced were demonstrated to be elliptical side lobes that were produced on each side of the bender element. An illustration of these lobes is illustrated in Figure 2.38 and they appear to be of similar shape to the lobes shown on photoelastic disks in Zhu et al. (1996). The resonant frequency of the bender element embedded in the soil was explored and it was found that the resonant frequency depended on the bender element stiffness for short cantilever lengths and on the soil stiffness for longer cantilever lengths. The issue of wave reflection inside the sample was explored and used to aid signal interpretation. A second estimate for travel time was found by measuring the time taken for the reflection of the shear wave to return to the transmitting bender element in a method known as auto-correlation. More information on this method can be found in Santamarina & Fratta (2005).

2.5.3 Key experimental studies using bender elements

The study by Kuwano & Jardine (2002) is particularly relevant to the current research. The cross-anisotropic, linear elastic assumption for soils was examined using Ham River sand and glass ballotini. High resolution triaxial tests were combined with multi-directional bender element experiments to explore anisotropic small-strain stiffness behaviour. The researchers identified a linear range of behaviour at very small strains typically less than 0.001%. \( S_{vh} \) and \( S_{hv} \), which are the shear waves propagating in different directions with different oscillation directions, should have the same value but were found to be different. This was inconsistent with a perfectly elastic response. It was also found that the shear moduli measured varied strongly with effective stress state and weakly with void ratio.

Jovičić & Coop (1997) used bender elements on samples of Dogs Bay sand, Ham River sand and decomposed granite to evaluate the evolution of \( G \) with confining pressure. The relationship between \( G \) and confining pressure was found and one such relationship is illustrated in Figure 2.39 for Dogs Bay sand. The researchers also investigated the influence of creep and loading history on the sample stiffness. These time effects are found to alter the sample stiffness.

Alvarado (2007) used bender elements to measure the small-strain stiffness, \( G_{vh} \), of Toyoura sand. Values calculated using different time and frequency domain methods were compared with values in the literature as observed on Figure 2.40. The frequency domain travel times was calculated from stacked phase versus frequency plots similar to Greening & Nash (2004), \( t_g \) on Figure 2.40. At higher confining pressures the values of \( t_g \) are found to be constant therefore \( t_{arr}(n) \) are estimated from the existing \( t_g \) values. These estimates were found by
considering the soil material to have a unique transfer function similar to Sanchez-Salinero et al. (1986). $n$ was used as an input into the calculation of the transfer functions and these estimates can be changed by specifying $n-1$ instead of $n$ to obtain better agreement with the existing data in the literature.

A recent study carried out in Yang & Gu (2013) is relevant to this study. Tests were carried out on ballotini of different diameters and particle size was found to influence the shape and frequency of the received signal; however, the wave speed was not affected. A threshold frequency was observed, shown on Figure 2.41, as the inputted frequency was increased and this was measured by measuring the “predominant” frequency in the frequency domain plots. This threshold frequency was found to be a function of particle size. The effect of varying $R_d$ and $\lambda/d_{50}$ was also investigated and a favourable band of $R_d$ values were found to lie between 2 and 4 while $\lambda/d_{50}$ values greater than 10 produced reliable results. This is in agreement with a number of other experimental and numerical studies. The relationship between the shear moduli of the samples and the confining pressure applied to the sample was investigated and found to be approximately $G \propto \sigma_0^{0.4}$. The theoretical Hertz-Mindlin contact model was investigated by Yang & Gu and there was no justification found for varying wave speed with varying particle size.

### 2.5.4 Key numerical studies using bender elements

#### 2.5.4.1 Continuum numerical analysis

Previous continuum numerical studies of the bender element test have usually been conducted with finite element analysis. Hardy (2003) carried out a two-dimensional plane strain finite element simulation of a bender element test in a triaxial cell apparatus. By specifying the input parameters it was possible to calculate the percentage errors on the material properties measured using bender elements. In initial simulations the time domain method was used to measure $G_{\text{max}}$ and in later simulations the frequency domain method was used. Comparisons were made between both methods. A layout of the sample is shown in Figure 2.42. The bender elements were modelled explicitly in the sample and had a stiffness value that was different to the surrounding soil. The transmitting bender elements were assigned a sinusoidal displacement and the displacement of the receiving bender element was recorded. Bender element tests were conducted on the sample for several $R_d$ ratios between 1 and 8. The values of wavelength relative to the element size vary from 94.5 to 11.8 when the $R_d$ ratios vary between 1 and 8 respectively. $R_d$ is the number of full shear wavelengths that
occur between the transmitting bender element and the receiving bender element. The frequency domain method was examined using a continuous signal as the input and phase sensitive detection obtains results. The values of shear wave speed were inaccurate for tests carried out with $R_d \leq 4$ and the values of wavelength divided by element size were always $> 10$.

Extending to three-dimensions, Arroyo et al. (2006) created a finite difference model (FDM) using FLAC3D. The layout of the model is shown in Figure 2.43. A three-dimensional cylindrical model of a soil sample was used with a prismatic region at one end to represent the bender element. The primary purpose of this model was to investigate the distortion of the signal by sample size effects and lateral boundary conditions. Two different sets of material properties were assigned in the model, one to the soil sample and a second to the bender element. Both materials were considered to be isotropic and elastic. The soil material properties used were for a typical medium to soft soil. The numerical model used for different geometries to adequately investigate the effect of sample size on signal propagation. Different lateral boundary conditions were applied to the cylindrical sample to investigate their effects on the sample. The parametric study represents an initial attempt to investigate, numerically, what effect varying some parameters has on bender element test results. The success of this numerical model to capture a lot of the features of the experimental bender element test is encouraging.

In Rio (2006) extensive finite difference modelling of bender element tests were conducted. It is important to carry out these numerical simulations to gain a better understanding of the system. The program FLAC3D was used to create the FDM model in this research. The sample properties and geometry were similar to the one in the paper mentioned above, Arroyo et al. (2006). Rio was able to distinguish between a direct propagated wave and a reflected propagated wave using the numerical analysis technique. Wave propagation simulations were conducted without the influence of reflections using FLAC3D’s “quiet” boundary conditions which damp out reflections using viscous dashpots. The effect of boundary conditions and particle diameter is shown on Figure 2.44. It should be possible to reproduce the effects which Rio (2006) observed in the FEM model in a future DEM model. It is also hoped that it will be possible to track the propagation of the signal through the DEM sample by measuring changes in grain displacement or velocity.
2.5.4.2 Discrete numerical analysis

A DEM model of a bender element test was created by Clement (2006). This model was a small-scale 2D model of a bender element test in the time domain using a single pulse excitation. The model layout is illustrated in Figure 2.45. A particle at the base of the sample was displaced to produce a signal and the displacement of a particle at the top of the sample was measured to determine the arrival time of the signal. A parametric study was carried out to determine some of the input parameters in the DEM model such as damping, friction and contact stiffness and, also, the properties of the input signal, such as frequency and amplitude. The seismic waves were tracked propagating though the sample at regular intervals and, from this, it is possible to demonstrate that many of the features of the experimental bender element test were present in this basic DEM model. The DEM model showed that both shear and compressional waves are produced during a bender element test and that complexities in the received signal are due to interference between these waves. A method of validating the attained value for the shear modulus using stress probes was presented and the results of the bender element tests can be critically assessed using this reference value.

Xu et al. (2012) developed a three-dimensional DEM simulation of a shear wave test similar to an experimental bender element test. The test layout is shown in Figure 2.46 and it is observed that the transmitter and receiver are larger than traditional bender elements meaning that they will transmit planar waves rather than the spherical shaped pulses transmitted by bender elements. Using this transmitter the authors transmitted torsional and shear waves in this sample. The propagation of the shear wave through the sample was visualised by the authors using individual particle velocities (Figure 2.47). Xu et al. investigated the differences between the measured shear wave velocities and the analytical solutions for a simple cubic packed and a randomly packed sample. It was found that there was good agreement between the shear wave velocity and the analytical solutions for the simple cubic packing but not for the randomly packed sample. The analytical solutions were obtained using effective medium theory. This highlights the difficulty in accounting for the local heterogeneities in the randomly packed sample using analytical solutions.
2.6 Small amplitude stress probes on granular material

Small amplitude stress probes can be used to calculate values of sample moduli at small-strain levels. Young’s modulus, $E_i$, in a particular direction can be calculated directly from calculating the slope of the axial stress versus axial strain curve which should be close to linear for small-strain levels. The Poisson’s ratio, $\nu_{ij}$, can be calculated from the negative of the slope of transverse strain versus axial strain. Shear moduli, $G_{ij}$, can be calculated by assuming isotropy in a particular plane and using the equation below.

$$G_{ij} = \frac{E_i}{2(1-\nu_{ij})}$$  \hspace{1cm} 2.30

Alternatively, shear stress could be applied to the sample and a plot of shear stress versus shear strain can be used to calculate the shear modulus. Ability to record stress and strain at such small levels has led to increasing ability to obtain small strain sample moduli using small amplitude stress probes.

2.6.1 Experimental stress probes on granular material

Cuccovillo & Coop (1997) and Tatsouka et al. (2000) measured small-strains in laboratory samples using LVDTs. These high-resolution instruments can measure strains at magnitudes as low as 0.0001% and are illustrated on Figure 2.48. This development allowed the stresses and strains to be determined at very small level of strain leading to the measurement of small strain stiffness that could be assumed to be still within the elastic Zone 1 mentioned in Section 2.3.1. LVDTs are sensitive enough to measure small inherent stiffness anisotropy in laboratory samples. Cuccovillo & Coop (1997) demonstrated the ability of LVDTs to measure small strain response using undrained tests on Kaolin clay samples. The LVDTs picked up a linear slope on the curve of deviatoric stress versus axial strain at small axial strain values.

Kuwano (1999) used small amplitude probes in her research on small strain soil parameters of Ham River sand, Dunkerque sand and glass beads. Static probes and dynamic tests were used to enable measurement of $E_v'$, $E_h'$, $\nu_{vh}$, $\nu_{hh}$ and $G_{vh}$. They comprise all the parameters that are needed for a cross-anisotropic description of soil. Stress probes were used to measure $E_v'$, $E_h'$, $\nu_{vh}$ and $\nu_{hh}$ with the remaining parameter, $G_{vh}$, measureable by bender element tests. Induced and inherent anisotropy of the different samples at small strain were
measureable using small amplitude stress probes. Inherent anisotropy was found to be present in the values of Young’s moduli where $E_h' < E_v'$ under isotropic effective stress in all materials. Values of Poisson’s ratio showed a consistent trend where $\nu_{vh} > \nu_{hv} > \nu_{hh}$ and the shear moduli exhibited anisotropy where $G_{hh} \neq G_{vh}$. It was possible to measure $E_h'$ and $\nu_{hh}$ from bender element tests and stress probes which allowed values to be compared.

Sadek (2006) examined the elastic properties of dry Hostun sand using a flexible bounded, true-triaxial cubical cell apparatus. In this research small amplitude stress probes and dynamic bender element tests were used to determine all the cross-anisotropic parameters in the stiffness tensor. Stress probes in different directions were used to build up stress response envelopes similar to the work carried out in Thornton (2000) on a numerical sample. Radial probing was carried out along twelve radial deviatoric stress paths. The stress response envelopes connect contours of equal shear or volumetric strain in stress space. From the results there is an indication of the inherent anisotropy of the pluviated Hostun sand sample. These stress probes were carried out on samples of initially isotropic and anisotropic stress states to examine the effect of induced anisotropy. The stress probe results were not directly compared with the results from the bender elements as they were used to ascertain different properties. Current research ongoing in the University of Bristol, Hamlin (2014), is making use of the cubical cell apparatus to explore wave propagation using bender elements and carry out stress probes.

Ezaoui & di Benedetto (2009) used their “Triaxial StaDy” apparatus to examine the quasi-elastic properties of dry Hostun sand in a lab setting. The apparatus was able to measure properties using very small axial cyclic static loadings, strain controlled, and four types of wave generated by piezoelectric sensors (bender elements). Three different sample preparation methods are used to compare different samples. They include simple pluviation, vibration method and tamping method. The strain amplitude used for the static tests was $10^{-5}$ m/m which is considered to be in the elastic or quasi-elastic range. Linear fits of the slopes plotted by $\Delta q$ against $\Delta \varepsilon_z$ give values for Young’s modulus, $E_z$, and linear fits of the slopes plotted by $\Delta \varepsilon_r$ against $\Delta \varepsilon_z$ give values for Poisson’s ratio, $\nu_{rz}$. These values were obtained using dynamic tests using shear and compressional waves propagating and oscillating in different directions. These waves are $V^P_z$, $V^S_z$, $V^P_r$, and $V^S_{r\theta}$ and the following equations are used to obtain the desired properties:
\[
\rho (V_{rz}^P)^2 = \frac{E_{r}^{dyn} (v_{rz}^{dyn} - 1)}{(v_{rz}^{dyn} - 1)E_{z}^{dyn} + 2v_{rz}^{2}E_{r}^{dyn}}
\]  
(2.31a)

\[
\rho (V_{rz}^{S})^2 = G_{rz}^{dyn}
\]  
(b)

\[
\rho (V_{r}^P)^2 = E_{r}^{dyn} \frac{v_{r}^{2}E_{r}^{dyn} - E_{z}^{dyn}}{(v_{r}^{2} - 1)E_{z}^{dyn} + 2v_{rz}^{2} (1 + v_{rz}^{dyn})E_{r}^{dyn}}
\]  
(c)

\[
\rho (V_{r}^{S})^2 = \frac{E_{z}^{dyn}}{2(1 + v_{r}^{dyn})}
\]  
(d)

where \( \rho \) is the sample density.

The static measurements \( E_{z}^{stat} \) and \( v_{rz}^{stat} \) were compared with the dynamic measurements \( E_{z}^{dyn} \) and \( v_{rz}^{dyn} \) and a good agreement was found. The coefficients of correlation between the static and dynamic results were very close to 1 (Figure 2.49).

### 2.6.2 Numerical stress probes on granular material

Magnanimo et al. (2008) used small strain probes to measure the elastic moduli of numerical granular samples. A small incremental strain was applied to the sample and then it was allowed to relax. The importance of this relaxation was previously highlighted by Makse et al. (2004) in Section 2.4.2. The friction coefficient in the simulation was set very high to avoid sliding occurring between the particles. The researchers applied a strain increment of \( \Delta \varepsilon_{12} \) and measured the stress response \( \Delta \sigma_{12} \) to obtain a value of shear modulus, \( G \), and an isotropic strain increment \( \Delta \nu = \Delta \varepsilon_{11} + \Delta \varepsilon_{22} + \Delta \varepsilon_{33} \) to obtain a value of bulk modulus, \( K \). Magnanimo et al. (2008) noted that the strain increment must be kept very small to ensure that the system remains in the linear response regime. Figure 2.50 illustrates the stress response when a strain increment of \( \Delta \varepsilon_{12} \) is applied to the sample. The strain increment was applied in one time step between points A and B on the graph. The system was allowed to relax until point C and the change in stress is measured from this point (Figure 2.50). The researchers examined \( G \) and \( K \) values for samples prepared with different coefficients of interparticle friction and found that both \( G \) and \( K \) vary depending on the preparation procedure.
In de Mol (2013) small amplitude stress probes were conducted in a DEM simulation and the constrained modulus, $M$, was calculated using Hooke’s law according to the following equation

$$M = \frac{Fl}{A\Delta l}$$

where $F$ was the force applied to the particles in the stress probe, $l$ was original length of the sample, $\Delta l$ was the change in length and $A$ was the cross-sectional area of the sample to which the force was applied.

### 2.7 Overall conclusions

Small-strain soil stiffness is an important parameter in geotechnical engineering. The movement of the ground during construction and during earthquake events can be accurately predicted only when the small-strain stiffness is accurately modelled. Constitutive models of soil behaviour are more accurate if they capture small-strain response of soil and this has been validated in laboratory and field observations by academia and industry. Bender elements are increasingly used to measure the small-strain stiffness of soil but the results are difficult to interpret. The existing travel time determination techniques often result in differing values of stiffness. The suitability of existing techniques needs to be critically assessed and there is scope for investigating alternative, more reliable techniques.

The origin of stress dependent stiffness of a granular material remains unclear. The stiffness of a granular material has been found to be linked to the contact force network. The contact force network is influenced by both inherent and induced anisotropy. The inability of contact models based on existing theory to capture this dependence accurately is a motivation for the current study. The influence of fabric on small-strain stiffness is poorly understood and needs to be investigated further.

Many of the existing wave propagation theories rely on the assumption of a homogeneous medium. Soil is rarely homogenous and the current study can create heterogeneous samples using the discrete element method. Fabric tensors were calculated from the particle scale data which can quantify heterogeneity with accuracy not available in previous studies.
2.8 Figures

Figure 2.1: A schematic of a typical DEM contact between two spherical particles from O’Sullivan (2011).

Figure 2.2: Characteristic stiffness-strain behaviour of soil with typical strain ranges for laboratory tests and structures from Atkinson (2000).
Figure 2.3: Comparison between the result from the Castlegate DEM model and test data of Alvarado (2007) from Cheung (2010).

Figure 2.4: Illustration of yield zones on $q$-$p'$ space from Jardine (1992).
Figure 2.5: Illustration of stresses acting on elements in the xy-plane (horizontal) and the zx-plane (vertical).

Figure 2.6: Distribution of contact normals: (a) assembly at initial (hydrostatic) stress condition; (b) initial distribution of contact normals; (c) assembly at peak stress ratio; (d) contact normals at peak stress ratio. Images taken from Rothenburg & Bathurst (1989).
Figure 2.7: Force chains shown experimentally using photo-elastic disks from Majmudar & Behringer (2005).

Figure 2.8: Young’s moduli plotted against confining pressure for a rough-surface contact model for packings with different degrees of anisotropy from Yimsiri & Soga (2000).
Figure 2.9: Comparisons between particle displacement fields (a) and (b) and particle rotation fields (c) obtained from the discrete method (left) and the continuum method (right). (a) is for loading case 1, (b) and (c) are for loading case 2 from Chang & Liao (1990).
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3 Implementation of user-defined contact model

3.1 Introduction

To date, in geomechanics most researchers have used either linear springs or a simplified Hertz-Mindlin contact model to describe the force-displacement relation at the contacts. As discussed in Chapter 2, and shown experimentally by Cascante & Santamarina (1996), shear wave speed can be highly dependent on the particle contact properties. Theoretically the shear wave speed should be affected by the contact model used. Effective medium theory as presented in Duffaut et al. (2010) predicts the shear modulus, $G$, of a granular packing to be a function of the contact stiffness in the normal and shear directions. $G$ will govern the speed of the shear wave propagating through our system. As illustrated in Figure 3.1 when two entities contact in a Discrete Element Method (DEM) simulation a contact normal vector lies between the centres of the two contacting particles and the normal contact force acts along this vector and is a function of the contact normal displacement (overlap). When the particles are spherical, as in the current study, a point contact exists. A tangential contact plane can be defined whose surface is perpendicular to the contact normal vector. The tangential force is a vector acting in this plane which is a function of the contact tangential displacement and normal force magnitude if Hertz-Mindlin is implemented. Where a linear spring is used to model contact, it can be thought of as a penalty spring whose role is to minimise penetration at the contact point. The simplified Hertzian contact model has a more developed theoretical basis and behaves as a non-linear elastic spring. This chapter discusses two refinements that were made to the Hertzian contact model on the basis of the experimental work of Cavarretta et al. (2010) and the theoretical/numerical work of Thornton & Yin (1991).

While Hertz (1896) proposed a widely accepted theoretical solution to the contact between two identical, elastic spheres, experimental observations carried out by Cavarretta et al. (2010) show that the response of real spheres is less stiff than Hertz theory predicts until a certain threshold pressure is reached. This is due to the presence of small asperities on the particle surface, as theoretically predicted by Greenwood & Tripp (1967) and found to affect sample stiffness in analytical work carried out by Yimsiri & Soga (2000). The
implementation of the Cavarretta-Mindlin model (CM) described in Section 3.2 uses the observations of Cavarretta et al. (2010) to propose an alternative force-displacement law for the normal direction.

From a theoretical perspective, a more accurate implementation of the tangential force-displacement law should account for the work of Mindlin (1949) and Mindlin & Deresiewicz (1953). Thornton and his colleagues have worked with the Hertz-Mindlin-Deresiewicz force-displacement model for a number of years e.g. Thornton (2000) and Thornton & Zhang (2010); however, it is not widely used in DEM simulations in geomechanics. The normal force-displacement model follows Hertzian theory and the tangential force-displacement model follows the theory proposed by Mindlin & Deresiewicz (1953). The key differences between the Hertz-Mindlin (HM) no-slip model implemented in most codes and the Hertz-Mindlin-Deresiewicz (HMD) model is that the simplified model does not model frictional energy loss due to micro-slip and does not account for the loading history of the contact. These differences may be subtle and may not measurably influence response at large strain levels, however it is likely to have a measurable influence for the small cyclic changes in tangential displacement that are a result of a small amplitude shear wave propagating through the granular medium.

The refined normal contact model is outlined in Section 3.2 while Thornton and Yin’s HMD model is discussed in Section 3.4. The implementation of these models and the verification exercises carried out are discussed in Section 3.5. The effects of different contact models on the results of a multi-particle simulation are discussed in Section 3.6. In these DEM models the effect of rolling resistance is not accounted for. Although Hertzian theory predicts a finite contact area the DEM model does not consider this finite area, consequently the rolling resistance that could be attained by having a finite contact area is never realized.

### 3.2 Hertz-Mindlin contact model

As noted above, Hertz (1896) developed an analytical expression to describe elastic deformations in the normal direction when two smooth, elastic spheres interact. Hertzian theory can be used to formulate a non-linear elastic DEM contact model. The parameters needed to implement a Hertzian contact model are the particle shear modulus, $G_{\text{particle}}$, the particle Poisson’s ratio, $\nu_{\text{particle}}$, and the particle radius, $R_{\text{particle}}$. Knowing the particle shear modulus and Poisson’s ratio the particle Young’s modulus, $E_{\text{particle}}$, was calculated. Hertz considered the circular contact area, $a$, that develops between two contacting spheres. As the
overlap, \( \alpha \), between the two particles increases the contact area also increases resulting in a non-linear force-displacement relationship at the contact. Referring to Thornton & Randall (1988) and Thornton & Yin (1991) the relevant equations are as follows where the subscripts \( \text{particle}_1 \) and \( \text{particle}_2 \) refer to the two particles in contact and \( k^n \) is the interparticle contact stiffness in the normal direction:

\[ k^n = 2E^* \alpha \]  \hspace{1cm} (3.1)

where

\[ \frac{1}{E^*} = \frac{1-v_{\text{particle}_1}^2}{E_{\text{particle}_1}} + \frac{1-v_{\text{particle}_2}^2}{E_{\text{particle}_2}} \]  \hspace{1cm} (3.2)

\[ a = \sqrt{R^* \alpha} \]  \hspace{1cm} (3.3)

and

\[ \frac{1}{R^*} = \frac{1}{R_{\text{particle}_1}} + \frac{1}{R_{\text{particle}_2}} \] \hspace{1cm} (3.4)

Finally the normal force, \( P \), is updated as follows where the tangential stiffness is multiplied by 2/3 to convert it to secant stiffness:

\[ P = \frac{2}{3} k^n \alpha \] \hspace{1cm} (3.5)

The relationship described by Equation 3.5 is plotted in Figure 3.2. This model is a non-linear elastic model; the non-linearity arises due to the change in contact area during deformation. Hertzian contact mechanics leads to a power law relationship between the average sample confining pressure, \( p' \), and the sample shear modulus, \( G \), of 1/3. As discussed in Chapter 2 experimental data tend to indicate \( G \) increasing more rapidly than \( p'^{1/3} \) (reported by Goddard (1990), Makse et al. (1999) and McDowell & Bolton (2001)) highlighting a shortcoming of the Hertz model.

The simplified Mindlin tangential contact model is governed by the following equation

\[ \Delta k_i = 8G^* \alpha \]  \hspace{1cm} (3.6)

where \( G^* \) is given by
\[ \frac{1}{G^*} = \frac{2 - \nu_{\text{particle}_1}}{G_{\text{particle}_1}} + \frac{2 - \nu_{\text{particle}_2}}{G_{\text{particle}_2}} \]

It is important to consider the incremental contact stiffness in the tangential direction. The incremental tangential force, \( \Delta T \), is related to the incremental tangential displacement, \( \Delta \delta \), by the following equation

\[ \Delta T = \Delta k \Delta \delta \]

### 3.3 Cavarretta-Mindlin contact model

In reality there is a possibility for plastic strain to occur at the contact point and elasto-plastic contact models have been proposed, an early example is Walton & Braun (1986) where a partially latching spring is considered, i.e. \( k_{\text{unload}} > k_{\text{load}} \). Thornton & Ning (1998) outlined an elasto-plastic normal force-displacement model based on particle yielding. At the small-strain level Cavarretta et al. (2010) proposed an elasto-plastic normal force displacement model, based on the yielding of particle asperities prior to the elastic loading of the particle which follows the theory of Hertz, that followed a series of physical experiments. This model also considers earlier observations in Greenwood & Tripp (1967) that at small deformations the normal interaction of two particles does not follow Hertz elastic theory. Greenwood & Tripp (1967) found that the response at small deformation was less stiff than Hertz predicted. Yimsiri & Soga (2000) analytically modelled the effects of these particle imperfections and found that it can affect sample stiffness and the relationship between sample stiffness and confining pressure. Cavarretta et al. (2010) experimentally demonstrated that there was some irrecoverable plastic deformation at the contact even at contact pressures below the yield pressure of the particle. The elastic Cavarretta model outlined below, the Hertz model and experimental data for a borosilicate glass ballotini particle under uniaxial loading are plotted in Figure 3.3. The ballotini used in this experiment had the following properties; particle shear modulus of 16.67GPa, particle Poisson’s ratio of 0.20, a hardness of 800MPa and a roughness of 0.03μm. The experimental determination of hardness and roughness is discussed in Cavarretta et al. (2010) and their influence on the model will be discussed below.

Two versions of the Cavarretta model were implemented in PFC, namely an elastic version and plastic version. The elastic version (Figure 3.4) loads, unloads and reloads along the
same curve. This curve is less stiff than the Hertz curve up to a threshold force, \( P_{GT} \), where the behaviour becomes Hertzian. The elastic version assumes that the crushing of the asperities is elastic and that the asperities return to their original shape after unloading. The plastic version (Figure 3.5) behaves elastically on the initial, less stiff, curve until \( P = P_{GT} \). Then the model follows the Hertzian curve for loading, unloading and reloading. This results in a plastic deformation of the particle once the contact force exceeds \( P_{GT} \). When the contact unloads the force goes to zero at a plastic deformation of \( \alpha_{p} \) which represents the full compression of the asperities.

In comparison with the Hertzian contact model the Cavarretta model requires two additional input parameters, the roughness (\( RMS_f \)) has units of length and the hardness (\( H_{particle} \)) has units of pressure. The displacement above which the contact area is large enough to exhibit some Hertzian elastic behaviour, \( \alpha_p \), is given by the following equation:

\[
\alpha_p = \frac{9R^*\pi^2}{16}\left(\frac{H_{particle}}{E^*}\right)^2
\]

\[\text{3.9}\]

\( P_{GT} \) is the threshold force above which the contact behaviour becomes fully Hertzian and given by:

\[
P_{GT} \cong 100(RMS_f)E^*[2R^*(RMS_f)]^{0.5}
\]

\[\text{3.10}\]

The overlap at which the force is equal to \( P_{GT} \) is \( \alpha_{GT} \):

\[
\alpha_{GT} = \left(\frac{3P_{GT}}{4\sqrt{R^*E^*}}\right)^{2/3}
\]

\[\text{3.11}\]

In equations 3.13 and 3.14 the exponential, \( b \), equals:

\[
b = 2E^*[R^*(\alpha_{GT} - \alpha_p)]^{0.5} \alpha_{GT} P_{GT}^{-1}
\]

\[\text{3.12}\]

For the elastic version the entire force-displacement model can be expressed as follows:

\[
P = P_{GT}\alpha_{GT}^b \alpha^b \quad \alpha < \alpha_{GT}
\]

\[\text{(a)}\]

\[
P = \frac{4}{3}\sqrt{R^*E^*} \left(\alpha - \alpha_{GT}\right)^{3/2} \quad \alpha \geq \alpha_{GT}
\]

\[\text{(b)}\]
For the plastic version the entire force-displacement model can be expressed as follows:

\[ P = P_{GT} \alpha_{GT}^b \alpha^b \]  
\[ (\text{Case 1: } P < P_{GT}, \alpha < \alpha_{GT}) \]  
\[ P = \frac{4}{3} \sqrt{R^*} E^* (\alpha - \alpha_{GT})^{3/2} \]  
\[ (\text{Case 2: } \alpha \geq \alpha_{GT}) \]  
\[ P = 0 \]  
\[ (\text{Case 3: Unloading after } P \text{ was previously } \geq P_{GT} \text{ during the loading history and } \alpha < \alpha_{GT}) \]

A parametric study was carried out to understand how hardness and roughness influence the response at a single contact. All particle parameters, i.e. shear modulus, Poisson’s ratio, density, friction angle, size, are kept the same except for the hardness and roughness values and these parameters are outlined in Table 3.1. The data in Figure 3.6 show that when hardness is doubled, \( \alpha_p \) is increased by a factor of 4 (see Equation 3.9). In Figure 3.7 the value of RMS\( \gamma \) was multiplied by a factor of ten to be 1.0\( \mu m \). A sphere with roughness of 1.0\( \mu m \) can be considered “rough” while the sphere with a value of 0.1\( \mu m \) is taken to be a smooth sphere. Altuhafi & Coop (2011) measured roughness values between 0 and 0.05\( \mu m \) for smooth sand particles and rough sand particles had values greater than that range. The rough spheres have a much higher value of \( P_{GT} \) and in Figure 3.7 it is observed that the rough spheres do not reach Hertzian behaviour. The plastic model never reaches the threshold contact force and therefore can be seen to behave similarly to the elastic model. The value of \( P_{GT} \) is much higher, however, and although the particle contacts don’t reach Hertzian behaviour they reach much higher contact forces for lower overlaps than the “base case” as the initial stiffness is higher.

### 3.4 Hertz-Mindlin-Deresiewicz contact model

As noted above, typically DEM codes use a simplified version of this theory that can be called a Mindlin no-slip tangential contact model. Mindlin & Deresiewicz (1953) proposed a contact model that includes micro-slip at the edges of the contact and takes account of the entire loading history of the contact. This model avoids the infinite tangential traction that is found at the edge of the contact area when no-slip is assumed prior to full sliding. The traction distributions acting on the contact area due to Hertz, Mindlin (no-slip) and Mindlin-Deresiewicz (partial-slip) are illustrated in Figure 3.8. The PFC software comes with the Hertz and Mindlin (no-slip) and Mindlin-Deresiewicz (partial-slip) model already implemented. Thornton & Randall (1988), and later Thornton & Yin (1991), outline a DEM contact model algorithm that incorporates the
work of Mindlin & Deresiewicz (1953). As is required for DEM implementation, the algorithm is displacement driven. This model dissipates energy due to frictional energy loss using the theory of micro-slip at the contact surface, as outlined in Johnson (1985) and Thornton & Randall (1988). The model requires the same input parameters as are used in the Hertz normal force-displacement model as well as a coefficient of friction, $\mu$. The equations presented in Thornton & Yin (1991) are given here and further explanation of the model is outlined below. This model differentiates between slipping and sliding in a way that other tangential models do not. Slip is the “micro-slip” that occurs before full sliding when Amontons’ law is invoked ($T = \mu P$). The model centres on calculation of a tangent stiffness at the contact point ($k'$), given by

$$k' = 8G^* \theta \pm \mu (1 - \theta) \frac{\Delta P}{\Delta \delta}$$

where $G^*$ is given by Equation 3.7 and

$$\theta^3 = 1 - \frac{T + \mu \Delta P}{\mu P} \quad \text{(loading)}$$

$$\theta^3 = 1 - \frac{T^* - T + 2 \mu \Delta P}{2 \mu P} \quad \text{(unloading)}$$

$$\theta^3 = 1 - \frac{T - T^{**} + 2 \mu \Delta P}{2 \mu P} \quad \text{(reloading)}$$

$\Delta \delta$ = the change in tangential displacement, $T^*$ = load reversal point where the tangential displacement starts to unload, $T^{**}$ = load reversal point where the tangential displacement starts to reload and the negative sign in the first equation is only invoked during unloading.

Finally the tangential force is updated as follows:

$$\Delta T = k' \Delta \delta$$

These equations are represented in graphical form in Figure 3.9 considering load, unload and reload conditions in the tangential direction. Figure 3.9 also illustrates the response under a changing normal force. As illustrated in Figure 3.10, the model assumes that an annulus of slip develops on the outside of the circular contact area. Inside this annulus there is a central circular sticking region that does not slip. Initially consider the case where the normal force
does not change as the tangential displacement in a particular direction increases the slip annulus grows while the stuck region shrinks. If the “stuck” region shrinks to zero so that the entire contact is sliding, the tangential force is set equal to the coefficient of friction multiplied by the normal force (Amontons’ law). If the tangential displacement changes direction and starts to unload the tangential traction required to initiate unload is twice that which is causing the loading (Figure 3.11). This means that the unloading curve is twice as stiff as the loading curve. The previous maximum traction under loading is indicated as $T^*$ on the force-displacement curves in Figure 3.9 is stored as a variable. A similar situation exists when reloading occurs and then both the maximum loading and minimum unloading forces indicated as $T^*$ and $T^{**}$, respectively, on Figure 3.9 are stored. Whether the tangential displacement is loading or unloading depends on the dot product of the new and old tangential displacement vectors. If the dot product is negative the tangential displacement is unloading relative to the old displacement vector. To test whether loading or reloading is occurring the value of the tangential force at the load reversal points is examined. If $T^*$ is not equal to zero then the initial loading has already happened and any subsequent loading is a reloading.

If the normal force value increases or decreases the contact area between the two particles also changes and thus the slip annulus and stick region change in size. The change in tangential force is given by $\mu \Delta P$. An increase in normal force will lead to a larger contact area which must be mobilised to cause slip and this leads to higher tangential forces for similar tangential displacements. The inverse is true for the case where the normal force decreases. When the normal force changes the tangential force-displacement curve moves onto a new curve which means that the load and unload reversal points $T^*$ and $T^{**}$ have to be updated to take the values on the new curve (Figure 3.9). If $\Delta P$ is increasing and $\Delta \delta$ is increasing,

$$\Delta \delta \geq \frac{\mu \Delta P}{8G^* a}$$

3.18

to ensure that a new loading curve is reached. Otherwise, $\theta = 1$ until Equation 3.19 is satisfied

$$8G^* a \sum |\Delta \delta| > \mu \sum \Delta P$$

3.19
The development of this tangential force-displacement model is non-trivial due to the large number of hysteretic parameters that must be stored for the complete duration. There is also the need to ascertain whether the direction of the tangential displacement is loading, unloading or reloading increasing the computational cost of the simulations.

To determine the difference in the time taken to run a simulation with different contact models a small scale test was carried out. A single particle impacted a second particle and the time taken for the simulation to run was measured. This simulation is identical to the simulations that will be outlined in Section 3.5.2 where a 15° impact angle was used. When the Hertz-Mindlin model was implemented the simulation took $97.0 \times 10^{-8}$ s and when the Hertz-Mindlin-Deresiewicz model was implemented the simulation took $97.013 \times 10^{-8}$ s.

The dissipation of energy due to micro-slip was explored by Mindlin (1951) in an experimental setting. They found that the HMD model correctly predicted the energy dissipation for magnitudes of $T^* / \mu P$ close to unity with $T^*$ being the maximum tangential force reached during the test and $P$ being a constant nominal force. For values of $T^* / \mu P$ close to zero it appeared that the HMD model over predicts the energy loss due to micro slip. This was recognised in Mindlin & Deresiewicz (1953) where the theory behind the HMD contact model is explained.

Previous studies have shown that the Hertz-Mindlin-Deresiewicz model can describe the tangential interaction of entities more accurately than the simplified Hertz-Mindlin no-slip solution. In Chung & Ooi (2011) “Test 5” simulates the impact of an elastic particle on an elastic wall of identical material properties. The results obtained from a DEM simulation using the Hertz-Mindlin simplified model did not accurately capture the normalised tangential surface velocity at low impact angles when compared with experimental observations and an analytical solution. The Hertz-Mindlin results tend to over-predict the tangential surface velocity and Chung & Ooi hypothesised that implementation of Hertz-Mindlin-Deresiewicz will produce more accurate results due to energy lost through micro-slip. Wu et al. (2003) had verified this hypothesis by showing that their finite-element simulations of an elastic particle impacting an elastic wall matched the output of a DEM simulation in which Hertz-Mindlin-Deresiewicz is implemented (Figure 3.12). They also match the analytical solutions of Maw et al. (1976) and the experimental observations by Kharaz et al. (2001). This short impact duration problem is common in process engineering applications but is much less common in geotechnical engineering applications. Therefore
the effect of using the Hertz-Mindlin-Deresiewicz model should be explored for geotechnical engineering applications.

### 3.5 Implementation of new contact models in PFC

PFC allows the implementation of a user-defined contact model (UDM) to replace the intrinsic linear elastic and Hertz-Mindlin contact models. The UDM for the CM and HMD model were developed in a step-wise fashion. Firstly the Hertzian normal force-displacement model was programmed. This was verified in two simple simulations involving ball-ball and ball-wall contacts in the normal direction. Next the simplified Mindlin no-slip tangential force-displacement model was programmed. This was tested using simple contact problems and comparing the results with PFC3D’s intrinsic Hertz-Mindlin model. Implementation of these pre-existing models enabled verification that the UDM interface was being used correctly, following from this the CM contact model was implemented and then the HMD contact model was implemented.

All of these UDM’s were programmed in C++ which is an object oriented programming language and each contact is treated as a different object from the same class. Each object is stored as long as the contact is active and when a contact becomes inactive the corresponding object is deleted. The UDM takes a number of inputs from the main DEM code. These include the contact overlap, the relative tangential displacement vector, the timestep, the contacting entities’ radii, etc. The UDM outputs the normal force magnitude and the tangential force vector to the main PFC program and these values are added to the resultant forces and moments acting on the two contacting particles. The stiffness calculated in the normal and tangential direction are stored for the next calculation cycle and are also used to calculate the critical timestep in the DEM simulation. The particle properties such as shear modulus, Poisson’s ratio and friction are set in the PFC program and these values are sent to the UDM during the PFC program.

#### 3.5.1 Cavarretta-Mindlin model – Implementation and verification

The Cavarretta model in the normal direction was programmed with a Mindlin no-slip tangential force-displacement model. This model was tested as outlined in the verification exercises below. The Cavarretta normal force-displacement model was implemented by modifying the Hertz normal force-displacement model to account for the lower stiffness
when the two entities first come into contact. In the plastic implementation a history parameter was used to record if the contact force rises above the threshold normal force to cause plastic deformation of the asperities.

To verify the elastic and plastic implementations of the Cavarretta model in the normal direction a series of tests were performed using two spheres. One was fixed in space while the other was set to overlap and separate from the fixed sphere a number of times to examine the load, unload and reload conditions. The curves in Figure 3.3 & Figure 3.4 were verified by considering the analytical solution to the contact between two particles using Equations 3.13 & 3.14 and comparing the output from PFC3D with the theoretical result obtained using MATLAB. This model was also validated against experimental data as can be seen in Figure 3.2.

### 3.5.2 Hertz-Mindlin-Deresiewicz model – Implementation and verification

The Mindlin-Deresiewicz tangential model was developed using the algorithms outlined in Thornton & Randall (1988) and Thornton & Yin (1991) as a guideline to development. In addition several discussions were held with Dr. Colin Thornton, and the correspondence with Dr. Thornton, including an examination of his GRANULE DEM code was instrumental in the development of this code.

**Test 1:**
Initially a ball was created and allowed to come to rest on a horizontal, elastic wall under gravity as shown in Figure 3.13. The parameters used in this simulation are outlined in Table 3.2. Once vibration in the normal direction had reduced to a negligible value the damping was set to 0.0 and the velocity in the horizontal x-direction was applied as shown in Figure 3.13. The resulting load-unload-reload responses are demonstrated in Figure 3.14 and are similar to results outlined in Thornton & Randall (1988) for an equivalent test shown on Figure 3.15. This simple test presents all the tangential loading conditions but did not involve any changes in normal force. If gravity is doubled in a new simulation the resulting load-unload-reload curves are seen to give higher tangential forces for the same displacements as is also observed in Figure 3.14. This is expected according to the theoretical curves outlined in Thornton & Randall (1988).
**Test 2:**
Thornton & Yin (1991) outlined a verification exercise involving an impact between two balls. Two balls impact at different angles of $\theta$ (Figure 3.16). The speeds of both particles were set at 0.05m/s in the $\pm z$-direction. The balls have identical properties as outlined in Table 3.3. The value of $\theta$ was varied from 15° to 75° in steps of 15°. The results are given in Figure 3.17 and Figure 3.18 and are compared with digitised data from the plots presented in the Thornton & Yin (1991) paper. There is good agreement between the two simulations with the exception of Figure 3.18 (a). This may be due to the fact that this particular plot is rather hard to isolate on the paper and the digitised data may be incorrect.

In carrying out this test the critical angle of impact was calculated at 63.72° and a simulation was run at $\theta = 63°$ and $\theta = 64°$ to test the robustness of our implementation. The critical angle is the angle of impact above which pure sliding occurs. The result can be seen in Figure 3.19 and it is clear that pure sliding occurs once the impact angle is greater than the critical angle of impact.

**Test 3:**
The third verification problem that was carried out was outlined in Thornton et al. (2011). This is a single ball impacting a flexible, horizontal wall at different angles of $\theta$. The ball is assigned different starting velocities depending on the angle $\theta$ (Figure 3.20). The velocity magnitude is always 5m/s and the ball is of diameter 50mm. The ball and wall have equal elastic properties (Table 3.4). The angle $\theta$ is set to 5°, 20° and 40° to give three sets of results. These results were compared to datasets provided by Dr. Thornton from Thornton et al. (2011) and the comparisons can be observed in Figure 3.21 and Figure 3.22. Figure 3.23 is a plot comparing the kinetic energy of the sphere against time. There was a good match between the datasets and the simulation data. The angular velocity about the y-axis is plotted in Figure 3.24 against time and there is, again, good agreement between the datasets and the simulation data.

### 3.6 Multi-particle comparisons
As stated in Section 3.1 it is unknown to what extent contact models will govern simulation results at the macro scale. To compare the effects of different force-displacement contact models at this scale an identical sample was tested with different contact models. The test represented an idealised version of the triaxial test experiment, and was performed by Rowe
(1962) and used in the validation of Trubal as outlined in Cundall & Strack (1979a). The goal was to ascertain whether different contact models affect the results of a particle simulation on a geotechnical scale. The particle properties, outlined in Table 3.1, were chosen to represent steel spheres to simulate previous experimental work carried out by Rowe (1962). The particle shear modulus, \( G_{\text{particles}} \), for all tests was 77.82GPa and the particle Poisson’s ratio, \( \nu_{\text{particles}} \), was 0.285 giving a particle Young’s modulus of 200GPa which is a realistic value for steel. The coefficient of friction was taken to be 0.123 which is friction angle of \( \gamma^o \). As illustrated in Figure 3.25 the particles were packed in a face-centred cubic lattice which is the densest possible packing of spheres and results in an average coordination number of approximately 12 (particles at the boundaries will have fewer contacts). The stability of the packing means the contacts have a long duration, as is likely to occur in geotechnical simulations in contrast to the short duration impact problems examined in chemical engineering, and used in prior validation studies. A constant stress is applied to the lateral boundary particles of the sample and the bottom layer of particles are fixed in space. Stress cannot be directly applied in a DEM simulation so the “exposure area” of a particle to the stress field is found by considering the particle’s position in the lattice. This area is multiplied by the desired stress to give a force which can then be applied to the particle’s centroid and directed towards the centre of the sample. (Further details of this test as well as sample PFC3D code can be found in the PFC3D manual, Itasca Consulting Group (2007) and in Cundall & Strack (1979b).) The top (at maximum z elevation) layer of particles in the lattice is moved down at a constant velocity (strain rate). The bottom layer of particles in the lattice are fixed (i.e. displacement is prevented). The effect of the contact models on the mechanics of the sample at the macro scale can be measured by examining the response by plotting the stress ratio against the axial strain. The effect of different contact models on the stress-strain behaviour is clear in Figure 3.26 where stress ratio, \( \sigma_1/\sigma_3 \), is plotted against strain in the principal direction, \( \varepsilon_1 \). The stress ratio is defined as the stress acting on the top, moving boundary divided by the applied stress to the lateral sides of the sample. In this example the intermediate stress, \( \sigma_2 \), is equal to the minor stress \( \sigma_3 \). The principal strain is defined as the change in position of the top layer relative to the initial position of this layer. The strain is defined by the velocity which is applied to these top particles.

The CM model appears to reach the same peak stress as the HM model; however the CM model reaches its peak stress at a strain of \( 7.23 \times 10^{-4} \) whereas the HM model reaches its peak stress at a strain of \( 3.50 \times 10^{-4} \). The CM model appears to maintain peak stress in line with the
HM model until a strain of $9.42 \times 10^{-3}$ is reached. At this point the stress ratio in the CM model gradually reduces until a strain of $17.83 \times 10^{-3}$ where it rapidly reduces. The HM model also reduces rapidly at this strain, although the stress ratio in the HM model drops to zero at a strain of 0.019, whereas the stress ratio in the CM model never drops to zero over the course of this test. The effect of a partial change in the normal force-displacement law is clear in this idealised triaxial test.

The behaviour of the HMD model in Figure 3.26 is seen to be very similar to the HM model at low strains as expected. The macro scale behaviour is assumed to be governed by the normal contact force behaviour and both models have identical normal force-displacement laws, i.e. Hertz. At a strain of 0.010 the stress ratio of the HMD model starts to drop below that of the HM model for the same strains. This is due to slip accumulating at the contacts. At a strain of 0.019 the stress ratio is seen to drop sharply and this behaviour is seen in the other two models.

This result shows that at low strain levels, while the packing remains relatively ordered, the results can be affected significantly by the normal force-displacement contact model. This is proven by the difference in results for the HM model and the CM model at these low strains. This is because the stiffness of the CM contact model is different from HM at low strains when the asperities are not crushed. As the strains increase the packing starts to become disordered as one layer tries to push into another. The tangential force-displacement contact model is seen to affect the results at these larger strains and this is proven by differences in the HM model and HMD model results. This is because the stiffness of the HMD tangential contact model will decrease with increasing tangential displacement while the HM tangential contact model will stay constant. The contact model chosen at the inter-particle level is seen to affect the results of a geotechnical test.

The effect of varying the CM model input parameters on the stress ratio vs. strain results is examined. The hardness and roughness values used are the same as the ones used earlier in the parametric study of the contact behaviour and are outlined in Table 3.1. Although results are only presented up to a strain of $1.5 \times 10^{-3}$ the effects of the contact model inputs at the geotechnical scale are clear in Figure 3.27. The spheres that have a H value of 3.0GPa do not reach peak stress until much later than the spheres with a H value of 1.5GPa as it takes more displacement to crush the asperities and reach Hertzian contact behaviour.
Different roughness values were also examined with smooth and rough spheres being implemented as seen in Figure 3.28 up to a strain of $1.5 \times 10^{-3}$. The rough spheres exhibit higher stress ratio for the same initial strain values compared to the smooth spheres. However, the rate of stress ratio increase is lower and the stress ratio for the smooth spheres increases at a much faster rate. Both spheres reach the same peak stress at similar strains.

**3.7 Conclusions**

Two interparticle contact models have been successfully implemented in the PFC3D software. The Cavarretta-Mindlin model accounts for the experimentally observed cracks and asperities on the particle surface. This model is closer to the observed response in experiments and produces a less stiff response under normal loading conditions than the Hertz-Mindlin contact model. The Hertz-Mindlin-Deresiewicz model considers the work of Mindlin & Deresiewicz (1953) and is a more theoretically correct implementation of the tangential contact model between two spheres in contact. This model accounts for micro-slip occurring at the edges of the contact and this micro-slip increases as the tangential displacement increases until full sliding occurs. The Hertz-Mindlin-Deresiewicz model produces a less stiff response under tangential loading conditions and is a more theoretically correct model for two ideal spheres in contact.

The contact models that were implemented are checked using numerous verification exercises available in the literature. The Cavarretta-Mindlin model was verified against the analytical equations in Cavarretta et al. (2010) and validated against the experimental data available in Cavarretta et al. (2012). The Hertz-Mindlin-Deresiewicz model was verified against theory and previous simulations carried out in Thornton & Randall (1988), Thornton & Yin (1991) and Thornton et al. (2011). For simplicity these verification exercises were carried out on single contact systems which are easier to understand.

The influence of the contact models on a multi-particle simulation of a triaxial test on a face-centred cubic packing was examined. The CM model affected the observed response on a deviatoric stress versus axial strain curve at low strains and the HMD model affected the observed response at higher strain levels. The inputs to the CM model, particle hardness and particle roughness, were found to influence the observed response, however, whether the elastic or plastic version of the model was implemented was found to have negligible influence. These findings have encouraged an examination of the effect of these contact models on a wave propagation simulation that will be discussed in Chapter 5.
3.8 Figures

Figure 3.1: General behaviour of two entities in contact in a typical DEM simulation from O’Sullivan (2011).

Figure 3.2: Hertzian normal force-displacement model for two particles in contact.
Figure 3.3: Comparison between Cavarretta model, Hertz model and experimental data for single contact loading of a borosilicate glass ballotini particle.

Figure 3.4: The Cavarretta normal force-displacement model, elastic implementation, over a single load and unload.
Figure 3.5: The Cavarretta normal force-displacement model, plastic implementation, over a single load and unload.

Figure 3.6: Effect of varying hardness, $H$, on the Cavarretta normal force-displacement model.
Figure 3.7: Effect of varying roughness, $RMS_f$, on the Cavarretta normal force-displacement model.

Figure 3.8: The traction distributions acting on the contact area due to (a) Hertz, (b) Mindlin (no-slip) and (c) Mindlin-Deresiewicz (partial-slip).
Figure 3.9: Plot of tangential force, $F_t$, versus tangential displacement, $\delta_t$, for varying tangential loading conditions and under varying normal forces from O’Sullivan (2011).

Figure 3.10: Contact area behaviour: slip/stick regions and tangential traction distributions for tangential loading from O’Sullivan (2011).
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Figure 3.12: Normalised angular velocity after impact versus normalised impact velocity before impact for elastic ball impacting a flat, horizontal elastic wall from Wu et al. (2003).
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Figure 3.14: Results for Test 1 for gravity set to g and 2g, where $g = 9.81 \text{m/s}^2$. 
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Figure 3.16: Simulation overview for Test 2.
Figure 3.17: Results for Test 2 (solid line) compared with digitised data from Thornton & Yin (1991) (points) for tangential force vs. normal force. (a) = 15°, (b) = 30°, (c) = 45°, (d) = 60° and (e) = 75°.

Figure 3.18: Results for Test 2 (solid line) compared with digitised data from Thornton & Yin (1991) (points) for tangential force vs. tangential displacement. (a) = 15°, (b) = 30°, (c) = 45°, (d) = 60° and (e) = 75°.
Figure 3.19: Examining the critical angle of impact (63.7186°) with (a) = 63° and (b) = 64°.

Figure 3.20: Simulation overview for Test 3.

Figure 3.21: Results for Test 3 (dashed line) compared with datasets from Dr. Colin Thornton (solid line) for tangential force vs. normal force. (a) = 5°, (b) = 20°, (c) = 40°.
Figure 3.22: Results for Test 3 (dashed line) compared with datasets from Dr. Colin Thornton (solid line) for tangential force vs. tangential displacement. (a) = 5°, (b) = 20°, (c) = 40°.

Figure 3.23: Results for Test 3 (dashed line) compared with datasets from Dr. Colin Thornton (solid line) for kinetic energy vs. time. (a) = 5°, (b) = 20°, (c) = 40°.
Figure 3.24: Results for Test 3 (dashed line) compared with datasets from Dr. Colin Thornton (solid line) for angular velocity about the y-axis vs. time. (a) = 5°, (b) = 20°, (c) = 40°.

Figure 3.25: Simulation approach to idealised triaxial test from Itasca Consulting Group (2007).
Figure 3.26: Stress ratio, $\sigma_1/\sigma_3$, versus strain, $\varepsilon_1$, illustrating the influence of different contact models on the behaviour of a simulation of an idealised triaxial test, HM – Hertz-Mindlin, HMD – Hertz-Mindlin-Deresiewicz, CM – Cavarretta-Mindlin (elastic).

Figure 3.27: Effect of different hardness, $H$, values on the behaviour of a simulation of an idealised triaxial test using both CM (elastic) and CM (plastic).
Figure 3.28: Effect of different roughness, $RMS_f$, values on the behaviour of a simulation of an idealised triaxial test using both CM (elastic) and CM (plastic).
### 3.9 Tables

Table 3.1: Simulation parameters to an idealised triaxial test simulation and the parameters used for a parametric study on the effects of hardness, \( H \), and roughness, \( \text{RMS}_f \), on the Cavarretta model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ball radius, ( R )</td>
<td>20 mm</td>
</tr>
<tr>
<td>Ball density, ( \rho )</td>
<td>2000 g/mm(^3)</td>
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<tr>
<td>Ball shear modulus, ( G )</td>
<td>77.82 GPa</td>
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<tr>
<td>Ball Poisson’s ratio, ( \nu )</td>
<td>0.285</td>
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<tr>
<td>Ball friction coefficient, ( \mu )</td>
<td>0.1228</td>
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<tr>
<td>Ball hardness, ( H ) (also used)</td>
<td>1.5 GPa (3.0 GPa)</td>
</tr>
<tr>
<td>Ball roughness, ( \text{RMS}_f ) (also used)</td>
<td>0.1(\mu)m (1.0(\mu)m)</td>
</tr>
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</table>

Table 3.2: Simulation Parameters used for Test 1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( g )</td>
<td>-9.81x10(^{-3}) mm/s</td>
</tr>
<tr>
<td>Ball radius, ( R )</td>
<td>0.50 mm</td>
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<tr>
<td>Ball density, ( \rho )</td>
<td>2.57x10(^{-3}) g/mm(^3)</td>
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<tr>
<td>Ball &amp; wall shear modulus, ( G )</td>
<td>28.68 GPa</td>
</tr>
<tr>
<td>Ball &amp; wall Poisson’s ratio, ( \nu )</td>
<td>0.20</td>
</tr>
<tr>
<td>Ball &amp; wall friction coefficient, ( \mu )</td>
<td>0.20</td>
</tr>
<tr>
<td>X-velocity applied to ball</td>
<td>10.0x10(^{-3}) mm/s</td>
</tr>
<tr>
<td>Local damping</td>
<td>0.7 until normal force stops vibrating and then set to 0.0</td>
</tr>
</tbody>
</table>

Table 3.3: Simulation Parameters used for Test 2.

<table>
<thead>
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<th>Parameter</th>
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<tr>
<td>Ball radius, ( R )</td>
<td>0.10 mm</td>
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<tr>
<td>Ball density, ( \rho )</td>
<td>2.65x10(^{-3}) g/mm(^3)</td>
</tr>
<tr>
<td>Ball shear modulus, ( G )</td>
<td>26.92 GPa</td>
</tr>
<tr>
<td>Ball Poisson’s ratio, ( \nu )</td>
<td>0.30</td>
</tr>
<tr>
<td>Ball friction coefficient, ( \mu )</td>
<td>0.35</td>
</tr>
<tr>
<td>(</td>
<td>v</td>
</tr>
</tbody>
</table>

Table 3.4: Simulation Parameters used for Test 3.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ball radius, ( R )</td>
<td>25.0x10(^{-3}) m</td>
</tr>
<tr>
<td>Ball density, ( \rho )</td>
<td>2.65x10(^{-4}) kg/m(^3)</td>
</tr>
<tr>
<td>Ball &amp; wall shear modulus, ( G )</td>
<td>26.923 GPa</td>
</tr>
<tr>
<td>Ball &amp; wall Poisson’s ratio, ( \nu )</td>
<td>0.30</td>
</tr>
<tr>
<td>Ball &amp; wall friction coefficient, ( \mu )</td>
<td>0.10</td>
</tr>
<tr>
<td>(</td>
<td>v</td>
</tr>
</tbody>
</table>
4 Two-dimensional discrete element modelling of bender element tests on an idealised granular material

4.1 Introduction

This Chapter presents the results of a series of discrete element method (DEM) simulations of bender element tests on a simple, idealised granular material. This was a preliminary study whose objective was to develop understanding of the problem prior to considering the more complex systems in Chapter 5 and Chapter 6. The material presented in this Chapter has already been accepted for publication in Granular Matter (O’Donovan et al., 2012) and so the Chapter follows closely the text of that paper. DEM simulations provide the opportunity to study the mechanics of the bender element testing approach in detail. In this Chapter the DEM model is shown to be capable of capturing features of the system response that had previously been identified in continuum-type analyses.

The work presented here is a development of the earlier preliminary simulations by Carter (2010) and Clement (2006). An ideal, relatively simple, system of hexagonally packed uniform disks was selected. Despite the ideal nature of the model used here the system response is complex, highlighting the pedagogical benefit of developing a fundamental understanding starting from consideration of a relatively simple system.

The particle velocity data indicate the migration of central S-motion accompanied by P-motion moving along the sides of the sample. Section 4.2 outlines the simulation approach and Section 4.3 describes the observed received signal response. As described in Section 4.4, the propagation of the wave was tracked by considering both the particle velocities and the representative particle stresses. Four alternative methods to determine the wave travel time are compared in Section 4.5. An approach based upon direct decomposition of the signal using a Fourier transform is shown to yield the most accurate results. The relationship between the particle-scale DEM model parameters and the shear wave speed recorded is explored in Section 4.6.
4.2 Simulation approach

The numerical code used in this project was the commercial DEM code PFC2D Version 3.1 (Itasca Consulting Group (2007)). The sample consisted of 759 hexagonally packed uniformly-sized disks of radius 2.9mm (Figure 4.1). A hexagonal packing is the densest packing that can be achieved for two-dimensional uniform circular disks and each disk had 6 contacts. The two-dimensional photoelastic disk packing used by Zhu et al. (1996) is comparable to this simulation. This type of grain packing was previously considered, from a soil mechanics perspective, by Rowe (1962), O’Sullivan et al. (2002) and Velický & Caroli (2002). The system is highly ideal, comprising uniform disks on a lattice packing and exhibits a mechanical response that differs from soil. Nevertheless, in an early three-dimensional study Thornton (1979) showed convincingly that insight into the mechanical response of granular materials can be obtained by considering uniform spheres on lattice packings. The effect of small geometrical perturbations of the lattice was considered by O’Sullivan et al. (2002) and Velický & Caroli (2002).

As was previously mentioned in Chapter 2 Santamarina & Cascante (1996) considered the stiffness of regular and irregular packings of monodisperse and polydisperse spheres. Their work included a review of the analytical relations between fabric, grain properties and the effective overall stiffness of three-dimensional regular assemblies of uniform spheres. The findings in Santamarina & Cascante can be directly compared with the three-dimensional work of Chapter 5 but there are some implications for the current two-dimensional work. Santamarina and Cascante observed similarities between the response trends predicted analytically for ideal systems and empirical relationships derived for real physical soils. Just as in the case of the work by Santamarina & Cascante (1996), the system chosen for consideration here is very stable and, under small perturbations, there is no change in contact configuration, i.e. the material can be considered elastic as plasticity is associated with contact breakage and sliding. Real granular materials are three-dimensional, however as argued by O’Sullivan (2011), in fundamental research studies there is merit in restricting consideration to a two-dimensional system. The two-dimensional analogue is particularly useful here as particle motion is restricted to one plane, enabling clear visualisation and understanding of the wave propagation through the sample. As outlined in Chapter 2 many researchers have demonstrated that invaluable insight can be gained from considering two-
dimensional analogue models of real soil; the most notable contributions include Oda et al. (1985), Kuhn (1999), Rothenburg & Bathurst (1989) and Zhu et al. (1996).

In Chapter 3 and Chapter 5 the interparticle contact models that are considered are non-linear. In this Chapter the contact force model is described by linear springs acting in parallel with viscous dashpots, both in the normal and shear directions, see Itasca Consulting Group (2007). A linear contact model was chosen to simplify this initial study on wave propagation. The normal force due to the spring \( F_{n,sp} \) is given by \( F_{n,sp} = k_n \alpha \), and the increment in the shear spring force \( \delta F_{s,sp} \) is given by \( \delta F_{s,sp} = k_s \delta \alpha \), where \( k_n, k_s \) are the normal and shear spring stiffness, \( \alpha \) is the grain overlap, and \( \delta \alpha \) is the increment in contact shear displacement. The force due to the dashpot \( D \) is added to the spring force. The magnitude of this force, whose direction is always opposite to the velocity vector, can be calculated through \( D = 2\beta \sqrt{mk|V|} \), where \( \beta \) is the critical damping ratio, \( m \) is the effective mass of the 2 grains in contact, and \( k \) is the contact spring stiffness and \( V \) is the (normal or shear) contact velocity. Table 4.1 lists the parameters used in the simulations. As noted elsewhere (Chapters 2 & 5), Hertzian contact mechanics shows that there is a non-linear relationship between force and displacement at elastic particle contacts, for small perturbations around the equilibrium position a Hertzian spring can be approximated by a spring with a stiffness equal to the tangent of the Hertzian curve at that point justifying the use of linear contact springs. The two-dimensional disks are assumed to have a unit thickness for the purpose of relating our two-dimensional system to three-dimensional elasticity equations. The sample was initially isotropically compressed to a stress of 1MPa using rigid wall boundaries on all four sides. Once this stress state had been achieved the side walls were removed and a numerical membrane was applied to simulate triaxial cell boundary conditions, as bender elements are most frequently deployed in triaxial test samples. The membrane algorithm used was detailed by Cheung & O’Sullivan (2008). Referring to Figure 4.1 forces are applied to the particles located along the lateral sides of the sample to achieve the specified confining pressure, while allowing free deformation as in a physical triaxial test sample. These applied forces were maintained constant during the wave propagation simulation.

Impedance mismatch is a measure of the ability of the sample boundaries to reflect the wave when it interacts with the boundary surface. The issue of impedance mismatch between the boundaries and the sample has been previously examined by Lee & Santamarina (2005) in an
experimental setting. In their work the large impedance mismatch between the rigid top and bottom boundaries and the sample was used to reflect the waves several times inside the sample. In the work presented here there is large impedance mismatch at the top and bottom boundaries as the elastic spheres are encountering rigid walls. This results in almost full reflection of the wave from the walls. The impedance mismatch between the balls and the simulated flexible boundaries is much lower as the boundary is simply applied forces to the boundary particles. This leads to lower reflection from the lateral boundaries and more absorption of the energy as work against the boundary forces.

As in the preliminary simulations of Carter (2010) and Clement (2006) the bender elements were modelled as single disks in the current study. A disk near the base of the sample was chosen to be the transmitting bender element and a disk near the top of the sample was chosen to be the receiving bender element (Figure 4.1).

The input wave was simulated by applying a single-period sine pulse displacement to the transmitter disk. The amplitude of the motion was 12.5\( \mu \)m, which is relatively small; the average overlap at the end of isotropic compression was of 6.65\( \mu \)m. While different types of pulses can be used, (e.g. Jovičić et al. (1996) used a square pulse); a single sine pulse is most commonly used and is recommended by Yamashita et al. (2009). Figure 4.2 illustrates the transmitted and received signals for a representative bender element test simulation. In principle a bender element test is applied to an elastic system. Here particle displacements large enough to cause (plastic) irreversible sliding were only experienced in the immediate vicinity of the bender element.

### 4.3 Analysis of received signal

As is the case in a laboratory bender element test, there are differences between the transmitted and received signals. The received signal has significantly lower amplitude and is of longer duration than the transmitted signal. As in laboratory testing the differences in shape between the received and transmitted signals mean that identifying accurately the travel time for the signal is non-trivial. Figure 4.2 bears similar characteristics to acoustical signals in a DEM sample measured by García & Medina (2007) and to the signal received during experimental tests; data from a representative experimental bender element test carried out by Viggiani & Atkinson (1995) are shown in Figure 4.3. In both Figure 4.2 and Figure 4.3 it is clear that a more complex signal was received than was transmitted. The added complexity
arose because there were a number of different waves and wave reflections influencing the receiver disk’s motion as will be discussed below in relation to Figure 4.4 - Figure 4.10. The received signal that resulted from these different waveforms had a smaller amplitude when compared with the transmitted signal (Figure 4.2). This smaller amplitude was a consequence of energy dispersion or dissipation, both mechanical and geometrical as discussed below. When carrying out a physical bender element test a number of checks are recommended to ensure the quality of the test as outlined in Alvarado (2007) and Lee & Santamarina (2005). These checks should also be applied to the test simulated in DEM. For example, the number of full shear wavelengths that occur in the sample, $R_d$, should be above 4 and the $R_d$ value in this simulation was 4.11. The value of wavelength, $\lambda$, divided by $d_{50}$ should also be as high as possible. The value of $\lambda/d_{50}$ for this simulation was 8.44 which is reasonably high.

When the bender element test was simulated using DEM, the sample was explicitly modelled as a multi-degree of freedom system. Trying to clearly identify and understand the different wave-forms present in the signal represents a significant challenge for this work and for experimental work carried out using bender elements. Care was taken to ensure the system remained elastic and relatively low values of viscous damping were used. All the contacts in the system were continuously monitored to confirm that there was little or no slippage of particles in the system, except for the transmitter particle, and no change in coordination number (i.e. average number of contacts per particle). Sliding of particles can lead to a permanent change in the arrangement of particles in the system resulting in a plastic deformation that will not be recovered. However, the small amounts of sliding particles (around the transmitter) moved back to their original position due to the regular packing proving that any strain induced by the transmitter disk is reversible and that the system behaviour can be considered to be elastic.

4.4 Overview of system response

4.4.1 Particle-scale measures considered

To understand the mechanisms underlying the observed macro-scale response at the receiver the particle-scale behaviour during the simulation was measured. As discussed further in Chapter 5, the sine wave pulse is a complex signal that includes a broad range of frequencies.
Snapshots of the system response at selected points were created for the simulated bender element test shown in Figure 4.2 and these are illustrated in Figure 4.4 to Figure 4.10. In Figure 4.4 and Figure 4.5 the particle velocities at 24 selected time points, labelled (a) to (x) are plotted as arrows, whose length is proportional to the magnitude of the particle velocity. Similarly Figure 4.7 and Figure 4.8 illustrate the normalised representative mean stresses acting on the particles at the same time points and Figure 4.9 and Figure 4.10 illustrate the relative representative particle shear stresses. These terms are explained below. These measures were selected as being the most sensitive or effective at picking up the passage of the disturbance through the specimen.

The stress distribution within the particles is obviously heterogeneous but the representative particle stress tensors were \( \left( \bar{\sigma}_{ij}^p \right) \) calculated in PFC2D by considering the contact forces that act on each particle following Potyondy & Cundall (2004), as follows:

\[
\bar{\sigma}_{ij}^p = \frac{1}{V^p} \sum_{c=1}^{N_c^p} f_j^c x_i^c
\]

where, \( f^c \) represents the contact force at location \( x^c \), \( V^p \) is the volume of the particle and \( N_c^p \) is the number of inter-particle contacts that act on particle \( p \). The representative mean stress for each particle \((p^p)\) in a two-dimensional system is then given by \( p^p = \frac{\bar{\sigma}_{xx}^p + \bar{\sigma}_{yy}^p}{2} \). The individual representative particle mean stresses were normalised by the initial representative mean stresses for the same particle, \( p^p_0 \), just before the bender element test was carried out when the system was in equilibrium under the applied isotropic confining pressure (point (a) the point at the origin of the time axis in Figure 4.4 to Figure 4.10). These normalised stresses, \( \left\langle p^p \right\rangle = \frac{p^p}{p_0^p} \), were used to isolate the effect of the stress wave on the particle stresses from the stresses induced by the applied confining pressure, which was kept constant for the duration of the test.

The particles are no longer in static equilibrium, there will be a resultant moment causing a rotational acceleration. The representative particle shear stresses were calculated as \( s^p = \frac{\bar{\sigma}_{xy}^p + \bar{\sigma}_{yx}^p}{2} \). The average was used as the stress tensor was not symmetric due to the presence of boundary conditions. The data presented in Figure 4.9 and Figure 4.10 are
the relative representative particle shear stresses, \( \langle s^p \rangle \), i.e. \( \langle s^p \rangle = s^p - s^p_0 \), where \( s^p_0 \) is the representative particle shear stress before the bender element test is carried out. Using relative shear stress produced clearer images of the passage of the disturbance than the normalised shear stress. The simulation was effectively quasi-static at the isotropic stress stage before the bender element test is begun. Therefore any changes seen in the shear stresses on the plots are due to the wave propagation through the sample.

There had been little prior discussion of the nature of the wave motion through the sample. However, Lee & Santamarina (2005) proposed that the transmitter bender element motion results in the cogeneration of a shear (S-) motion in a central wave lobe and compressional (P-) motion in side wave lobes in the sample. Analysis of the particle velocities, the normalised representative particle mean stresses and the relative particle shear stresses allow exploration of this hypothesis.

**4.4.2 Particle velocities**

As noted above, the particle velocity snapshots are illustrated in Figure 4.4 and Figure 4.5. Over the duration captured in Figure 4.4 the displacement of the transmitted particle causes a small amplitude stress wave to develop in the sample. Figure 4.4 (b)-(d) illustrates S-motion forming a circular lobe around the transmitter disk. This is indicated by the dominant horizontal orientation of particle velocities, i.e. orthogonal to the direction of wave propagation. In Figure 4.4 (e)-(f) it is clear that as this shear wave moves up through the sample a corresponding P-motion is developing at the sides of the sample. This compressional wave is illustrated as particle velocities which have a direction parallel to the direction of wave propagation. The net result is a complex, vortex-like motion within the sample, with the central particles moving from left to right and the outer particles moving vertically; to the right of the bender particle they move upwards, to the left downwards. The particles close to the right boundary of the sample have a horizontal velocity component directed away from the sample centre and a vertical component that is directed upwards. In the prior DEM simulations described by Li & Holt (2002) a planar S-wave was input using a large body of particles as a transmitter. Particle velocity measurements also clearly showed a vortex-like pattern in the motion of the particles which were positioned further along the sample. This vortex-like pattern has been observed by Xu et al. (2012) in three-dimensional DEM simulations of shear wave propagation through a cylindrical sample.
In Figure 4.4 (g)-(l) the propagation of P-motion and S-motion through the sample is clearly illustrated as particles further up the sample start to move and multiple subsystems of interacting disks whose velocities form vortex-like patterns are observed. As the first shear wave moves further from the transmitter disk (Figure 4.4 (g)) a second shear wave is seen to develop behind it. As both the shear and compressional waves become more established it is observed that the compressional wave travels at a higher speed than the shear wave and leads the shear wave by Figure 4.4 (k). The smaller amplitude of the P-motion makes it harder to observe than the S-motion. In Figure 4.4 (j) in the top half of the sample the particles towards the right side move upwards, while the particles towards the left side move downwards indicating the P-motion has propagated through the sample.

Figure 4.5 shows the time period from the point at which the previous Figure 4.4 (l) was generated to the arrival of both P- and S-motion at the receiver disk. The striking difference between Figure 4.5 (m) and Figure 4.5 (x) is the reduction in magnitude of the particle velocity. This loss in magnitude is a result of a loss of energy from the system. Some of the energy loss is due to the viscous damping model (a dashpot) used at the contacts in the simulation. The flexible boundaries on the lateral sides of the sample absorb some energy too as body work done by the applied forces in opposition to the boundary particle motion. These sources of energy dissipation are coupled with the geometric effects of energy radiating from a point source. The ability to observe this attenuation of the seismic wave by consideration of particle velocities in the sample during propagation is a feature unique to DEM. Using particle scale data for a column of particles connecting the transmitter to the receiver the attenuation of the wave was found to be systematic. The velocity squared in the oscillating direction, which is equivalent to the kinetic energy, decreased in proportion to $1/r$ where $r$ is the distance from the transmitter. This decrease in kinetic energy is illustrated on Figure 4.6 and the dashed line is the line produced by decrease exactly proportional to $1/r$. The fluctuations in the numerical data near the maximum position is a result of reflections off the wall boundary of the sample. Throughout this latter stage of the simulation, the complexity of the response remains evident with multiple subsystems with vortex-like displacement patterns developing through the sample. The complexity of the response inhibits interpretation on the basis of affine and non-affine components of motion as was considered by Makse et al. (2004). Furthermore, when this sample is deformed the significance of the non-affine motion will be greatly influenced by the regular lattice packing used.
4.4.3 Normalised representative particle mean stresses

The plots of the normalised representative particle mean stresses $\langle p^p \rangle$ in Figure 4.7 and Figure 4.8 complement the observations of particle velocities. Referring to Figure 4.7 (b), the particles immediately to the right of the bender (moving to the right, with a positive x-displacement) experience an increased compressive stress as the bender moves to the right, while particles immediately to the left experience a decreased compressive stress. The anti-symmetrical nature of the response is more clearly visible than it was when considering the velocity vectors. When the motion of the bender particle reverses, Figure 4.7 (d), the distribution of stresses reversed. Thus, immediately to the right of the now left moving bender particle, there is a zone of reduced compressive stress. Further to the left there is a transition to a zone of increased compressive stress as a consequence of the earlier bender movement to the right. At point (f) there is once again a reversal of the stresses as the bender is moving to the right from a time of 0.09ms until the end of the period. From points (f) to (x) the stress response is more complex as the particle stresses respond to the particle motion.

The magnitude of the compressive stress is directly related to the strain energy and there is clearly an ongoing conversion of kinetic energy into strain energy and vice-versa as the wave propagates through the system. Energy loss can be observed in Figure 4.8 (m)-(x) as the light and dark patches become steadily less pronounced. Figure 4.8 (r) clearly shows quite a number of alternating light and dark patches in the sample indicating continuing propagation of the disturbance inside the sample. By comparing Figure 4.8 (r) to the directions of the arrows in Figure 4.5 (r) a clearer picture of the stress wave behaviour can be presented. The velocity data (Figure 4.5 (r)) indicate the presence of both S-motion and P-motion. P-motion is shown to be located primarily on the sides of the sample and S-motion is located in the centre of the sample. The velocities and stresses can be correlated to some extent; considering the counter-clockwise vortex just above the sample mid-height (Figure 4.5 (r)) the particles at the left of the sample move downwards and inwards, corresponding to an increase in mean stress (in comparison to the initial value), while the particles at the right move upwards and outwards, corresponding to a decrease in mean stress. A similar observation is made by comparing Figure 4.5 (v) and Figure 4.8 (v), i.e. where the particles are moving inwards towards the sample centre there is an increase in mean stress and vice-versa.
4.4.4 Relative representative particle shear stresses

Upon movement of the transmitter disk the magnitudes of the relative representative particle shear stresses $\left<s^p\right>$ are shown to change. Initially the observed magnitude of the shear stress increase spreads symmetrically from the transmitter disk (Figure 4.9 (a-b)). However, upon reversal of the disk motion direction (Figure 4.9 (c)-(d)) the response loses symmetry and becomes more complex. In response to the reversal of motion a second shear wave grows around the transmitter disk. By Figure 4.9 (f) a third shear wave is seen to develop and the transmitter disk now stops moving. Throughout the rest of Figure 4.9 up to point (l) the propagation of the wave through the sample is observed. There is a concentration of shear stress in the centre of the sample and this can be explained by the central motion of the shear wave travelling through the centre of the sample as already discussed.

Figure 4.10 offers interesting insight into the arrival of the shear stress disturbance at the receiver disk. Regions of increased relative shear stress magnitude propagate through the sample. An initial region of non-zero relative shear stress magnitude is seen to arrive at the receiver disk at Figure 4.10 somewhere between snapshots (p) and (n). This corresponds with the point at which a signal registers. However, a second zone of with larger relative shear stress magnitude is seen to arrive at appoint point (r). This corresponds to the first local minimum shown on the received signal which is taken as the arrival point when using the start-start method of travel time determination as outlined below. The stress wave is seen to be heavily attenuated in Figure 4.10 and the wave amplitude represented by the change in relative representative particle shear stresses is shown to decrease from Figure 4.10 (m) to Figure 4.10 (x). The reduction in energy in the system has been explained above and the shear stress plot in Figure 4.10 offers further proof of this loss of energy. Observation of Figure 4.10 (m) to (x) again highlights the complexity of the response, there now are a number of areas of increased shear stress propagating through the centre of the sample and along the sides.

4.5 Calculating sample stiffness

The data presented in Figure 4.2 to Figure 4.10 indicate that the model can capture key elements of bender element response as observed in the laboratory and predicted from continuum analyses. The idealised nature of the system considered here (i.e. an elastic
system with perfect contact between bender element and tested material) makes it well-suited to use in a fundamental study on how best to interpret bender element data. To calculate $G_{\text{max}}$ using Equation 2.3 it is necessary to know the overall sample density ($\rho$) and the S-wave velocity ($V_S$). The sample dimensions were used to calculate the sample area and using this area and the summation of the individual masses of the particles the overall sample density was calculated as:

$$\rho = \frac{A_{\text{solids}} \times \rho_{\text{solids}}}{A_{\text{total}}}$$

4.2

To calculate $V_S$ the travel distance and travel time must be measured. The travel distance was given by the distance between the receiver and transmitter disk centroids, which are marked on Figure 4.1. Determining the travel time was less straightforward, as has been discussed by Viggiani & Atkinson (1995) amongst others. Different methods can be used to identify the arrival of the shear wave and these include start-start (or point of inflection), peak-peak and cross-correlation. Researchers who have explored measuring seismic wave velocity and have demonstrated prior use of the methods considered here include Jovičić & Coop (1997); Arulnathan et al. (1998) and Alvarado (2007).

The travel time determination methods that were considered in the current study are:

1. Start-start,
2. Peak-peak,
3. Signal decomposition,

The $G_{\text{max}}$ obtained for each method was compared with the $G_{\text{max}}$ measured in a biaxial compression test on the same sample configuration.

4.5.1 Start-start

This method was used by Jovičić & Coop (1997) amongst others. The start of the S-motion at the receiver, and thus the arrival time, is taken to be the point of first local minimum. Figure 4.2 illustrates the point of first local minimum on the received signal. The travel time is then taken as the time difference between the start of the transmitter signal and this arrival.
time. On Figure 4.3 it is the time difference between points A to A’. The theory behind this method is that the initial deflection is the arrival of the faster P-motion and the change in direction of the received signal marks the arrival of the S-motion. However, as experimentalists have not been able to track the waves propagating through the sample this differentiation between P- and S-motion arrivals is hypothetical. To date, use of this method can only be justified by the fact that it has been used many times and on many different samples and has often given reasonably accurate results. As outlined above in the discussion related to Figure 4.10 there seems to be some correlation between the magnitude of the relative shear stresses and the received signal. This is preliminary evidence that there is a rationale for using this method, however further analyses considering more complex configurations (random assemblies of three-dimensional particles) is needed.

4.5.2 Peak-peak

This method involves analysis of both the transmitted and received signals. The peak-peak travel time is taken to be the time difference between a peak on the transmitted signal and its equivalent peak on the received signal. As illustrated in Figure 4.2 the location of the equivalent peak on the received signal is often not clear. For example, referring to Figure 4.3, there are two possible peak-peak measurements i.e. B to B’ and C to C’. In previous studies, such as Leong et al. (2005), the equivalent peak has been taken to be either the first peak on the received signal or the maximum peak on the received signal. Often these different peaks represent a large difference in the computed travel time. This method offers the advantage that identification of a peak is not affected by noise in the received signal but its use is difficult to justify due to this ambiguity.

4.5.3 Signal decomposition

A complete decomposition of the received signal is a simple method for determining the travel time of the shear wave in the sample that is not widely used. A fast Fourier transform (FFT) was performed on the signal in Figure 4.2 in Matlab. The FFT essentially calculates the amplitudes ($A$) and phase angles ($\phi$) of the constituents of the signal if this was to be expressed as a sum of a number of sinewaves of different frequencies ($\omega$).

When using this method care needs to be taken so that the sampling rate used for the output signal is not too low. The signal was sampled with a period $T_{sampling}$ which here is directly
related to the mechanical timestep of the DEM simulation (constant in this case). The mechanical timestep needed to be small enough to ensure that the received signal could be plotted as a relatively smooth waveform. If it was too large the waveform would appear too jagged and it would not be possible to accurately decompose it to its constituent parts, as the largest frequency that can be calculated with the FFT is equal to half the sampling frequency. The mechanical timestep chosen here was therefore significantly smaller than the critical time step required for stable DEM analysis.

The resultant waveforms were then plotted together on Figure 4.11 in order to compare the frequencies and amplitudes of each of the constituent cosine waves. The constituent parts can be summed together to inspect the validity of the decomposition. If the waves summed to a good approximation of the original signal then the signal decomposition was considered accurate enough. The decomposition was successfully validated by selecting the lowest 15 frequencies to represent the majority of the signal’s amplitude. Figure 4.11 includes the received signal, the 5 cosine waves with the lowest frequencies as well as summation of the 15 cosine waves with the lowest frequencies. The wave with the largest amplitude was taken to represent the waveform from the transmitted signal. In this case it was the waveform with the third lowest frequency, $\omega_3$. The point where this waveform first crosses the x-axis represents the arrival of this waveform at the receiver end of the sample.

In using the signal decomposition approach care must be taken to ensure an accurate result. Specifically an appropriate length of signal should be considered in the decomposition. Here the signal length selected was the maximum time period for which the first 15 components, when summed together accurately captured the signal upon inversion. The amplitudes and phases of the summation and of the original received signal were compared and the decomposition was considered valid as the percentage errors were smaller than 10% in either of these checks. This check ensured that the received signal was decomposed to a high degree of accuracy and gave confidence in the arrival time which was subsequently determined from this method. It should be noted that this technique seems to work well, but as it seems not fully justified theoretically more research is required on this topic.

### 4.5.4 Cross-correlation method

The cross-correlation method is a more conventional use of the fast Fourier transform in signal analysis and has been proposed in a number of papers. Implementation of the method
in the current study followed the procedure outlined in Viggiani & Atkinson (1995) and Arulnathan et al. (1998). As in method (c) the sampling rate, $T_{\text{sampling}}$, can affect the accuracy of the cross-correlation method. $T_{\text{sampling}}$ should be as low as possible so that all the relevant constituent waves are included in the decomposition. A discrete fast Fourier transform (FFT) of both transmitted and received signals was computed. These two FFT’s were divided and then an inverse FFT of the result was taken. This represents the cross-correlation function which was then plotted in Figure 4.12. The absolute maximum of this function was taken to represent the point of arrival of the predominant wave-form and that represents the travel time of the shear wave in the sample. The shear wave is generally considered by those using bender elements to be the predominant wave-form at the receiving end as this is the wave-form that is input to the sample by the transmitter element. The implementation of the cross-correlation function used here was validated against code developed and used by Alvarado (2007) on experimental bender element signals.

4.5.5 Calculating $G_{\text{max}}$ from biaxial compression test

A static biaxial compression test to find a reference $G_{\text{max}}$, and using Equation 4.3 a reference $V_S$, was performed on the sample of disks. The boundary conditions were identical to those used in the bender element test, and the transverse stress was kept at a constant value. The top rigid wall platen was moved vertically down at a constant velocity until a set axial strain value was reached. From a biaxial compression test it was possible to plot deviator stress, $q$, versus axial strain (Figure 4.13). It is a straight line as a linear elastic contact model is used and there was no slippage at the particle contacts. The slope of this graph gave a value for Young’s Modulus, $E$.

$$E = \frac{dq}{d\varepsilon_{\text{axial}}}$$  \hspace{1cm} 4.3

where $q$ is the deviatoric stress ($\sigma_y - \sigma_z$) and $\varepsilon_{\text{axial}}$ is the axial strain during the compression test. Comparison of this type of static probe with bender element data was also carried out by Sadek [3].

By monitoring the transverse strain during the simulation it was possible to plot transverse strain vs. axial strain on Figure 4.13. The Poisson’s Ratio, $\nu$, was calculated using Equation 4.4:
\[ \nu = -\frac{de_{\text{trans}}}{de_{\text{axial}}} \]

where \( e_{\text{trans}} \) is the transverse strain during the compression test. In order to calculate a Poisson ratio value the axial versus transverse strain curve was approximated by a straight line. The calculated Poisson ratio was very small (0.0035), but this is expected due to the regular packing of the sample, and the fact that the normal and shear spring stiffness are identical. The extremely low values of Poisson’s ratio mean that any changes in Poisson’s ratio due to non-linearity will lead to negligible differences in the calculation of \( G_{\text{max}} \). The values of Young’s modulus and Poisson’s ratio were used to calculate \( G_{\text{max}} \) for the sample using Equation 4.5:

\[ G_{\text{max}} = \frac{E}{2(1 + \nu)} \]

4.6 Sensitivity of system response to DEM model parameters

A parametric study in which the DEM model parameters (contact stiffness, particle density and viscous damping coefficient) were systematically varied was carried out to assess the influence of these parameters on the wave propagation velocity and to compare the various options available for travel time determination. The frequency of the input signal was also adjusted as different frequencies are often used in laboratory bender element tests.

The “base case” of simulation parameters is listed in Table 4.1. Then the chosen parameter was adjusted separately, maintaining the other parameters at the base value. Both the normal and tangential stiffness’s were kept equal to one another when varied from the “base case” value. Table 4.2 summarises the \( R_d \) and \( \lambda/d_{30} \) values for each of the configurations used in this parametric study.

The results for varying contact stiffness are shown in Table 4.3 and Figure 4.14 (a). Considering Table 4.3, there are some large percentage errors in the results obtained from the different methods. Such large errors have been previously observed in studies such as Yamashita et al. (2009), Hardy (2003) and Greening et al. (2003). In Yamashita et al. (2009) a large dataset of tests on one sand type was prepared, different travel time determination
approaches were used and for a given void ratio differences in the calculated $G$ value were as large as 50%. In Hardy (2003) a reference $G_{\text{max}}$ is calculated from the input parameters of the finite difference model, $E$ and $v$. When travel times for a parametric study on bender element input frequency were calculated errors exceeding 20% were noted when using the start-start method of travel time determination for a signal of a given frequency. When the frequency domain method was used, namely the phase sensitive detection method, these errors could rise to be as much as 140%. Greening et al. (2003) reported differences of as much as 30% between shear wave velocity measurements obtained using first arrival time and frequency domain methods. As $G_{\text{max}}$ is proportional to $V_S^2$ any difference in travel time determination provides a much larger difference in $G_{\text{max}}$ values. The variation in the measured shear wave velocity ($V_S$) as a function of the interpretation approach used show the values for the signal decomposition method to be the most consistent and are within 10% error of the value for $G_{\text{max}}$ measured using biaxial compression on identical samples.

The $V_S$ values were used as the metric to assess the sensitivity of the system response to the input parameters. The travel time values used were those obtained using the signal decomposition method which had been proven to be the most accurate method. As would be expected for this elastic system, referring to Figure 4.14 (a) and (b) $V_S$ was proportional to the stiffness, $\sqrt{K}$ (where $K = k_n = k_s$) and inversely proportional to $\sqrt{\rho}$. Considering the sample to be a system of particles connected by springs of stiffness $K$, it is reasonable to expect that the overall shear stiffness, $G$, would be linearly proportional to the root of the contact stiffness, $\sqrt{K}$. The linear relationship between $V_S$ and $1/\sqrt{\rho}$ was also expected as a consequence of Equation 2.3. For low values of viscous damping, $< 0.01$, the system response appeared relatively insensitive to damping and this can be seen in Figure 4.14 (c). However at larger damping values, the measured $V_S$ values were sensitive to viscous damping. Finally the effect of bender element frequency on shear wave speed was explored. The results for this study can be found in Figure 4.14 (d). The sensitivity to frequency might be due to the use of the viscous damping model at the contacts. Viscosity at the inter-particle contacts leads to dispersion of the signal as it travels through the sample as outlined in Sadd et al. (1993). This dispersion can be observed in Figure 4.2 as the received signal is “broader” than the transmitted signal.
4.6.1 Frequency domain analysis

The transmitted and received signals are compared in the frequency domain for samples with different values of interparticle contact stiffness \((K)\), Figure 4.15, and different values of particle density \((\rho)\), Figure 4.16. It appears that the frequency content of the received signals is reduced compared to the frequency content of the transmitted signals in all cases indicating that the sample is acting as a frequency filter as discussed in Chapter 2. There was a correlation between the value of interparticle contact stiffness and the “threshold” frequency at which frequency filtering occurs on Figure 4.15. There was also a correlation between the value of particle density and this “threshold” frequency on Figure 4.16. The relationship was observed by picking a characteristic point on the frequency signals on the plots on Figure 4.15 and Figure 4.16. The characteristic point was the last local maximum peak on the plots. The frequency values with increasing stiffness were 5.05kHz, 7.15kHz and 10.00kHz and the frequency values with increasing density were 10.15kHz, 7.20kHz and 5.85kHz. The frequencies were increasing or decreasing in line with the expected \(f \propto \sqrt{K/M}\) trend. The effect of stiffness on frequency filtering will be further examined in Chapter 5 and Chapter 6 as the values of interparticle contact stiffness are dependent on the confining pressure when non-linear models are used.

The effect of varying one of the directions of the interparticle contact stiffness was investigated. In Figure 4.17 the effect of varying the contact stiffness in the normal direction \((k_n)\) was investigated in isolation while the contact stiffness in the shear direction \((k_s)\) was kept constant. The maximum “threshold” frequency was observed to be influenced by the value of \(k_n\). When the value of \(k_s\) is varied independently of \(k_n\) in Figure 4.18 there was little effect on the “threshold” frequency observed. This indicated that the value of \(k_n\) was controlling the changing frequency filtering that was observed on Figure 4.15.

A plot of frequency versus position is illustrated in Figure 4.19 shows that a small amount of frequency filtering was occurring as the wave propagated through the sample. The initial band of frequencies propagating in the sample reduces from a peak value of approximately 20.29kHz to 17.42kHz as the wave was tracked through the sample. This shows that the sample was behaving in a dispersive way. Figure 4.20 plots angular wavelength \((2\pi f)\) against wavenumber \((2\pi/\lambda)\) and is created by carrying out a two-dimensional fast Fourier transform of the wave propagating through time and space. There appears to be a linear relationship
between wavenumber and angular velocity illustrating a shear wave propagating with a speed equal to the slope of that linear relationship. There was also a maximum frequency above which no waves were propagating with higher frequency and there was a maximum wavenumber. These frequency domain plots will be explored in more detail in the three-dimensional simulations carried out in Chapter 5.

4.7 Conclusions

In this Chapter a simple, idealised, elastic system of disks was considered. The DEM simulation data captured the main features of response that are observed in laboratory bender element tests. A more simple interparticle contact model was considered here compared to those outlined in Chapter 3 so that initial simulations to develop the algorithm and wave interpretation techniques could be developed quickly. The algorithm used to input the wave using a single particle was adapted in later work for three-dimensional simulations outlined in Chapter 5.

A key advantage of the two-dimensional DEM simulation was the ability to visually examine particle scale response to the bender element input wave. Examining this micromechanical data illustrated the wave propagation motion in a way that was previously not possible. The assumptions of Lee & Santamarina (2005) were seen to hold true for this two-dimensional case, however the response is highly complex. The reversal of the direction of the transmitter disk particle added to the complexity of the response. Circular shear wave lobes were seen to travel through the centre of the sample and P-motion wave lobes were seen to travel along the sides of the sample. A relation was observed between the changes in shear stress and the received signal. Sub-systems of particles formed within the sample that interacted to generate vortex-like particle velocity patterns as has been observed in Li & Holt (2002). The particle velocities and representative particle mean stresses were linked; in general when the particle velocities were directed towards the centre of the sample the stress increased, and vice-versa. These visualisation techniques developed here were used on work considering three-dimensional packings of particles in Chapter 5.

Four different methods of travel time determination were critically assessed using DEM and many of the existing methods were shown to be unreliable even when applied to this very simple system. A new method, proposed here, involves the Fourier decomposition of a received signal as a means to determine the arrival time of the shear wave at the receiver disk.
This method has shown promise and there is good agreement between results of this method and the results of a biaxial compression test on the sample. These travel time determination techniques will be examined for a three-dimensional packing in Chapter 5 and new travel time determination techniques are developed.

Frequency filtering was observed in this two-dimensional sample. The amplitudes of the received signal were associated with waves of lower frequencies than the amplitudes of the transmitted signal. The maximum frequency above which filtering occurred, a “threshold” frequency, was found to be a function of the particle densities and the interparticle contact stiffness. Isolating the normal and shear directions of the interparticle contact model, it was observed that the normal contact stiffness was more influential than the shear contact stiffness on the value of “threshold” frequency.
4.8 Figures

Figure 4.1: Illustration of DEM test sample configuration.

Figure 4.2: Transmitted and received signal from a representative numerical bender element test carried out on the DEM sample, key points on the received signal used to calculate $V_S$ are illustrated as is the arrival time predicted based on the measurement of $G$ in a static probe. $\sigma_0 = 1\text{MPa}, f_{\text{trans}} = 8.20\text{kHz}, R_d = 4.11$ and $\lambda/d_{50} = 8.44.$
Figure 4.3: Representative experimental bender element signal from Viggiani & Atkinson (1995). The clean sinusoid A-B-C is the transmitted signal. A-A' represents the travel time for the start-start method. B-B' and C-C' represent the travel time for alternative implementations of the peak-peak method.

Figure 4.4: Particle velocity vectors for time points (a) to (l) where (a) represents the start of the bender element test and (l) represents a point that is 2.2 input wave periods (0.027s) after the start of the test. The length of each arrow is proportional to the magnitude of the particle velocity. $\sigma_0 = 1$MPa, $f_{trans} = 8.20$kHz, $R_d = 4.11$ and $\lambda/d_s = 8.44$. 
Figure 4.5: Particle velocity vectors for time points (m) to (x) which are 2.4 and 4.6 input wave periods (0.030s and 0.057s) respectively after the start of test. The length of each arrow is proportional to the magnitude of the particle velocity. $\sigma_0 = 1\text{MPa}$, $f_{\text{trans}} = 8.20\text{kHz}$, $R_d = 4.11$ and $\lambda/d_{50} = 8.44$.

Figure 4.6: The decrease in maximum velocity squared of particle as a function of the particle’s position along the propagation axis. The dashed line is a line with a slope inversely proportional to the position. $\sigma_0 = 1\text{MPa}$, $f_{\text{trans}} = 8.20\text{kHz}$, $R_d = 4.11$ and $\lambda/d_{50} = 8.44$. 
Figure 4.7: Particles coloured according to normalised representative particle mean stresses, $<p^r>$ for time points (a)-(l). $\sigma_0 = 1\text{MPa}$, $f_{trans} = 8.20\text{kHz}$, $R_d = 4.11$ and $\lambda/d_{so} = 8.44$.

Figure 4.8: Particles coloured according to normalised representative particle mean stresses, $<p^r>$ for time points (m)-(x). $\sigma_0 = 1\text{MPa}$, $f_{trans} = 8.20\text{kHz}$, $R_d = 4.11$ and $\lambda/d_{so} = 8.44$. 
Figure 4.9: Particles coloured according to relative representative particle shear stresses, $\langle \dot{s} \rangle$ for time points (a)-(i). $\sigma_0 = 1$MPa, $f_{trans} = 8.20$kHz, $R_d = 4.11$ and $\lambda/d_{50} = 8.44$.

Figure 4.10: Particles coloured according to relative representative particle shear stresses, $\langle \dot{s} \rangle$ for time points (m)-(x). $\sigma_0 = 1$MPa, $f_{trans} = 8.20$kHz, $R_d = 4.11$ and $\lambda/d_{50} = 8.44$. 
Figure 4.11: A plot of the received signal and the five constituent waveforms with five lowest frequencies for the numerical bender element test simulation considered in Figs. 4.2, 4.3, 4.4, 4.5, 4.6, 4.7 and 4.8. $\sigma_0 = 1\text{MPa}$, $f_{\text{trans}} = 8.20\text{kHz}$, $R_d = 4.11$ and $\lambda/d_{50} = 8.44$.

Figure 4.12: The cross-correlation function plotted as a function against time for the numerical bender element test simulation considered in Figs. 4.2, 4.3, 4.4, 4.5, 4.6, 4.7 and 4.8. $\sigma_0 = 1\text{MPa}$, $f_{\text{trans}} = 8.20\text{kHz}$, $R_d = 4.11$ and $\lambda/d_{50} = 8.44$. 
Figure 4.13: A plot of $q$ versus axial strain where $q = \sigma_y - \sigma_x$ and a plot of transverse strain versus axial strain.

Figure 4.14: Results for a parametric study carried out on the DEM sample. (a) $V_S$ versus $\sqrt{K}$ ($K$ is the interparticle contact spring stiffness); (b) $V_S$ versus $1/\sqrt{\rho}$ ($\rho$ is the particle density); (c) $V_S$ versus viscous damping ratio; (d) $V_S$ versus bender element frequency.
Figure 4.15: Normalised amplitude versus frequency for (top) transmitter and (bottom) receiver for signals transmitted through samples with different interparticle contact stiffness values, $K$.

Figure 4.16: Normalised amplitude versus frequency for (top) transmitter and (bottom) receiver for signals transmitted through samples with different particle density values, $\rho$. 
Figure 4.17: Normalised amplitude versus frequency for (top) transmitter and (bottom) receiver for signals transmitted through samples with different interparticle contact stiffness values in the normal direction, $k_n$, and the same values in the shear direction, $k_s$.

Figure 4.18: Normalised amplitude versus frequency for (top) transmitter and (bottom) receiver for signals transmitted through samples with different interparticle contact stiffness values in the shear direction, $k_s$, and the same values in the normal direction, $k_n$. 
Figure 4.19: Plot of frequency versus position coloured by amplitude. Black indicates higher amplitude than white. $\sigma_0 = 1$ MPa, $f_{\text{trans}} = 8.20$ kHz, $R_d = 4.11$ and $\lambda/d_{50} = 8.44$.

Figure 4.20: Plot of angular velocity versus wavenumber (inverse of wavelength) coloured by the magnitude of the x-velocity. Black indicates higher wave energy than white. $\sigma_0 = 1$ MPa, $f_{\text{trans}} = 8.20$ kHz, $R_d = 4.11$ and $\lambda/d_{50} = 8.44$. 
### 4.9 Tables

Table 4.1: The sample and bender element properties used for a representative bender element test on the DEM sample.

<table>
<thead>
<tr>
<th>Model Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle Density</td>
<td>2.6x10⁵ kg/m³</td>
</tr>
<tr>
<td>Particle Radius</td>
<td>0.0029 m</td>
</tr>
<tr>
<td>No. of Particles</td>
<td>759</td>
</tr>
<tr>
<td>Viscous Damping Ratio</td>
<td>0.01</td>
</tr>
<tr>
<td>Normal Contact Stiffness (ball-ball) &amp; (wall-ball) (kₙ)</td>
<td>1x10⁹ N/m</td>
</tr>
<tr>
<td>Shear Contact Stiffness (ball-ball) &amp; (wall-ball) (kₙ)</td>
<td>1x10⁷ N/m</td>
</tr>
<tr>
<td>Friction Coefficient (ball-ball)</td>
<td>0.65</td>
</tr>
<tr>
<td>Frequency of Bender Element</td>
<td>8.20 kHz</td>
</tr>
<tr>
<td>Amplitude of Bender Element</td>
<td>12.5x10⁻⁶ m</td>
</tr>
<tr>
<td>Travel distance (d)</td>
<td>0.2007 m</td>
</tr>
</tbody>
</table>

Table 4.2: Summary of Rₙ and λ/dₒ values for the various configurations used during the parametric summary. (Only four of the viscous damping values are listed below to illustrate the scatter in results).

<table>
<thead>
<tr>
<th>K = kₙ = kₛ [kg/s²]</th>
<th>ρ [kg/m³]</th>
<th>Viscous damping [-]</th>
<th>f [kHz]</th>
<th>Rₙ [-]</th>
<th>λ/dₒ [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0x10⁰</td>
<td>2.6x10⁵</td>
<td>0.01</td>
<td>8.20</td>
<td>4.11</td>
<td>8.44</td>
</tr>
<tr>
<td>1.0x10⁰</td>
<td>2.6x10⁵</td>
<td>0.01</td>
<td>4.10</td>
<td>2.38</td>
<td>14.55</td>
</tr>
<tr>
<td>1.0x10⁰</td>
<td>2.6x10⁵</td>
<td>0.01</td>
<td>12.3</td>
<td>5.42</td>
<td>6.38</td>
</tr>
<tr>
<td>1.0x10⁰</td>
<td>2.6x10⁵</td>
<td>0.01</td>
<td>8.20</td>
<td>12.63</td>
<td>2.74</td>
</tr>
<tr>
<td>1.0x10⁰</td>
<td>2.6x10⁴</td>
<td>0.01</td>
<td>8.20</td>
<td>1.29</td>
<td>26.88</td>
</tr>
<tr>
<td>1.0x10⁰</td>
<td>2.6x10⁴</td>
<td>0.01</td>
<td>8.20</td>
<td>13.02</td>
<td>2.66</td>
</tr>
<tr>
<td>1.0x10⁰</td>
<td>2.6x10⁴</td>
<td>0.01</td>
<td>8.20</td>
<td>1.50</td>
<td>23.06</td>
</tr>
<tr>
<td>1.0x10⁰</td>
<td>2.6x10⁴</td>
<td>0.1</td>
<td>8.20</td>
<td>4.11</td>
<td>8.44</td>
</tr>
<tr>
<td>1.0x10⁰</td>
<td>2.6x10⁴</td>
<td>0.3</td>
<td>8.20</td>
<td>3.72</td>
<td>9.30</td>
</tr>
<tr>
<td>1.0x10⁰</td>
<td>2.6x10⁴</td>
<td>0.5</td>
<td>8.20</td>
<td>4.06</td>
<td>8.53</td>
</tr>
</tbody>
</table>
Table 4.3: Comparison of values of $G_{max}$ calculated from the bender element test using different travel time determination techniques for three different interparticle contact spring stiffness’s with the $G_{max}$ value obtained in a static probe.

<table>
<thead>
<tr>
<th>Varying Stiffness</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>K (N/m)</td>
<td>Method</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>$1 \times 10^8$</td>
<td>First Inflection</td>
</tr>
<tr>
<td></td>
<td>Peak-Peak</td>
</tr>
<tr>
<td></td>
<td>Signal Decomposition</td>
</tr>
<tr>
<td></td>
<td>Cross-Correlation</td>
</tr>
<tr>
<td>$1 \times 10^9$</td>
<td>First Inflection</td>
</tr>
<tr>
<td></td>
<td>Peak-Peak</td>
</tr>
<tr>
<td></td>
<td>Signal Decomposition</td>
</tr>
<tr>
<td></td>
<td>Cross-Correlation</td>
</tr>
<tr>
<td>$1 \times 10^{10}$</td>
<td>First Inflection</td>
</tr>
<tr>
<td></td>
<td>Peak-Peak</td>
</tr>
<tr>
<td></td>
<td>Signal Decomposition</td>
</tr>
<tr>
<td></td>
<td>Cross-Correlation</td>
</tr>
</tbody>
</table>
5 Regularly packed granular medium under isotropic confining pressure

5.1 Introduction

The study described in this Chapter builds on previous studies of wave propagation through a granular material using a discrete element method (DEM) approach. Previous researchers, including Hazzard et al. (1998), Li & Holt (2002) and Somfai et al. (2005) amongst others, have demonstrated that DEM can capture the propagation of a stress wave through a granular sample by considering individual particle and interparticle contact force data. These researchers exploited the micromechanical data available for each discrete element in a DEM simulation. From these data insight was gained into the wave propagation mechanism through a granular sample. Li & Holt (2002) found that the particle velocity vectors adopt a vortex like pattern when a planar shear wave is propagated through a granular medium. Somfai et al. (2005) compared contact force data with particle velocity data to conclude that the strong force chain network did not influence wave propagation. Hazzard et al. (1998) investigated a bonded particle model approximating a chalk and a granite sample and were able to relate the number of inter-particle bond breakages to the macro stress versus strain data. They also illustrated the propagation of seismic events, due to these bond breakages, through the sample by considering the velocity data for individual particles.

This research uses three dimensional DEM simulations to investigate the wave propagation mechanism in a bender element test. A bender element test is a common stress wave test conducted in geotechnical engineering laboratories to measure soil properties at small strain and is outlined in more detail in Chapter 2. The research described here is an extension to the previous two-dimensional work described in Chapter 4 and uses the contact models outlined in Chapter 3.

The simulations aim to characterise the waves that are produced by a point source bender element transmitter as they propagate through a granular medium with boundary conditions that match a physical laboratory apparatus, namely the cubical cell apparatus. To focus the analysis on these key points the samples considered are idealised and they largely remain
elastic due to the elastic Hertzian contact law and the lattice packings of monosized particles. Some plasticity may occur due to contact sliding.

Section 5.2 describes the samples including their properties, boundary conditions and the method of inputting a stress wave. Section 5.3 discusses the particle-scale interactions to visualise the wave lobes that are produced by the movement of the transmitter particle. Section 5.4 uses and show particle data to build up a picture of how the waves propagate through the samples including how geometric spreading and boundary reflection play key roles. Section 5.5 outlines analytical solutions that are used to estimate sample stiffness and in turn provide an estimate for the arrival time of the wave. The received signals are analysed in Section 5.6 using methods from the literature that are enhanced by including the observations made in Section 5.4. The sample stiffness is measured by considering the wave propagation speed in Section 5.7 and a parametric study is carried out on variations in macroscale and microscale properties.

5.2 Samples under consideration

5.2.1 General overview

The commercial DEM code PFC3D, Itasca Consulting Group (2007), was used to carry out all the simulations documented in this Chapter. The samples consisted of monosized spheres packed in a face-centred cubic lattice. This is the densest possible packing of uniform spheres that can be created and each sphere contacted twelve other spheres with the exception of spheres at the sides and edges which had fewer contacts. This packing was previously considered by Rowe (1962), Thornton (1979) and O’Sullivan et al. (2002). They used this packing to study quasi-static response and showed convincingly that insight into granular materials can be obtained by considering uniform spheres on a lattice packing. The work of Mouraille et al. (2006) and Mouraille & Luding (2008) is relevant as they considered the propagation of waves through long-short-short face-centred cubic packings of monodisperse spheres. They provide an alternative stiffness tensor based on a fourth order fabric tensor. Santamarina & Cascante (1996) considered the stiffness of regularly packed monodisperse samples and included a review of the analytical relations between grain properties and the effective overall system for three-dimensional regular assemblies of uniform spheres, widely known as effective medium theory, EMT (see Chapter 2). As particle properties are used as
inputs for a DEM simulation it allows direct comparison between these results and the analytical solutions and this comparison is detailed in Section 5.5.

5.2.2 Production sample

A small sample containing 2,673 particles was initially used to develop the code used in the simulations. Sample size effects must be considered and so all of the data presented here are for a much larger sample consisting of 81,576 particles of diameter 2.54mm. The sample measured 99.04mm in the x- and y-directions and 99.51mm in the z-direction. Figure 5.1 presents an overview of the production sample. The ratio of particle diameter to sample size was similar to what was used in laboratory work carried out in the University of Bristol. The production sample was sufficiently large to obtain reasonable $R_d$ values when signals using laboratory frequencies are inputted. Defining a reasonable $R_d$ value has been subjective with different researchers arriving at different conclusions for a correct minimum value. In the analytical work of Arroyo et al. (2003) a value greater than 1.6 was recommended to avoid near-field interference, in the numerical work of Hardy (2003) a value of 4 was recommended and in the experimental work of Jovičić et al. (1996) a value greater than 8.1 was used. The material modelled here was the larger ballotini particles used in the laboratory experiments and the property values outlined in Table 5.1 were obtained from Cavarretta et al. (2012). In conjunction with the default Hertz-Mindlin contact model in PFC3D two user-defined models were used in different samples of the same size. These were Cavarretta-Mindlin and Hertz-Mindlin-Deresiewicz and they are outlined in more detail in Chapter 3. These three contact models were coupled with a viscous damping dashpot model to dissipate energy as in the prototype sample.

5.2.3 Achieving a stress state

Due to numerical rounding errors the placement of the particles was not in a perfect face-centred cubic packing initially but by allowing the particles to slide, by setting the coefficient of friction to zero and applying isotropic stress, they converged to a face-centred cubic packing during isotropic compression. The samples were contained using rigid face wall elements which operated using a servo-controlled algorithm outlined in Cheung & O’Sullivan (2008). These servo-controlled walls were used to compress the sample to the desired confining pressure which was set at 100kPa initially. The compression took place very slowly to insure that there were no dynamic effects as is outlined in O’Sullivan (2011). By examining the stresses in a representative element volume of the sample it was confirmed that
the stress states were reached in a quasi-static manner. The quasi-static manner was checked by examining the increase of stress with time and ensuring that there were no fluctuations. This type of compression and the need to avoid dynamic effects has been considered previously by Ng (2006) and Kuhn (1999). Once the stress acting on the walls reached $\pm 2.50\%$ of the desired confining pressure the compression was stopped. The particle friction was set to the respective material parameter once the compression was stopped.

5.2.4 Boundary conditions

Once the samples reached the required stress state the rigid wall elements were removed and replaced with flexible boundary conditions. At each face a projected area was calculated for each of the outermost particles. This area was calculated using the same method as was used in the triaxial cell example in the PFC manual for a face-centred cubic lattice as outlined in Itasca Consulting Group (2007) and Cundall & Strack (1979b). On the faces perpendicular to the $z$-axis each particle had an equal area associated with it, however, at the other faces the area associated with each particle was dependent on its position in the lattice. This area was multiplied by the desired stress to calculate a force that was applied to the centroid of each particle. The force was directed parallel to the global coordinate direction which pointed towards the sample’s centre. The stress was chosen to match the stress state that had being created with the servo-controlled rigid walls, i.e. 100kPa. Figure 5.2 shows there was good agreement between the stresses applied by the flexible boundary and the stress measured in a representative element volume given by a measurement sphere. They matched to within 1% after an initial fluctuation. Figure 5.1 illustrates the applied forces acting on the particles for each of the samples under consideration here. It shows that only the outermost particles have an applied force and the particles along the edges of the sample have a higher applied force as they have forces acting on them from two and possible three directions.

5.2.5 Creating a stress wave

A disturbance was used to create a stress wave in a soil sample. In the simulations presented here a disturbance was created by translating an individual particle in the middle of one face. This particle was chosen to be mid-way along the $z$-axis, mid-way along the $y$-axis and near zero on the $x$-axis (Figure 5.3). A particle inside the boundary particles was chosen as a transmitter as the bender element tests would be inserted into the sample a given penetration length. This approach has been used in previous DEM analysis of bender elements such as the study outlined in Chapter 4, Carter (2010) and Clement (2006). It differs from DEM
simulations of wave propagation through granular material by Xu et al. (2012) who used a large transmitter that produces a plane wave rather than a point source wave. The frequency of the bender element in the production sample is shown in Table 5.1 and was chosen to keep the value of $R_d$ high. It has been shown by experimental work of Alvarado (2007), the numerical work of Hardy (2003) and the analytical work of Arroyo et al. (2003) that a high value of $R_d$, usually greater than 4, leads to better quality received signal and avoids excessive near field effects. Near field effects have been discussed in Lee & Santamarina (2005) who considered experimental studies and in earlier analytical work by Sanchez-Salinero et al. (1986) who considered the waveform equations and sample transfer functions to provide a theoretical basis for the observed effect. The amplitude of the sine wave was 0.000125mm and was chosen to be very low to avoid any change in the sample packing in both the production and prototype samples. The amplitude was selected after a parametric study which compared how much a given amplitude disturbed the packing of the sample and whether the received signal was large enough to be visible among the quasi-static fluctuations of the particle velocities.

An example DEM received signal is shown on Figure 5.4 (a) for a transmitted single sine pulse at a frequency of 30kHz. There is low amplitude response at 0.2ms, rising to a higher amplitude at around 0.4ms and a lower, fluctuating amplitude after this time. This signal is compared with a received signal for a laboratory sample carried out on the same ballotini particles modelled in the DEM simulation. This received signal was produced by a transmitted single sine pulse at a frequency of 15kHz. The received laboratory signal also has initial lower amplitude response, followed by a higher amplitude part and then lowering in amplitude again. The frequency is lower than the DEM received signal but this is expected due to the difference in transmitted frequencies. The DEM received signal arrives before the laboratory signal as it is regularly packed and therefore stiffer than the laboratory sample. The micromechanical data outputted by the DEM simulation are used to explain the complexities observed on the received signal in Section 5.3 and Section 5.4. Compared to the transmitted signals the received signals exhibit dispersion (frequency reduces during propagation), diffusion/attenuation (amplitude reduces during propagation) and the presence of the near field effect observed as initial small amplitude fluctuations on the received signal before the shear wave arrival.
5.2.6 Preserving the elasticity of the sample

The movement of the transmitter particle produced no change in coordination number and some sliding contacts in the samples. Figure 5.5 illustrates the average global coordination number and the number of contacts sliding during a bender element test on the production sample. It is important to preserve the elasticity of the sample as it is an underlying assumption of body wave propagation theory which was outlined in Chapter 2. The value of the average coordination number remained unchanged and there was no change in particle positions large enough to either break contacts or create new contacts. The small number of sliding contacts was unavoidable to produce a seismic wave that had an amplitude significantly above the particle motions that constantly happen in a quasi-static simulation. The sliding contacts were not expected to overly affect the elasticity assumption as the wave propagates through the system; however it must be acknowledged.

5.3 Waveforms generated by disturbance

5.3.1 Overall waveform

In all samples a shear wave was propagated as this is repeatedly reported in the literature as a difficult wave to determine a travel time where bender elements were used, Blewett et al. (2000). A single particle in the DEM simulation was displaced in the y-direction and the direction of wave propagation was the x-direction (Figure 5.3). Previous laboratory research by Lee & Santamarina (2005) indicated that the experimental bender element test resulted in the formation of a central shear wave lobe which was spherical in shape and in two compressional wave side lobes. The figure from their paper has been reproduced here as Figure 5.6.

In Figure 5.7 the particles which have a rotational velocity about the z-axis above 0.05rad/s were plotted, which captures the particles experiencing higher shear stresses in the x-y plane. This snapshot was taken at a time of 9.172x10^{-5}s into the simulation. The plan and elevation view clearly show a spherical shear wave front, the speed of which was a function of $G_{xy}$. The rotational velocities were chosen to illustrate the shear waves as the shear stresses they induced were related to the rotational velocities of the particles. Figure 5.8 also considers the system at a time of 9.172x10^{-5}s, but it plots the particles that have reached a velocity in the x-direction of magnitude greater than 0.1mm/s. This illustrates the compressional wave side lobes that were propagating diagonally out from both sides of the point-source, just as was
observed in Lee & Santamarina’s paper. The compressional wave side lobes were a function of the constrained modulus, $M_x$.

The DEM data allowed a three-dimensional visualisation of the mechanics. Figure 5.9 plots the particles which had a rotational velocity about the x-axis greater than 0.04rad/s. Two spherical fronts spread from the transmitter towards the top and bottom faces of the sample and their speed was a function of $G_{yz}$ of the sample. Figure 5.10 plots the particles which had a rotational velocity about the y-axis greater than 0.04rad/s. Four arc fronts spread from the transmitter towards the corners of the sample at a speed that was a function of the sample $G_{xz}$. As well as isolating the particles with significant velocities in the x-direction, the particles with significant velocities in the y- and z-directions were isolated in Figure 5.11 and Figure 5.12. The threshold used was for a particle to have a speed above 0.1mm/s. Figure 5.11 shows that particles with velocity in the y-direction generally followed the shear wave lobe pattern in Figure 5.7. Figure 5.12 shows particles with higher speed in the z-direction followed the shear waves propagating towards the corner of the sample. Figure 5.9 to Figure 5.12 are plotted at the same time point as Figure 5.7 and Figure 5.8 to be comparable.

5.4 Propagation of wave through sample

Individual particle velocity vectors

The particle velocity vectors are plotted on Figure 5.13 and Figure 5.14. Although the sample was three-dimensional and therefore has three vector components only the components in the shear plane, i.e. x and y, are plotted for clarity. To aid interpretation only velocities less than 0.5mm/s are plotted as the larger velocities created at the transmitter cloud the propagation of the wave. The plots presented on Figure 5.13 and Figure 5.14 are a plan view of the sample considering a slice 5mm thick which is approximately twice the particle diameter. The arrows are scaled by the magnitude calculated from the x and y velocity components only. On Figure 5.13 compressional waves are observed to propagate from the transmitter towards the boundaries of the sample. The compressional waves appear to be oppositely polarised which is expected based on observations made in Chapter 4. A circular shear wave lobe is observed to propagate towards the receiver through the centre of the sample. Reflections are seen to initiate from the boundaries at time point (f). Figure 5.14 presents the later time points in the signal propagation which includes the shear wave arrival. Shear waves continue to propagate through the centre of the sample. Reflections propagate
diagonally towards the receiver from the boundaries. Movement of the receiver occurs between time points (i) and (j) which appears from the plots to be before true shear wave arrival at time point (l). The loss in magnitude of the velocity vectors at later time points is a result of a loss of energy from the system and geometric effects. Some of the energy loss was due to the viscous damping model (a dashpot) used at the contacts in the simulation. There was also some energy loss due to frictional energy dissipation. This occurred due to the sliding contacts that were caused by the movement of the transmitter particle as outlined previously. Another source of energy dissipation was the flexible boundary conditions. The body work done by the applied forces in opposition to the boundary particle motion absorb some energy. The geometric effects of energy radiating from a point source are coupled with these sources of energy dissipation.

**Representative particle shear stresses**

Figure 5.15 and Figure 5.16 plot the representative particle shear stresses as the wave propagates through the system, similar to the visualisation used for the two-dimensional simulations in Chapter 4. A circular shear wave lobe propagates from the transmitter along the central axis of the sample. The circular region is seen to develop at time point (b) and by time point (f) it is over half-way through the sample. The propagating shear wave comprises of bands of alternating positive and negative changes in shear stress corresponding to the peaks and troughs of the propagating wave. The shear stresses are related to the particle rotations which are explored later in this Section. Reflections from the boundaries appear in Figure 5.16 and initiate from the corners at the transmitter end of the sample. The shear wave lobe leads the reflections through the sample but it is clear that they will play a role in the movement of the receiver later in the simulation. At time point (l) on Figure 5.16 it appears that the shear wave has arrived at the receiver end of the sample.

**Representative particle mean stresses**

Figure 5.17 and Figure 5.18 plot the relative representative particle mean stress which was computed in a similar way to the normalised representative particle mean stress in Chapter 4; however in this case the values at each time point are subtracted from the initial time point rather than divided. The side lobes produced are clearly observed in Figure 5.17 and they propagate towards the sample edge. As discussed before in Chapter 4 they alternate between positive and negative and this is dependent on the direction in which the transmitter has moved. These side lobes of relative mean stress are taken to represent the compressional
wave lobes produced by the motion of the transmitter particle. After interacting with the boundaries in Figure 5.18 reflected waves are observed to propagate towards the centre of the sample. As mentioned in Chapter 4 the magnitude of the compressive stress is directly linked to the strain energy and there is clearly an on-going conversion of kinetic energy into strain energy and vice-versa as the wave propagates through the system. Energy loss can be observed in Figure 5.18 as the light and dark patches become steadily less pronounced.

**Particle translational velocities**

Figure 5.19 and Figure 5.20 isolate the particle velocities in the y-direction and complement the previous observations. The motion of the particle velocities in the y-direction produces images that match the changes in representative particle shear stress. The shear stress is caused by an initial movement of the transmitter particle in the y-direction so this is intuitive. Again, in Figure 5.19 the development and production of a central shear wave lobe is observed. On Figure 5.20 the y-velocities have not captured the reflections as clearly as the representative particle shear stresses. This is because the reflections are not motion just in the y-direction but will contain significant motion in the x-direction. As before, an arrival at time-point (l) can be inferred.

The particle velocities in the x-direction are captured on Figure 5.21 and Figure 5.22. They are seen to complement the observations in Figure 5.17 and Figure 5.18. In Figure 5.21 motion in the x-direction forms side lobes that are propagating towards the edge of the sample. They have alternating sign due to the motion of the transmitter particle. Figure 5.22 plots the reflected waves from the sample boundaries more clearly than the relative particle mean stress and this could be due to the addition of the reflected shear waves adding motion in the x-direction. The reflections propagate towards the centre of the sample (Figure 5.18).

**Particle rotational velocities**

Another interpretation method is illustrated on Figure 5.23 and Figure 5.24 where rotational velocities about the z-axis are considered. The shear stresses that result from the motion of the particle in the y-direction are likely to cause a rotation of the particle about the z-axis by inducing a moment on the particle. Consequently the plots of particle rotational velocity that are shown in Figure 5.23 and Figure 5.24 agree with the earlier plots of relative shear stress quite well. The central lobe and reflections are both clearly captured using this method. On the received trace in the centre of the figures there is some initial motion before the arrival of the shear wave lobe. This was examined by considering the plot of the particles for time
point (j) at a much higher colour scale resolution, ±0.005 rad/s, instead of ±0.05 rad/s. This image is plotted at Figure 5.25 and it can be seen that the reflections have travelled faster along the particles close to the boundary and interacted with the boundary at the receiver end of the sample to produce a disturbance. This disturbance travelled out from the boundary particles and caused the fluctuation of the receiver particle seen before arrival of the wave front. This is clear as there are a number of particles between the wave front and the receiver particle that are not rotating. Therefore, the wave front has not reached those particles and the fluctuation at the receiver particle must be coming from the boundary conditions.

Elevation view
Figure 5.26 and Figure 5.27 plot and elevation view of the cross-section xz showing the rotational velocities about the z-axis. The three-dimensional spherical central lobe produced is clearly observed in Figure 5.26. The geometric spreading of the wave is seen to occur in this direction also. Figure 5.27 illustrates reflections produced by interaction with the bottom and top boundaries and then these reflections propagate in towards the centre of the sample much like what happened in Figure 5.23 and Figure 5.24 for the cross-section xy.

Summary
From this Section it is concluded that the compressional waves are best observed using representative particle mean stresses and the x component of individual particle velocities. The shear waves are best observed using representative particle shear stresses, y component of individual particle velocities and particle rotational velocities about the z-axis. It is found that the shear wave lobe is spherical and travels through the centre of the sample in agreement with the preliminary findings in the previous Section. The arrival of the shear wave is clouded by the presence of a disturbance that has travelled around the boundaries of the sample and is not the true shear wave arrival. The compressional waves are found to propagate diagonally towards the boundaries as observed in Chapter 4. The flexible bounded sample produces reflections that travel towards the receiver and will influence its motion.

5.5 Analytical estimates of sample stiffness
There are a number of analytical solutions that can be applied to the face-centred cubic packing to quantify values of stiffness or wave propagation speed. The stiffness values attained using these analytical solutions can be compared to results of DEM simulations more readily than laboratory tests. The analytical solutions contain simplifications and
idealisations that mean that the results from these methods will differ from those observed in the simulations and in the experiments. This has been previously reported in Chapter 2. These solutions also can be compared for a sample at different confining pressures to see how they change over different confining pressures. The following analytical solutions are examined: effective medium theory, principle of virtual displacement and dispersion relation theory. These solutions are outlined in the Sections below and the resulting values of Young’s modulus and shear modulus are shown for comparison on Figure 5.28 and Figure 5.29 respectively. It is important to compare these solutions in terms of their magnitudes and in the relationship they provide between elastic moduli calculated and confining pressure. In addition there is a theory for predicting the near field effect and that is outlined in Section 5.5.4.

5.5.1 Effective medium theory

Effective medium theory (EMT) can be used to get an approximate stiffness for the face-centred cubically packed sample and is explained in detail in Chapter 2. EMT has often been used to describe the stiffness of a granular packing for example in Duffy & Mindlin (1957) and Walton (1987). The equations used for the face-centred cubic packing are summarised in Santamarina & Cascante (1996), and are used to calculate the sample shear modulus, $G_{FCC}$, and the sample Poisson’s ratio, $\nu_{FCC}$, are given by:

$$G_{FCC} = \frac{(4 - 3\nu) \left[ \frac{3\sigma_0 G_{\text{particle}}^2}{2(1 - \nu_{\text{particle}})^2} \right]^{1/3}}{2(2 - \nu_{\text{particle}})}$$

5.1

$$\nu_{FCC} = \frac{\nu_{\text{particle}}}{8 - 5\nu_{\text{particle}}}$$

5.2

where $G_{\text{particle}}$ and $\nu_{\text{particle}}$ are the particle shear modulus and Poisson’s ratio and $\sigma_0$ is the sample confining pressure. This analytical solution cannot account for different contact forces between the particles or boundary conditions or for changes in the contact force network. There are additional equations in Santamarina & Cascante (1996) for other regularly packed samples to obtain sample shear moduli and Poisson’s ratio. Figure 5.28 and Figure 5.29 show that the relationship between Young’s modulus and confining pressure and between shear modulus and confining pressure is 0.333 (1/3) for both as predicted by Hertzian contact mechanics.
5.5.2 Principle of virtual displacement

In Mouraille et al. (2006) and de Mol (2013) a method known as the principle of virtual displacement was used to produce a fourth order stiffness tensor from which the elastic moduli can be extracted. The theory behind this approach has been outlined in Chapter 2 and here the equation is expanded to include the effects of particle friction as

\[
C_{\alpha\beta\gamma\delta} = \frac{1}{V} \sum_{p \in \mathcal{V}} \left( k_n \sum_{c=1}^{C} \left( l^2 / 2 \right) n^c n^c n^c n^c + k_t \sum_{c=1}^{C} \left( l^2 / 2 \right) t^c t^c t^c t^c \right)
\]

where \( n^c \) is the unit vector in the normal direction of contact, \( t^c \) is the unit vector in the tangential direction of contact, \( k_n \) is the normal contact stiffness, \( k_t \) is the tangential contact stiffness, \( l \) is the branch vector (~ the particle diameter) and \( V \) is the Voronoi volume. To solve this for a face-centred cubic packing a unit lattice is used by taking a single particle in the system and the twelve particles contacting it. This method has the advantage over EMT of being able to account for anisotropies in the stiffness of a face-centred cubic packing. The solution for a face-centred cubic packing sample illustrates the cubic anisotropy of the sample as outlined by Lings (2013) and in Section 5.7.7 of this Chapter. Norris (2006) is an example of where equations governing the directional dependence of parameters can be found.

Table 5.2 shows where the fourth order tensor values fit into a second order stiffness tensor, where 1 = x-direction, 2 = y-direction and 3 = z-direction.

Table 5.3 shows the values calculated for the production sample confined at 100kPa isotropically. Due to cubic anisotropy the equalities in Section 5.7.7 were observed. This theory cannot account for sliding contacts or changes in particle packing and cannot account for boundary conditions. Figure 5.28 shows the relationship between Young’s modulus and confining pressure and Figure 5.29 shows the relationship between shear modulus and confining pressure. The data indicate that \( E_x \propto \sigma_0^{0.336} \) and that \( E_x \) calculated by the principle of virtual displacement is below the value obtained using effective medium theory. The magnitude of \( E_z \) was found to be higher than \( E_x \) and the relationship was \( E_z \propto \sigma_0^{0.337} \). \( G_{xy} \propto \sigma_0^{0.394} \) is observed in Figure 5.29 and the magnitude is close to that of effective medium theory. The power law relationship for \( E_x \) is quite similar to that obtained through effective medium theories but the relationship between \( G_{xy} \) and \( \sigma_0 \) is not as similar to effective medium theory. \( G_{yz} \propto \sigma_0^{0.299} \) and \( G_{zx} \propto \sigma_0^{0.337} \), which are close to the expected 1/3 values. The
magnitude of $G_{yz}$ was found to be greater than $G_{zx}$ which in turn was larger in magnitude than $G_{xy}$.

5.5.3 Dispersion relation theory

The second analytical method outlined in Mouraille et al. (2006) and de Mol (2013) is known as dispersion relation theory. This theory has been explained in the literature review and considers a unit lattice to calculate the relationship between wavenumber ($k$) and angular velocity ($\omega$) of a wave propagating through a granular material. When the eigenvalue problem presented in Chapter 2 is solved for frictional particles, 6 eigenvalues are obtained for each value of wavenumber inputted to the system. The 6 eigenvalues are the angular velocities of the compressional wave, two shear waves and three rotational waves. The slope of the plot of angular velocity versus wavenumber gives a value of wave speed for the chosen wave. This wave speed can be then used to calculate an elastic modulus depending on the wave propagation and oscillation direction. $E_i$ is plotted against different confining pressures on Figure 5.28 and the magnitudes of the moduli are similar to those obtained from effective medium theory and the principle of virtual displacement. The power law relationship between $E_x$ and $\sigma_0$ is 0.351 and between $E_z$ and $\sigma_0$ is 0.336 and both of these were close to the expected 1/3. $G_{ij}$ are plotted on Figure 5.29 where the magnitudes of values obtained from dispersion relation theory are generally above those of the other two methods. $G_{xy} \propto \sigma_0^{0.292}$ is close to the trend of the other methods. $G_{yz} \propto \sigma_0^{0.336}$ and $G_{zx} \propto \sigma_0^{0.336}$ which show close agreement with the expected 1/3 value. The full set of dispersion relation results, for waves propagating in different directions, indicate that the sample packing is cubic anisotropic. Whereas elastic isotropy only requires two independent parameters, cubic anisotropy requires three independent parameters. The magnitude of $G_{yz}$ was found to be greater than $G_{zx}$ which in turn was larger in magnitude than $G_{xy}$.

Figure 5.30 illustrates that the dispersion relation curve predicts frequency filtering. Frequency filtering is when waves with frequencies above a certain pass band do not propagate through the system. This has been outlined in Chapter 2. The peak observed for both the compressional wave (black) and the shear wave (blue) indicates that no higher frequencies would propagate in this system. The wave at the peak is a standing wave with a given angular velocity and wavenumber. Suiker et al. (2000) showed that this is predicted even for a one-dimensional granular chain and that a truly linear elastic material would not plateau but continue with a constant positive slope. This shows that a regularly packed
granular material is not a liner elastic material when considering wave propagation. Suiker et al. stated that the region which comprises the waves that are physically permissible is from the origin to the first peak and this is called the “Brillouin region”.

5.5.4 Near-field effect

The near-field effect observed in experimental and numerical simulations can be analytically predicted using the work of Sanchez-Salinero et al. (1986). The solution to this analytical solution, which is obtained by calculating a transfer function for the sample, can be compared with the numerical DEM results for a face-centred cubic packing confined at 100kPa. It shows good agreement with the time at which the near-field effect occurs on Figure 5.31. The magnitudes of the displacement of the analytical solution and the DEM simulation do not agree, however, and the Sanchez solution is scaled by $10^7$. An input wave speed is needed to calculate the near-field effect solution and the wave speed chosen here is from EMT for a face-centred cubic sample confined at 100kPa. The analytical solution implemented here did not have a material damping value as the numerical simulation had a very low value of damping.

5.6 Determining the travel time

A key goal of this research is to critically assess travel time determination techniques using micromechanical data. The received signal is firstly considered; this is directly analogous to laboratory bender element testing data analysis (Section 5.6.1). Then, the detailed information on the passage of the wave through the sample was analysed, giving additional information on shear wave arrival time, as detailed in Section 5.6.2.

5.6.1 Analysis of the received signal

Characteristic points

The received signal for a single sine pulse transmitted at 30kHz is plotted against time on Figure 5.32. Some small amplitude oscillations preceded the arrival of the shear wave as indicated by the micromechanical data presented above. Figure 5.24 and Figure 5.25 show that the reflections striking the corner of the sample were causing this fluctuation before the true shear wave arrived. This first fluctuation was ignored when first arrival travel time determination technique was used such as first zero crossing. Figure 5.33 plots the x and y components of the receiver motion as the wave arrives. It illustrates the movement that can
occur in the x-direction even though the transmitter was moved in the y-direction. The movement in the x-direction was of smaller amplitude than the movement in the y-direction.

Signals transmitted at different frequencies and with different waveshapes were examined in this research. The waveshapes examined were a single sine pulse, a single triangular pulse, a single sine pulse with a 270° phase angle and a square pulse. The single sine pulse was transmitted with the frequencies 7kHz, 15kHz, 20kHz and 30kHz (Figure 5.34). Figure 5.35 compares the transmitted and received signals for different waveshapes (single sine pulse, single triangular pulse, single sine pulse with phase angle and square pulse) all transmitted at 20kHz. None of these changes to the waveform should change the stiffness of the sample, therefore the wave speed measured should be similar in all these cases. The amplitude of the received signal was observed to decrease as the frequency of the sine wave increased. The choice of waveshape was also observed to affect the amplitude of the receiver. All received traces were observed to be at zero initially; however, there was a deviation before the expected shear wave arrival in all signals, indicating the arrival of a wave component at the receiver. As the wave causing this deviation was faster than the predicted shear wave but slower than the predicted compressional wave it could be a compressional wave that had gone on a circuitous route through the sample and not in the straight line from transmitter to receiver. This clouded the arrival of the shear wave. Choosing the first zero crossing as before, based on Figure 5.25, gave different results depending on the wave shape and frequency picked and it was this dependence that needed to be avoided. The range of calculated arrival times goes from $1.859 \times 10^{-4}$s to $2.492 \times 10^{-4}$s resulting in stiffness values that range from 387.62MPa to 215.71MPa. When the 7kHz waves were removed from consideration based on their low $R_d$ values the range of stiffness values dropped, now between 387.62MPa and 333.56MPa. This was still a large range indicating that the first zero crossing may not be a suitable wave speed measurement technique.

A number of first arrival techniques were examined, namely the point of first local minimum, first point where the first derivative equals zero and second point where second derivative equals zero (the second point was picked to avoid the near-field effect), to see if a reduction on the sensitivity to frequency seen using zero crossing was achieved. The locations of these characteristic points on a typical numerical received signal are plotted on Figure 5.36. The recorded travel times for all methods exhibited sensitivity to frequency and to the chosen waveshape. The travel time was observed to reduce as the frequency was increased. A dependence on the waveshape chosen was also observed where the sine wave was always
faster than the triangular wave which in turn was faster than the sine wave with phase. These results are summarised in Table 5.4 and Table 5.5. Based on these recorded discrepancies further work was carried out to examine the received signal to see if this apparent dependence on frequency and wave shape can be avoided. The signal decomposition method, outlined in Chapter 4, was utilised on these signals to see if it could be used to obtain travel times that were not a function of frequency. As can be observed on Table 5.4 and Table 5.5 the shear moduli values obtained from this method were just as much a function of frequency and wave shape as any of the other methods. Although this method appeared to work well for the two-dimensional sample outlined in Chapter 4 it did not improve, i.e. reduce, the frequency dependence observed using the other methods. A plot of the dependence of shear modulus on frequency is plotted in Figure 5.37 where the shear modulus was calculated from the sine pulse and averaged over the time domain methods. The frequency dependence recorded here was also reported by Leong et al. (2009). In their experimental work on sand samples and residual soil samples the recorded shear wave speed increased as the excitation frequency used was increased. These data are included on Figure 5.37. Frequency dependence was also observed by Blewett et al. (2000).

Cross-correlation
Cross-correlation is outlined in Chapter 2 and in Santamarina & Fratta (2005) and is a signal processing operation that permits similarities between noisy signals to be identified. The resulting signal in the frequency domain was transformed into the time domain and plotted alongside the original received signal (Figure 5.38). The arrival time was chosen by picking a peak on the cross-correlation function near an existing first arrival characteristic point on the received signal such as first zero-crossing or first point of inflection. As mentioned in Chapter 2, Mohsin & Airey (2003) argued that this method gave a more reliable result compared to picking the maximum peak on the cross-correlation function as previous researchers had done, e.g. Viggiani & Atkinson (1995). Yang & Gu (2013) have used this method with some success. Cross-correlation results for different frequencies and wave shapes are included in Table 5.4 and Table 5.5 and were dependent on both frequency and wave shape.

Amplitude versus frequency plots
Figure 5.39 and Figure 5.40 compare the signals of various transmitted frequency and waveshape in the frequency domain in terms of normalised amplitude versus frequency. The
frequency content of the received waves was affected by the transmitted wave frequency. It appears on Figure 5.39 that as the frequency content of the transmitter increased the frequency content of the receiver increased to match it. Evidence for the decreasing amplitude of the received signals with increasing frequency in the time domain can be found in the non-normalised frequency domain plot on Figure 5.41. As the frequency content for the transmitter broadened, the amplitude is reduced. This caused reduction in the corresponding received amplitude. Differences in received amplitude measured in the frequency domain were also observed to be functions of different waveshapes as shown on Figure 5.42.

In Figure 5.39 to Figure 5.42 the maximum peak in all signals in the frequency domain occurred at approximately 12.621kHz. A bender element test simulation was carried out on the sample using this frequency as the transmitted frequency. The results are presented in both time and frequency domains on Figure 5.43. In the time domain the received signal associated with the 12.621kHz transmitted signal has a higher amplitude than all other received signals. The received wave also appears to oscillate with a more consistent frequency. In the frequency domain the peak in amplitude for the received signal associated with the transmitted 12.621kHz frequency was larger than all other peaks. The frequency 12.621kHz appears to be related to a resonant frequency of the system as there was less diffusion when this frequency was used.

A continuous (10) cycle input signal was considered, and the number of oscillations influenced the response in the time and frequency domains (Figure 5.44). Both signals appeared to arrive at a similar time but the amplitude of the received signal resulting from the ten pulse transmitted signal was larger than the amplitude of the received signal resulting from the single pulse transmitted signal. In the frequency domain the transmitted pulse that was cycled ten times was a narrower peak over the transmitted frequency. This resulted in the received signal having a maximum peak over the transmitted frequency value of 30kHz. There is still a local maximum occurring at a frequency of approximately 12.62kHz providing robust evidence that there is a fundamental sample mode at that frequency.

The frequency domain plots were affected by signal length in the time domain. It affected both the amplitude and the frequency resolution. For the comparisons carried out above the signal length in the time domain was limited to a low value. The length of the transmitted 7kHz signal was varied to discover the effect of the signal length on the frequency domain
plots. Figure 5.45 compares the two signal lengths in the time domain where the short signal is approximately 0.3ms and the long signal is approximately 1.3ms. The frequency domain plots are shown on Figure 5.46 where the FFT of the longer signal shows many more peaks and seems to be more limited by the transmitted signal frequency content than the shorter signal. The longer signal captured the sample response through the reflections that were generated whereas the shorter signal captured the frequency of that initial oscillation, found to be 12.621kHz in the previous analysis. The particle scale visualisations in Section 5.4 showed that the first oscillation after the near-field arrival was the true shear wave.

Frequency filtering was not observed with the frequencies chosen here. Figure 5.40 shows that the frequency content of the receiver changed with the transmitted waveshape. As the frequency content of the transmitted waveshape increased or decreased the frequency content of the received waveshape also increased or decreased. The transmitted triangular waveshape on Figure 5.40 (b) shows relatively high amplitude values at high frequencies compared to the other transmitted signals. The received signal, however, reduced in amplitude greatly when the frequencies were above 50 – 60kHz. This indicates that this may be the “threshold” frequency at which frequency filtering would occur in this face-centred cubically packed sample. As the highest transmitted frequency used here was 30kHz none of these signals would have large amplitudes occurring at frequencies above 60kHz. This limits the certainty with which a “threshold” frequency can be picked.

The small prototype sample used in model development (2,763 particles) was used to prove that frequency filtering could happen on a sample with a face-centred cubic lattice packing of particles. Two high frequency transmitted waves were propagated through the prototype sample. The frequencies used were 400kHz and 800kHz. Figure 5.47 illustrates that frequency filtering can occur when such high frequency waves are transmitted through a face-centred cubic packing and the “threshold” frequency was found to be approximately 285kHz for both the 400kHz and 800kHz transmitted waves. This value should not be compared with previous production sample results as the model parameters for the prototype sample were different.

By comparing the plots for transmitted and received signals the effect of frequency filtering in a granular system was clearly observed as previously noted by Zhu et al. (1996) and Lawney & Luding (2013). This is observed in Figure 5.48 for the production sample at different isotropic confining pressures. The transmitted signal was always a shear pulse in
the xy-plane with a frequency of 30kHz and an amplitude of 0.000125mm. The frequency domain plot of the transmitted pulse shows an amplitude versus frequency curve that peaks at 30kHz and contains significant amplitude content up to 60kHz. The transmitter moved at a range of frequencies causing the propagation of waves of different frequencies. The plot for all received signals shows little or no frequency content above ~55kHz. This implies that the granular system was not allowing higher frequency values to propagate through the system which could be offering some interesting insight into the system’s behaviour.

**Phase versus frequency plots**

The travel time of the shear wave can be determined in the frequency domain. The method outlined in Greening & Nash (2004) was used. The stacked phase was calculated using the Matlab functions ANGLE and UNWRAP to calculate the angle of the complex numbers present in the Fourier transform and then these phase angles were stacked on top of each other. A plot of stacked phase versus frequency was created and the secant slope of this graph equalled to the phase travel time of the shear wave. In Equation 5.4 the phase, \( \phi \), is divided by the angular velocity, \( 2\pi f \), to give a value of travel time, \( t_{arr} \), for the wave.

\[
t_{arr} = \frac{\phi}{2\pi f}
\]

Two wave velocities could be ascertained using the plots of stacked phase versus frequency. The phase velocity obtained from the secant slope of the graph of stacked phase versus frequency was the speed at which the phase of any one component frequency of the wave travelled. The group velocity obtained from the mean of the tangent slopes of the graph was the velocity with which the overall shape of the wave’s amplitudes propagated through the system. The values for group velocity were found to be more scattered than the phase velocities and were not included in this study. Figure 5.49 plots the stacked phase against frequency for the sample confined at 100kPa. For nondispersive systems the value of group velocity equals the value of phase velocity but even one-dimensional chains of particles were seen to behave in a dispersive nature in Lawney & Luding (2013). This dispersion indicated that the system may not be not linear elastic, although there are many sources of dispersion. The values of phase velocity are shown on Table 5.6 and Table 5.7 for waves that were propagated at different frequencies and with different waveshapes.
The phase versus frequency plots were used to calculate $G_{\text{max}}$ values for signals propagating through the sample at various frequencies (7, 15, 20 & 30 kHz) and wave shapes (sine, triangular, sine + 270° phase and square). The results are summarised on Table 5.6 and Table 5.7. The phase versus frequency plots provided results that appear in all cases to be very different from previously calculated time-domain results. This method seems to be unreliable for the system considered here.

5.6.2 Temporal – spatial analysis of system

Time-domain contour plots

A DEM simulation provides a large amount of grain scale data as observed in the previous Section 5.4. By plotting contour plots of these data such as the particle incremental displacements the propagation of the wave was observed. Particles consisting of a central column between the transmitter and receiver were chosen to create this contour plots. Figure 5.50 has position as y-axis and time as x-axis and the slope of a contour line gives the wave speed for a sine pulse of 15kHz. The effect of reflections was observed at higher time values. One of the problems with this method is that the contours can give a number of different slopes and judgement must be used to decide which slope should be used. Generally one of the initial slopes is a better choice as reflections can influence a later slope. Also, the contour line should have a reasonably uniform slope. If these conditions were met a reasonably consistent result was obtained. The effects of frequency and wave shape on the contour plot method were investigated in Table 5.4 and Table 5.5 and the results show a dependency on frequency and wave shape. Figure 5.51 illustrates the contour plot information on a three-dimensional surface plot to highlight the attenuation of the wave amplitude as it travelled through the system. The reflection off the receiver end boundary is also clearly observable in the figure. The reduction in kinetic energy as the wave propagates through the system is further visualised using Figure 5.52 where the maximum particle velocity in the y-direction reached was squared and was plotted against that particle’s position on the propagation axis (x-direction). The solid points indicate the location of the particles and the non-linear reduction in the maximum velocity squared attained is clear. The square of the velocity was indicative of the kinetic energy ($KE$) and the decrease in velocity squared was proportional to $r^{-2.15}$ where $r$ was the position of the particle along the propagation axis. Therefore an approximate relationship is that $KE \propto 1/r^2$, which is represented by the dashed line. This
relationship is related to the area of a sphere indicating that a spherical lobe is propagating through the system.

**Frequency versus position plots**

As mentioned in Chapter 2 Mouraille et al. (2006) examined the phenomenon of frequency filtering in their numerical sample by producing frequency versus position plots that were coloured by amplitude so that the filtering of the frequencies was observed as the wave travelled through the sample. This plot was created for the production sample at 100kPa and is illustrated in Figure 5.53. The observation from these plots was that the higher frequencies were quickly filtered by the system as they did not survive for very long along the position axis. To create these plots data were needed for the interval particles between the transmitter and receiver so a numerical simulation was needed to achieve this. This frequency filtering was observed on a one-dimensional chain of particles in numerical simulations carried out by Lawney & Luding (2013) and in experimental work carried out by Zhu et al. (1996) using photoelastic disks.

**Two-dimensional fast Fourier transform**

It is possible to identify a travel time using a two-dimensional fast Fourier transform after Mouraille et al. (2006) and de Mol (2013). These plots were created using the variation of the signal over time and space. Particles were chosen along a “column” of particles connecting the transmitter and receiver and the time was from the start of transmission to just before arrival at the receiver. This prevented the inclusion of reflected waves which would lead to a noisier plot. The two-dimensional fast Fourier transform allowed a contour plot of position versus time coloured by ball velocity or displacement to be reconsidered in the frequency domain into a plot of angular velocity \( (\omega) \) versus wavenumber \( (k) \), inverse of wavelength multiplied by \( 2\pi \), coloured by wave energy. Figure 5.54 displays a schematic of the process used to create a 2D FFT of the signal propagating through a sample. It considers a one-dimensional line of particles to simplify the schematic but as a column of particles is considered in the full implementation this would be an accurate simplification. This schematic also illustrates the theory behind the fft2d function in MATLAB. In MATLAB the temporal and spatial variation of the propagating signal is stored in a matrix which is inputted into the fft2d function such as the transformation from the contour plot to the dispersion relation illustrated in Figure 5.54. This can be considered as a three stage process. Firstly, the displacements or velocities versus time plots for each particle are transformed into the
frequency domain. Secondly, the displacements or velocities versus position plots for each time point are transformed into the frequency domain. Finally, product of these two transformations creates a dispersion relation. This process is also illustrated in Figure 5.54. The resolution of the angular velocity (Δω) is a function of the overall length of the signal recorded. The resolution of the wavenumber (Δk) is a function of the distance between the transmitter and receiver. The maximum angular velocity is a function of the timestep (Δt) and the maximum wavenumber is a function of the separation between two particle centroids (approximately the diameter of a particle). Figure 5.55 gives this plot and there appeared to be an almost linear relationship between frequency and wavenumber, the slope of which gave a value of wave speed. The maximum wavenumber that can be recorded was equal to 1/2Δx where Δx was the distance between two particles. The wavenumber resolution, Δk, was equal to 1/X where X was the position of the particle furthest from the transmitter. This was analogous to the determination of Nyquist frequency and frequency resolution discussed in Chapter 4. The best-fit linear slope of this plot gave a value of wave speed. This plot gave us other information about the sample such as the highest frequency and the highest wavenumber (shortest wavelength) that was propagated through the system. The advantages of using the two-dimensional fast Fourier transform is that it gives a robust determination of wave speed and illustrates the range of angular velocities and wavenumbers that can propagate through the system. The disadvantage is that the spatial variation of the wave as it propagates must be known which would imply the use of many transducers along the propagating length in the sample.

The effect of the number of signal cycles in the time domain on the results of this method was considered when ten input sine waves were inputted. Figure 5.56 plots the two-dimensional fast Fourier transform of angular velocity against wavenumber. As the transmitted wave of frequency 30kHz (ω = 188.50x10³ rad/s) was cycled continuously for ten cycles there is a dark band on Figure 5.56 at this angular velocity. Along this dark band a darker region is observed at a wavenumber of 403.70 rad/m and if the angular velocity was divided by this wavenumber the resulting wave speed was 466.93 m/s. This was close to the value calculated for a single sine pulse. Figure 5.57 used a signal length in the time domain that is 1ms longer than the signal length used in Figure 5.55. Both plots are remarkably similar and the speed of the shear wave calculated using Figure 5.55 was 476.30 m/s and the speed of the shear wave calculated using Figure 5.57 was 473.10 m/s.
The two-dimensional fast Fourier transforms were used to calculate $G_{\text{max}}$ values for signals propagating through the production sample at various frequencies (7, 15, 20 & 30 kHz) and wave shapes (sine, triangular, sine + 270° phase and square). It was not possible to calculate a two-dimensional fast Fourier transform result for the square wave. This was due to the noise on the plot which made it impossible to calculate a clear slope in the plot. The results are summarised on Table 5.6 and Table 5.7. The two-dimensional Fast Fourier transform results were very consistent where it was possible to carry out the analysis. They did not show the dependence on frequency or wave shape previously observed in the time-domain analysis. The value calculated for $G_{\text{max}}$ from this method under predicted the stiffness compared with previous time-domain methods and the analytical solutions implemented. Due to its independence from transmitted frequency, however, it gave a more accurate value of sample stiffness than other methods.

5.7 Sample stiffness measurements

5.7.1 Establishing the cubic anisotropy of the sample

The simulations in this Section were completed with the aid of Mr. Philip Vautier who completed a MEng research project on wave propagation in Imperial College London from February 2012 to June 2012. Shear waves were propagated in different directions through the production sample confined at 300kPa isotropically. The wave speed was calculated using the two-dimensional fast Fourier transform methods and the density of the sample is $1.60 \times 10^3$ kg/m$^3$. Using the wave speed and the sample density the value of constrained moduli and shear moduli in different axial directions and different shear planes were calculated. The results are as follows:

\[
M_x = M_y = 1,649.89\text{MPa}
\]

\[
M_z = 1,682.41\text{MPa}
\]

\[
G_{xy} = G_{yx} = 402.93\text{MPa}
\]

\[
G_{xz} = G_{yz} = 422.27\text{MPa}
\]

\[
G_{zx} = G_{zy} = 428.08\text{MPa}
\]

The fact that $(M_x = M_y) \neq M_z$ and $(G_{xz} = G_{yz}) \neq (G_{zx} = G_{zy})$ indicated that the sample packing can be considered cubic anisotropic and this will influence the calculation of results from the
stress probes in Section 5.7.7. The value of $G_{xy}$ is 5% smaller than $G_{xz}$ and $G_{xz}$ is ~1.5% smaller than $G_{zx}$. Although these differences are small enough to be obscured by uncertainty in travel time there is a trend whereby no matter what method is used or what the confining pressure is: $(G_{xy} = G_{yz}) \neq (G_{xz} = G_{yz}) \neq (G_{zx} = G_{zy})$. Therefore the cubic anisotropy of the sample can be inferred.

5.7.2 Assessing sensitivity of response to confining pressure

It is common practice in geotechnical engineering to plot the relationship between the measured value of sample shear modulus, $G$, and the confining stress applied to the sample, $\sigma_0$. Consider, for example, McDowell & Bolton (2001) and Goddard (1990) who examined how sample shear modulus and wave speed respectively are affected by confining pressure. As already outlined in Chapter 2 Hertzian contact mechanics predicts that the sample shear modulus should be proportional to the confining pressure to the power of 1/3. While laboratory observations frequently measure sample shear modulus proportional to the confining pressure to the power of 1/2. The particle-scale imperfections were predicted to dominate the response at low confining pressures while increasing coordination number was predicted to dominate at higher confining pressures. Figure 5.58 shows different $G$ values for different confining pressures using different travel time determination techniques. The signal here was a wave propagating in the x-direction and oscillating in the y-direction. A single sine pulse was transmitted at 30kHz. While there was some scatter among the results from the different techniques a relationship between $G$ and confining pressure that was close to $G \propto \sigma_0^{1/3}$ was observed. The phase versus frequency results were seen to be far below the other methods in magnitude of shear modulus and there was too scattered to calculate a reliable best-fit slope. The magnitudes of the sample shear moduli calculated from the first derivative equal to zero and first local minimum were found to be greater than the other methods and the effective medium theory. Figure 5.58 shows that this DEM simulation can successfully achieve the predicted response of a lattice packed granular medium to stress wave propagation.

5.7.3 Bender versus extender test

As well as using the single particle motion to generate shear waves, compression waves can also be induced by moving the particle in the positive x-direction. A compressional wave, P-wave, was propagated through the production sample by carrying out an extender test on the sample. The wave was created by displacing the same transmitter particle as before in the x-
direction, which was the direction of wave propagation. The displacement took the form of a sine wave to allow comparison with the shear wave.

**Received signal**

The displacement of the receiver particle was tracked during the extender test and plotted against the displacement of the receiver particle due to the “base case” bender test on Figure 5.59. The compressional wave travelled faster than the shear wave and its first arrival was not clouded by small amplitude oscillations as happened with the shear wave first arrival. The arrival time agreed well with one predicted by the analytical equations (EMT – see Chapter 2) in Santamarina & Cascante (1996) and there was little or no noise affecting the arrival of the compressional wave. The relationship between compressional wave speed and shear wave speed is related by the following equation:

\[
\frac{V_P}{V_S} = \sqrt{\frac{2(1-\nu)}{1-2\nu}}
\]

5.5

The analytical solution for the sample Poisson’s ratio from effective medium theory, \(\nu\), was 0.029 and this gave a value of \(\frac{V_P}{V_S}\) equal to 1.44. Using the two-dimensional fast Fourier transform method the value of \(V_P\) equalled 673.72m/s and the value of \(V_S\) equalled 476.47m/s. This gave a value of \(\frac{V_P}{V_S}\) was measured as 1.41 which deviates from the predicted value by less than 2.13%. This wave speed was close to that obtained from the first zero crossing method which was 489.16m/s. This provided further evidence that the small amplitude oscillations observed before the shear wave arrival should be ignored when picking the first arrival of the shear wave. The clarity of the arrival time of the compressional wave also shows that it was correct to expend more time on researching the shear wave whose arrival time was not as clear.

**Micromechanics**

Figure 5.60 plots the relative representative shear stress and relative representative mean stress for the “base case” bender test carried out on the production sample for two time points (d) and (l) to capture the initial wave lobes formed and the reflections that resulted. For comparison Figure 5.61 plots the relative representative shear stress and relative representative mean stress for the extender test and the base case bender test for the same two time points. The central wave lobe in the extender test was best visualised using the mean stresses indicating that it was a compressional wave. The side lobes were shear wave lobes.
as shown by the relative shear stresses. It appeared that the body waves have reversed their respective lobe patterns. The bender test produced a symmetrical wave lobe visualised using relative representative shear stresses and an antisymmetric wave lobe visualised using relative representative mean stresses. Whereas, the extender test produced a symmetric wave lobe visualised using relative representative mean stresses and an antisymmetric wave lobe visualised using relative representative shear stresses. At time point (l) the compressional wave had already arrived at the receiver due to its faster speed and complex wave patterns were observed in both shear stresses and mean stresses following the initial wave lobes.

5.7.4 Plane wave propagation

Comparisons were made between plane wave propagation and point source wave propagation. A plane wave was propagated through the sample by isolating all the particles in the same plane as the transmitter and moving these particles together. The receiver was a single particle as before. The wave inputted was a shear wave propagating in the x-direction and oscillating in the y-direction and the sample used was the production sample confined at 300kPa. The two-dimensional fast Fourier transform diagrams were used to calculate a wave speed for both the point source and plane wave propagation tests. The plane wave propagated at a higher speed than the point source wave. The plane wave speed was 573.44m/s while the point source wave speed was 560.04m/s.

Received signal

The received signals are compared using the displacement of the receiver particle when a point source transmitter was used and when a plane wave transmitter was used. The amplitude of the received signal was much larger for the plane wave than for the point source wave (Figure 5.62). The point source received signal must be scaled by a factor of 25 to be observable with the plane wave received signal. The near-field effect was observed on the received signal for both wave types; however, the plane wave produced a received signal that appeared to oscillate more uniformly than the point source wave.

Micromechanics

The plane wave propagation was visualised using individual particle velocity vectors. Figure 5.63 plots the velocity vectors for individual particles that are scaled by velocity magnitude and directed using the vector components. The slice considered was a 5mm thick slice midway along the z-axis of the sample. Only the x and y components were plotted and only they
were used to calculate the magnitude of the velocity. In addition particles with velocities greater than 10mm/s were not plotted so that the wave components could be more clearly observed. A vortex pattern was observed forming in the sample as the wave propagated through the system. The effect of the boundary conditions on the wave was observed at time point (b). The plane wave arrived between time points (d) and (e). The attenuation of the received signal is observed to be much less when a plane wave is propagated as it does not need to be scaled to be observed with the transmitted wave. The plane wave is observed to propagate centrally through the sample and the boundaries are seen to affect the edges of the plane wave. At time point (c) this effect is seen to move ahead of the plane wave and is likely to be the source of the initial fluctuation observed on the received signal. The vortex motion of the particle velocities matches the earlier observations of Li & Holt (2002) for a plane wave and the earlier observations in this Chapter for a point source wave. The plane wave arrives between time point (d) and (e) and following the plane wave reflected waves can be observed on time points (e) and (f).

The surface plot on Figure 5.64 was coloured and scaled by particle displacement in the y-direction. Comparing Figure 5.64 and Figure 5.51 this confirmed that the amplitude did not decrease much after the plane wave was inputted. A clear reflection off the receiver end boundary of the sample was observed. As the amplitude remained large the small amplitude noise resulting from the wave propagation was not observable on Figure 5.64. The colour scale used on Figure 5.64 was ten times larger than the colour scale used on Figure 5.51 and the wave was clearly observable highlighting the larger amplitude wave that the plane wave transmission produced.

5.7.5 Sensitivity of system response to boundary conditions

It is important to understand the sensitivity of the system response to the boundary conditions. This complements the analysis of sensitivity to sample size carried out by Marketos & O’Sullivan (2013). Different boundary conditions were considered including rigid wall boundaries and periodic cell boundaries (Figure 5.65). The sample was compressed to an isotropic stress state of 100kPa using rigid wall elements. To carry out a bender element simulation with rigid walls the stage where the rigid wall boundaries are replaced by flexible boundaries was simply not carried out. The numerical bender element algorithm was run with the sample contained by rigid walls on all six sides. PFC3D modelled the contact between balls and walls using a similar methodology to the contact
between two balls; however, the “wall ball” was assigned an infinite radius and infinite Young’s modulus. This resulted in normal contact stiffness between ball and wall that was \(2\sqrt{2}\) times stiffer than the normal contact stiffness between identical balls. The friction coefficient of the walls was maintained at zero and therefore there was no tangential contact stiffness between ball and wall elements in this implementation which meant that the balls were free to slide along the walls.

As mentioned above the interaction contact forces developed between ball-wall contacts are different from those developed between ball-ball contacts and this is explored in a small scale test. The particles used are similar in all respects to the ones used in the large scale simulations except that they have a unit radius rather than 2.54mm. Four cases are examined in which the moving balls have a velocity of 5mm/s and are placed just in contact with the stationary elements.

**Case 1:** Moving ball impacts a stationary ball for which an applied force is calculated based on the negative of the out of balance force that the ball experiences due to the impact. The out of balance force is the resultant force of all the forces acting on a ball. In this case it is equal to the contact force.

**Case 2:** Moving ball impacts a stationary ball that is fixed in space.

**Case 3:** Moving ball impacts a stationary ball that experiences a stress field of 100kPa (i.e. the “base case” confining pressure in the above simulations) when displaced from its original position. The stress field is removed and the ball motion is stopped when it is returned to its original position.

**Case 4:** Moving ball impacts a stationary wall face element that is fixed in space.

These four cases are illustrated in Figure 5.66 and their results are in Figure 5.67. The plot is of displacement in the z-direction versus time. As can be seen the ball-wall contact behaves differently to all ball-ball contacts and all ball-ball contacts behave similarly regardless of the properties of the stationary ball. Closer inspection of Figure 5.67 shows that the slopes, i.e. velocities, of the particles in all simulations are the same implying that the difference in displacement is due to the ball-wall contact reaching a repelling contact force sooner than the ball-ball contact. However, all contacts reach the same repelling contact force in the end. This implies that the reflections generated by these different boundary conditions may be
very similar and that there is no difference in impedance mismatch (see Chapter 4) when comparing ball-ball and ball-wall contacts as boundaries.

Periodic boundary conditions map any particle volume that is outside the predetermined periodic space to the other side of the sample. While the particle centroid is inside the periodic space it is considered a “master” particle and the ball that is remapped to the opposite side is considered a “slave” particle. Should the “master” particle move further outside the periodic space so that its centroid is outside the periodic space then the “master” particle becomes the “slave” particle and the previous “slave” particle becomes the “master” particle. Figure 5.68 illustrates the periodic boundary conditions implemented on all sides of a two-dimensional sample. As the wave could propagate in the reverse direction the periodic boundary conditions were only applied to the faces that were perpendicular to the y- and z-axes and rigid wall elements were maintained on the two faces that were perpendicular to the x-axis. The rigid walls were removed from the sides when the sample was compressed to 100kPa isotropically. The periodic boundary conditions were added such that the overlap between the original ball element and the remapped ball element produced forces that matched those present between the ball and wall elements. This maintained the compression at 100kPa. There was some slight fluctuation due to the change in boundary conditions; however, this was quickly reduced by the viscous damping dashpot model. When a wave was transmitted in this sample it was visualised as a wave transmitted by many benders acting in parallel.

**Received signal**

The received signals are plotted on Figure 5.69 for the three different boundary conditions implemented here. The speed of the shear waves propagating through the flexible bounded sample, the wall bounded sample and the periodic bounded sample were measured using the two-dimensional fast Fourier transform method. The values were 476.47m/s, 477.09m/s and 475.88m/s respectively which were all very close in value. The shear wave speed, measured using the point of first zero crossing, was seen to be unaffected by the boundary conditions; however the amplitude of the signals was affected. The amplitude was related to the geometric spreading of the wave so it was observed that rigid wall boundaries caused more geometric spreading and thus a larger reduction in amplitude compared to periodic boundary conditions as was seen when comparing Figure 5.70 and Figure 5.71. The flexible boundary conditions acted like an intermediary of the rigid and periodic boundary conditions.
Interestingly the arrival of the shear wave in all boundary condition cases was clouded by a small amplitude half-oscillation. This had being observed in the previous analysis of the flexible bounded sample and it was not clear how big a part the boundary condition played in this. What was common to all boundary conditions considered here was a defined end to the sample in the x-direction. Either a rigid wall or applied force boundary was used making the system finite in the x-direction. The impact of the shear wave on this boundary must have caused the oscillations observed in Figure 5.69 before the arrival of the true shear wave.

**Micromechanics**

It is important to understand the sensitivity of the system response to the boundary conditions. Figure 5.70 plots the relative representative shear stresses and relative representative mean stresses for the wall bounded sample for time points (d) and (l) so that they could be compared with the base case flexible bounded sample (Figure 5.60). The initial shear wave lobes were seen to develop in much the same way as previously found with the flexible boundary. The reflections were also seen to progress in much the same way although their reflected directions seemed to be more directed towards the opposite side of the sample than the centre. As expected based on the small-scale single contact test in Figure 5.67 there is little difference in the reflections generated by the wall bounded sample and the flexible bounded sample. Figure 5.71 repeats the same plots but instead of the wall bounded sample the periodic bounded sample is compared with the flexible bounded one. Again there seems to be no difference in the initial wave lobes that were produced as visualised by both the relative mean stresses and relative shear stresses. The reflected shear stress waves were more directed towards the receiver than the waves in the flexible bounded sample.

**5.7.6 Absorbing boundary conditions**

As mentioned in Chapter 2 previous finite difference work on wave propagation used an absorbing or “quiet” boundary as part of a parametric study, e.g. Rio (2006). Absorbing boundaries were found in previous work to remove some of the complications that cloud the arrival of the shear wave. The initial fluctuation highlighted in Figure 5.25 were removed or greatly reduced in the finite difference work with absorbing boundaries. The finite difference code used was FLAC3D and this code contains a “quiet” boundary condition. There is no such boundary condition in DEM so a small-scale test was carried out first to develop the absorbing DEM boundary.
Small-scale test to develop absorbing boundary condition

FLAC3D uses viscous damping dashpots to create boundaries that absorb impacts and do not produce reflections. The viscous damping dashpots were used as a base to which develop absorbing boundaries in DEM. Initially a single contact system was used to examine the effect of different critical viscous damping dashpot ratios, $\beta$. This test is outlined in Figure 5.72 and consisted of a single three-dimensional particle placed in contact with a horizontal wall face element. Gravity at 10m/s was turned on and the fluctuations in contact force with time were examined for different values of $\beta$. The horizontal line is the static solution to the contact force that would be generated by gravitational loading and the value is 191.34μN. The results are illustrated on Figure 5.73 and when $\beta$ is 0.01 the contact force oscillates repeatedly around this value. This decreases as $\beta$ increases. When $\beta = 1.5$ the system appears to be critically damped, however a $\beta$ of 10 seems to overly affect the system response. It must be noted that $\beta$ will affect the contact stiffness at that contact and its influence on contact stiffness is illustrated on Figure 5.74. Once the value of $\beta$ was greater than approximately 1 it seemed to greatly affect the value of contact stiffness. The new contact stiffness is calculated by multiplying the value of contact stiffness calculated by the Hertz-Mindlin contact model and the lambda factor calculated using the value of $\beta$.

Received signals

The absorbing boundary was created by assigning a $\beta$ value of 1.5 to any contacts that included a membrane particle. A plane wave was inputted as this wave is less complex than the point source waves created by the bender element and therefore it was easier to analyse the effectiveness of the boundaries using this wave. The plane wave received signal for the production sample with a standard, reflective flexible boundary and the received signal for the production sample with an absorbing flexible boundary are plotted in Figure 5.75. In both cases the initial fluctuation of the received signal can be observed. The absorbing boundary that was created in the DEM sample was not as effective as the FLAC3D “quiet” boundary at removing this fluctuation. A $\beta$ value of 3.0 was also used but the fluctuation remained with this value as well.

Micromechanics

Figure 5.76 uses the same criteria as Figure 5.63 to plot the plane wave propagating through the sample with absorbing flexible boundaries. At time point (c) it appears that the boundaries are affecting the wave propagation similarly to the previous figure. Again, the
plane wave arrives between time points (d) and (e), however, the reflected waves are not observed on time points (e) and (f).

**Surface plots**

Three dimensional surface plots were created using a column of particles connecting the transmitter to the receiver and are illustrated on Figure 5.64 and Figure 5.77. The wave can be observed to travel through time and space in both figures. The fluctuations near the transmitted end of the sample that are observed in Figure 5.64 are damped out by the absorbing boundaries in Figure 5.77. A reflected wave is observed in both figures at the receiver end of the sample but in Figure 5.77 it is noticed that the reflected wave appears reduced compared to Figure 5.64. However; the absorbing boundaries have not absorbed as much of the reflections as would be expected and this is linked to the initial fluctuation.

**Wall bounded sample**

The work outlined above was repeated for the production sample confined at 300kPa using wall boundaries. The reason for this is that the wall bounded sample is less complicated than the flexible boundaries. In this simulation a $\beta$ value of 1.5 is applied to any contacts that involve a wall element. The received signal for a sample with standard wall boundaries and the received signal for a sample with absorbing wall boundaries are plotted against time in Figure 5.78. Again, the fluctuation is not removed in the simulation with absorbing boundaries. This simulation was repeated using a $\beta$ value of 3.0 but this did not remove the fluctuations. It appears that more research is needed to successfully implement an absorbing boundary in DEM software that could be used for wave propagation simulations in order to simplify the received signals.

### 5.7.7 Sensitivity of system to different interparticle contact models

The contact models considered in this research were Hertz-Mindlin (HM), Hertz-Mindlin-Deresiewicz (HMD) and Cavarretta-Mindlin (CM). The implementation and verification of these models has been explained in detail in Chapter 3 and a brief summary is presented here. The HM model is the default interparticle contact model in most DEM codes and is a non-linear elastic contact model that includes energy loss due to frictional sliding. The HMD model implements the theory of Mindlin & Deresiewicz in the tangential direction that includes energy loss due to micro-slip before full sliding occurs. This is more accurate based on the theory of two ideal spheres in contact. The CM model assumes that the interparticle
contact stiffness in the normal direction is reduced at small overlaps due to the effect of particle imperfections and asperities.

**Received signals**

Figure 5.79 confirmed the findings above by plotting the HM, HMD and CM received signals on the same time axis for three samples confined at 100kPa. If the first initial small amplitude oscillations were ignored in line with previous observations for the production sample then the arrival time for HM is seen to be before HMD which was before CM. The amplitudes and frequencies of the received signals vary considerably.

**Micromechanics**

The Cavarretta-Mindlin (CM) model was compared with the Hertz-Mindlin (HM) model for two time points (d) and (l) using relative representative particle shear stress and relative representative particle mean stress on Figure 5.80, which can be compared with Figure 5.60. The initial lobes produced by the disturbance were less defined for the CM contact model. Consequently the reflections from the boundaries are much harder to perceive due to their lower amplitude. The relative shear stresses did show a faint lobe propagating through the sample. It had progressed to three-quarters of the way through the sample when the HM shear wave had arrived at time point (l) indicating the slower wave speed in a sample with this model implemented.

The Hertz-Mindln-Deresiewicz (HMD) model was compared with the Hertz-Mindlin (HM) model for time points (d) and (l) using the same parameters as above on Figure 5.81, which can be compared with Figure 5.60. There did not seem to be any observable changes in the wave lobes produced by the same initial disturbance when the HMD model was used. In examining the relative representative shear stresses for time point (l) the HMD shear wave lobe appeared to be lagging behind the HM shear wave lobe. This indicates that the shear wave speed was lower in the HMD sample than in the HM sample.

**Sample stiffness versus confining pressure**

The effect of different interparticle contact models on the wave propagation simulation was examined using the production sample. The normal force-displacement law and tangential force-displacement law were varied. The contact model will affect the relationship between sample shear modulus, $G$, and confining pressure, $\sigma_0$, as proven empirically by Cascante & Santamarina (1996) and numerically by Yimsiri & Soga (2000). As the Cavarretta-Mindlin
model takes account of asperities on the particle surface it tests the first of Goddard’s hypotheses for why the relationship between $G$ and $\sigma_0$ is not the same between DEM and equivalent experimental studies. As the sample packing is face-centred cubic it would be impossible for new contacts to form so only one hypothesis will be tested here.

Figure 5.82 plots $G$ against $\sigma_0$ for three samples with three different contact models implemented at six different confining pressures (100kPa, 200kPa, 300kPa, 500kPa, 750kPa and 1MPa). This range of pressures was chosen to provide statistically meaningful results for trying to characterise the relationship between $G$ and $\sigma_0$. The travel time determination technique used here was the two-dimensional fast Fourier transform. It was observed that the sample with the HM contact model showed the highest values of $G$ and $G \propto \sigma_0^{0.30}$. The HMD model showed the next highest values of $G$ and $G \propto \sigma_0^{0.32}$ while the CM model showed the lowest values of $G$ and $G \propto \sigma_0^{0.40}$. From these results it was concluded that changing either the normal stiffness or tangential stiffness will have an effect on the shear wave speed through the sample and thus the shear stiffness of the sample. It was interesting that a change even in the tangential stiffness will produce different $G$ values. Changing the normal stiffness produced a greater change than changing the tangential stiffness. The variation in the trend between $G$ and confining pressure also provided insight into the effect of a contact model on the system as a whole. The HM and HMD models exhibited similar trends between sample shear modulus and confining pressure at 0.30 and 0.32 respectively and both were within ±10% of the predicted 1/3 for a sample with a Hertz-Mindlin contact model. This showed that changes to the tangential contact model will affect the value of $G$ obtained but not the subsequent relationship between $G$ and the confining pressure. The CM model exhibited a trend of 0.40 between sample shear modulus and confining pressure. This showed that a change in the normal contact model will affect both the obtained value for $G$ and the relationship between $G$ and the confining pressure.

The CM model appears to have two behaviour regimes, one relationship held true at the lower confining pressures and another held true at the higher confining pressures. This is illustrated on Figure 5.83 where two slopes are presented for the CM model results. The slope calculated when the result for confining pressures from 100kPa to 300kPa was 0.55 and the slope calculated when the result for confining pressures from 500kPa to 1MPa was 0.33. This illustrates the change in contact model behaviour as the contact stiffness increase when the simulated asperities are crushed. When the asperities are crushed the contact model behaves as a Hertz-Mindlin contact model producing the relationship between elastic moduli
and confining pressure of 1/3 as found by Yimsiri & Soga (2000) in their analytical model and in experimental work summarised in Goddard (1990).

**Stress probe results**

The stress probes were carried out using the servo-controlled wall algorithm developed for earlier isotropic compression of the sample. The tolerance for the final stress that needed to be reached was lowered for the stress probe simulation by a factor of ten to 0.0025 and the stress change in a chosen principal direction was 10kPa. Lings (2013) presented the relationships between elastic parameters for cubic anisotropic materials such as the face-centred cubically packed sample. The minimum number of elastic parameters required to calculate all other elastic parameters is three, Young’s modulus in the z-direction (\(E_z\)), Poisson’s ratio in the zx-plane (\(\nu_{zx}\)) or zy-plane (\(\nu_{zy}\)) and Young’s modulus in the x- or y-directions (\(E_x\) or \(E_y\) as they are assumed to have equal values due to the packing). The remaining values of shear moduli (\(G_{ij}\)), Poisson’s ratios and constrained moduli (\(M_i\)) were calculated from these three parameters using Equations 5.6 to 5.11 and using the following conventions for a cubic anisotropic material:

<table>
<thead>
<tr>
<th>(E_x = E_y)</th>
<th>(G_{zx} = G_{xy} = G_{yz})</th>
<th>(v_{zx} = v_{zy})</th>
<th>(M_x = M_y)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(G_{xy} = G_{yx})</td>
<td>(v_{xy} = v_{xy})</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[
G_{zx} = \frac{E_z E_x}{4E_z - 2E_x (1 - \nu_{zx})} \quad 5.6
\]

\[
G_{xy} = \frac{E_z}{2(1 + \nu_{zx})} \quad 5.7
\]

\[
v_{zx} = \frac{\nu_{zx} E_x}{E_z} \quad 5.8
\]

\[
v_{xy} = \frac{E_z - E_x (1 - \nu_{zx})}{E_z} \quad 5.9
\]
\[
M_z = \frac{(1 - \nu_{zx})E_z}{(1 + \nu_{zx})(1 - 2\nu_{zx})}
\]
\[5.10\]

\[
M_x = \frac{(E_z - \nu_{zx}^2)E_z}{(1 + \nu_{zx})(1 - \nu_{zx})[2E_z - E_x(1 - \nu_{zx})]}
\]
\[5.11\]

Stress probes were carried out in the z-direction to obtain a value of \(G_{xy}\) which could be compared with wave propagation results.

Two measurement regions were considered, namely the entire sample and the measurement sphere which was centrally located in the sample and had a diameter that is 80% of the length of the cubical cell. The sample stress tensor was calculated by an averaging procedure using the representative particle stress tensors which is outlined in the PFC3D manual and in Cundall (1988). The sample strain tensor was calculated using the best fit method which is outlined in O'Sullivan (2011) and in Marketos & Bolton (2010). By plotting the particles’ displacements against positions a best fit line was found using least squares regression of which the gradient represents the sample strain. The stress and strain tensors calculated from these stress probes were principal stress and principal strain. Probes were carried out on the Hertz-Mindlin sample at isotropic confining pressures of 100kPa, 500kPa and 1MPa.

The resulting \(G_{xy}\) values from stress probe tests were plotted against the results from wave propagation tests that were used in earlier comparisons between samples with different contact models on Figure 5.84. In general the results calculated from the measurement sphere were larger than the results calculated from the whole sample and the alpha value was higher. There was good agreement between the two methods of interpreting stress probe results and the wave propagation tests. The results from the stress probes were always within 10% of the wave propagation test results calculated using the two-dimensional fast Fourier transform method.

### 5.8 Conclusions

The lobes that were produced by a point-source were measured using the particle rotational velocities and translational velocities.

- The lobes that were produced to visualise the \(G_{xy}\) lobe and the \(M_x\) lobes matched the shear and compressional wave lobes found in the experimental work of Lee & Santamarina (2005).
The numerical results revealed that the more than one type of shear wave and one type of compressional wave were produced. Shear wave lobes were produced that propagated in all shear planes and compressional wave lobes were produced that propagated in each of the principal directions.

This research also found that a three-dimensional wave was produced by the point-source.

Wave were visualised propagating through the sample using particle-scale measurements.

The interpretation methods used are as follows:

- particle velocity vectors,
- representative particle shear stresses,
- representative particle mean stresses,
- particle y-component velocities,
- particle x-component velocities,
- particle rotational velocities about the z-axis.

The propagating shear waves were found to be easily visualised by the particle velocity vectors, the representative particle shear stresses, the particle y-component velocities and the particle rotational velocities about the z-axis.

The propagating compressional waves were found to be easily visualised by the particle velocity vectors, the representative particle mean stresses and the particle x-component velocities.

Reflected waves were observed to be propagating from the boundaries and a wave that seemed to travel faster along the boundaries was observed to arrive at the receiver before the true shear wave arrival.

The elevation view showed that the shear wave remained three-dimensional as it propagated through the sample.

Analytical models were found to accurately capture the stiffness of the sample, the wave speed and the occurrence of the near-field effect.

Effective medium theory (EMT) was found to overpredict the magnitude of both the Young’s modulus and shear modulus in comparison to the wave propagation and stress probe data. It did not account for the cubic anisotropy of the sample that
resulted in slight variations in magnitude when different directions and different shear planes were considered.

- The principal of virtual displacement (PVD) was found to predict both the magnitude of the elastic moduli and the cubic anisotropy of the sample using a single particle and the twelve contacts around it.
- Dispersion relation theory (DRT) predicted the magnitude of the elastic moduli of the sample, the cubic anisotropy of the sample and gave a theoretical background for frequency filtering that will be discussed more in Chapter 6.
- The Sanchez-Salinero analytical solution accurately predicted the occurrence of a near-field effect and the time, relative to the true shear wave arrival, at which the effect would occur.

The effect of different transmitting frequencies and waveshapes on the received signal was examined and a number of findings can be noted.

- The amplitude of the received signals in the time domain decreased as the transmitting frequency increased. This was confirmed by examining plots in the frequency domain.
- The amplitude of the received signals in the time domain varied as the transmitted waveshape varied. The sine pulse with 270° phase angle produced a received signal with the largest amplitude, followed by the sine pulse with no phase angle, the triangular wave and the square wave. This was confirmed by examining the amplitudes of the frequencies in the time domain.
- The range of frequencies contained in the received signal was found to increase with increasing frequency.
- The range of frequencies contained in the received signal was found to vary with changing waveshape. Similar to the increasing frequency of the sine wave, if the frequency range of the transmitted signal increased due to waveshape then the frequency of the received signal also increased.
- Frequency filtering was observed when high frequency signals were transmitted through the prototype regularly packed sample.

Different travel time determination techniques were critically assessed during the course of the research on the regularly packed sample. A number of techniques were examined in both time and frequency domains.
• All travel time determination methods with the exception of the two-dimensional fast Fourier transform method produced results that were dependent on the frequency of the transmitted wave. As frequency of the sine wave increased the wave speed measured increased.

• All travel time determination methods with the exception of the two-dimensional fast Fourier transform method produced results that were transmitter waveshape dependent. The single sine pulse was consistently found to be the fastest wave followed by the triangular wave, the square wave and the sine pulse with a 270° phase angle.

• The different travel time determination methods were used to calculate sample stiffness and the calculated sample stiffness at different confining pressures were compared. The values calculated using first local minimum equal to zero and first derivative equal to zero consistently produced over estimates of sample stiffness while the phase versus frequency plots consistently produced under estimates of sample stiffness. Based on the investigations the two-dimensional fast Fourier transform method was deemed the optimal travel time determination technique while recognising that it could not be used for standard bender element test set-ups as the spatial variation of the wave needed to be known.

A number of parametric studies were carried out on the system varying both macro-scale and micro-scale parameters.

• The difference between a propagating shear wave and compressional wave was examined in terms of their received signals and the micromechanics of the wave propagation. The compressional wave propagated faster than the shear wave and faster than the near-field effect. The first deviation of the received compressional wave signal from zero was the true compressional wave arrival. The relationship between compressional wave speed and shear wave speed was a function of the sample Poisson’s ratio.

• The differences between plane wave propagation and point source wave propagation was examined. The received plane wave had much higher amplitude than the received point source wave due to the increased kinetic energy that was inputted to the sample. A vortex like pattern was observed in the micromechanical analysis of
the plane wave that was similar to the patterns observed on Chapter 4. This was not observed for the point source wave in the three-dimensional sample.

- The effect of boundary conditions on the sample was examined. The boundary conditions considered were the flexible boundaries, the rigid wall boundaries and the periodic boundaries. It was found that the shear wave speed was not influenced greatly by the boundary conditions but that the reflections produced were influenced by them. The micromechanical analysis illustrated the effect of the boundary conditions on the propagating wave in terms of wave amplitude and reflections.

- The effect of the different interparticle contact models was examined. Three interparticle contact models were considered, namely the default Hertz-Mindlin (HM) model, the rough surface Cavarretta-Mindlin (CM) model and the frictional energy dissipating Hertz-Mindlin-Deresiewicz (HMD) model. The shear wave velocity was found to be particularly sensitive to the interparticle contact model in the normal direction which was varied when the CM model was considered. The shear wave velocity was found to be sensitive to the interparticle contact model in the tangential direction which was varied when the HMD model was considered. When the 2D FFT was used the exponent relationship between shear modulus and confining pressure was found to be a function of the normal contact model but was not much affected by the tangential contact model. The exponent relationship between shear modulus and confining pressure appeared to have two regimes depending on whether the low confining pressures or high confining pressures were considered. At low confining pressure the exponent relationship was approximately 1/2 while at the higher confining pressures it was closer to 1/3.

There was good agreement between the results calculated from dynamic wave propagation tests and stress probe tests. The sample considered was the base case sample with the Hertz-Mindlin contact model and the results were always within 10% of the wave propagation test results.
5.9 Figures

Figure 5.1: Layout of production sample with particles coloured by applied force.

Figure 5.2: Comparison between applied stresses to the flexible bounded sample and the internal measurement region stresses.
Figure 5.3: Layout of bender element test with single particle transmitter and single particle receiver.

Figure 5.4: A received signal for (a) the face-centred cubically packed DEM simulation and (b) the randomly packed laboratory sample (University of Bristol). Both samples are of equal size and contain particles of similar size and material properties. DEM: $\sigma_0 = 100$kPa, $f_{trans} = 30$kHz, $R_d = 5.63$ and $\lambda/d_{10} = 6.40$. 
Figure 5.5: Measures of plasticity (a) global average coordination number, (b) sliding contacts, occurring in the sample during the bender element test. $\sigma_0 = 100\text{kPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 5.63$ and $\lambda/d_{50} = 6.40$.

Figure 5.6: The waveforms that are expected to form during a bender element test.
Figure 5.7: Visualisation of $G_{xy}$ shear wave lobe by plotting particles with rotational velocities about the z-axis above 0.05rad/s at a time of $9.172 \times 10^{-5}$s. $\sigma_0 = 100$ kPa, $f_{trans} = 30$ kHz, $R_d = 5.63$ and $\lambda/d_{50} = 6.40$.

Figure 5.8: Visualisation of $M_{xx}$ compressional wave lobes by plotting particles with velocities in the x-direction above 0.1 mm/s at a time of $9.172 \times 10^{-5}$s. $\sigma_0 = 100$ kPa, $f_{trans} = 30$ kHz, $R_d = 5.63$ and $\lambda/d_{50} = 6.40$. 
Figure 5.9: Visualisation of $G_{xz}$ shear wave lobes by plotting particles with rotational velocities about the x-axis above 0.04 rad/s at a time of 9.172 x $10^{-5}$s. $\sigma_0 = 100$ kPa, $f_{trans} = 30$ kHz, $R_d = 5.63$ and $\lambda/d_{50} = 6.40$.

Figure 5.10: Visualisation of $G_{yz}$ shear wave lobes by plotting particles with rotational velocities about the y-axis above 0.04 rad/s at a time of 9.172 x $10^{-5}$s. $\sigma_0 = 100$ kPa, $f_{trans} = 30$ kHz, $R_d = 5.63$ and $\lambda/d_{50} = 6.40$. 
Figure 5.11: Visualisation of $M_{zz}$ compressional wave lobe by plotting particles with velocities in the z-direction above 0.1mm/s at a time of $9.172 \times 10^{-5}$s. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_{10} = 6.40$.

Figure 5.12: Visualisation of $M_{yy}$ compressional wave lobes by plotting particles with velocities in the y-direction above 0.1mm/s at a time of $9.172 \times 10^{-5}$s. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_{10} = 6.40$. 
Figure 5.13: Individual particle velocity vectors (x & y components) scaled by magnitude considering x and y components of velocity only. View is a plan view of a 5mm thick cross-section through the sample. Only particle velocities less than or equal to 0.5mm/s magnitude are plotted to prevent larger velocities from "clouding" the system response. Time points (a) to (f) are shown in this plot. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_0 = 6.40$.

Figure 5.14: Individual particle velocity vectors (x & y components) scaled by magnitude considering x and y components of velocity only. Time points (g) to (l) are shown in this plot. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_0 = 6.40$. 
Figure 5.15: Relative representative particle shear stresses (average of $\sigma_{xy}$ and $\sigma_{yx}$) illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along z-axis. Time points (a) to (f) are shown in this plot. $\sigma_0 = 100\text{kPa}$, $f_{trans} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_{50} = 6.40$.

Figure 5.16: Relative representative particle shear stresses (average of $\sigma_{xy}$ and $\sigma_{yx}$) illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along z-axis. $\sigma_0 = 100\text{kPa}$, $f_{trans} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_{50} = 6.40$. 
Figure 5.17: Relative representative particle mean stresses, average of $\sigma_{xx}$ and $\sigma_{yy}$ and $\sigma_{zz}$, illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along $z$-axis. Time points (a) to (f) are shown in this plot. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_{10} = 6.40$.

Figure 5.18: Relative representative particle mean stresses, average of $\sigma_{xx}$ and $\sigma_{yy}$ and $\sigma_{zz}$, illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along $z$-axis. Time points (g) to (l) are shown in this plot. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_{10} = 6.40$. 

\[\sigma_0 = 100\text{kPa}, \quad f_{\text{trans}} = 30\text{kHz}, \quad R_d = 5.63 \quad \text{and} \quad \lambda/d_{10} = 6.40.\]
Figure 5.19: Relative particle y-velocity component illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along z-axis. Time points (a) to (f) are shown in this plot. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_0 = 6.40$.

Figure 5.20: Relative particle y-velocity component illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along z-axis. Time points (g) to (l) are shown in this plot. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_0 = 6.40$. 
Figure 5.21: Relative particle x-velocity component illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along z-axis. Time points (a) to (f) are shown in this plot. $\sigma_0 = 100\text{kPa}, f_{trans} = 30\text{kHz}, R_d = 5.63$ and $\lambda/d_{dp} = 6.40$.

Figure 5.22: Relative particle x-velocity component illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along z-axis. Time points (g) to (l) are shown in this plot. $\sigma_0 = 100\text{kPa}, f_{trans} = 30\text{kHz}, R_d = 5.63$ and $\lambda/d_{dp} = 6.40$. 
Figure 5.23: Relative particle rotations about the z-axis illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along z-axis. Time points (a) to (f) are shown in this plot. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_0 = 6.40$.

Figure 5.24: Relative particle rotations about the z-axis illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along z-axis. Time points (g) to (l) are shown in this plot. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_0 = 6.40$. 
Figure 5.25: Time point \((j)\) from Figure 5.24 at a lower colour scale to illustrate movement of receiver before true shear wave arrival. \(\sigma_0 = 100\text{kPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 5.63\) and \(\lambda/d_{30} = 6.40.\)
Figure 5.26: Relative particle rotations about the z-axis illustrating wave propagation through the sample (elevation view). The cross-section through the packing is at mid-way along y-axis. Time points (a) to (f) are shown in this plot. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_{50} = 6.40$.

Figure 5.27: Relative particle rotations about the z-axis illustrating wave propagation through the sample (elevation view). The cross-section through the packing is at mid-way along y-axis. Time points (g) to (l) are shown in this plot. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_{50} = 6.40$. 
Figure 5.28: Calculated values of Young's modulus in the x-direction ($E_x$), in the y-direction ($E_y$) and in the z-direction ($E_z$) for different confining pressures using different analytical methods. EMT - effective medium theory, PVD - principle of virtual displacement and DRT - dispersion relation theory.

Figure 5.29: Calculated values of shear modulus in the xy-plane ($G_{xy}$), yz-plane ($G_{yz}$) and zx-plane ($G_{zx}$) for different confining pressures using different analytical methods. EMT - effective medium theory, PVD - principle of virtual displacement and DRT - dispersion relation theory.
Figure 5.30: Analytical dispersion relation for a compressional wave (black) and shear wave (blue) propagating through the production sample. The peak reached on the angular velocity axis indicates frequency filtering and the "Brillouin region" which represents the waves that are physically permissible is from the origin to the peak.

Figure 5.31: A recorded signal from a numerical bender element test compared with the result from the Sanchez-Salinero equations. The Sanchez-Salinero solution is scaled by 1x10^7 so that it can be observable with the recorded signal. EMT arrival time is indicated by a vertical line. Recorded signal: $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_{50} = 6.40$. 
Figure 5.32: Two time-domain travel time determination methods. Peak-peak is from the peak on the transmitted signal to the first peak on the received signal. First arrival is from the start of the transmitted signal to the point of first zero-crossing on the received signal. Received signal: \( \sigma_0 = 100 \text{kPa}, f_{\text{trans}} = 30 \text{kHz}, R_d = 5.63 \) and \( \lambda/d_{50} = 6.40 \).

Figure 5.33: The displacement of the receiver particle (x- and y-components) for a bender element test carried out on the production sample. \( \sigma_0 = 100 \text{kPa}, f_{\text{trans}} = 30 \text{kHz}, R_d = 5.63 \) and \( \lambda/d_{50} = 6.40 \).
Figure 5.34: Comparison of transmitted signals (dashed) and received signals (solid) transmitted with a single period sine pulse at different frequencies in the time domain (a) 7kHz ($\sigma_0 = 100\text{kPa}$, $R_d = 1.31$ and $\lambda/d_{50} = 27.4$), (b) 15kHz ($\sigma_0 = 100\text{kPa}$, $R_d = 2.81$ and $\lambda/d_{50} = 12.8$), (c) 20kHz ($\sigma_0 = 100\text{kPa}$, $R_d = 3.75$ and $\lambda/d_{50} = 9.60$), (d) 30kHz ($\sigma_0 = 100\text{kPa}$, $R_d = 5.63$ and $\lambda/d_{50} = 6.40$).

Figure 5.35: Comparison of transmitted signals (dashed) and received signals (solid) transmitted with different waveshapes in the time domain (a) single sine pulse, (b) single triangular pulse, (c) single sine pulse with a 270° phase angle, (d) single square pulse. $\sigma_0 = 100\text{kPa}$, $f_{trans} = 20\text{kHz}$, $R_d = 3.75$ and $\lambda/d_{50} = 9.60$. 
Figure 5.36: Location of characteristic arrival points on a typical numerical received signal. $\sigma_0 = 100$ kPa, $f_{trans} = 30$ kHz, $R_d = 5.63$ and $\lambda/d_{so} = 6.40$. 

\[ \text{Normalized Displacement} \] 

\[ \text{Time - [s]} \times 10^3 \]
Figure 5.37: Variation of sample shear modulus with frequency average over the time-domain travel time determination methods. Values are compared with frequency dependence of shear wave speed observed in Leong et al. (2009).

Figure 5.38: Cross-correlation function, received signal and transmitted signal plotted on normalised amplitude versus time plot. Red arrow indicates the peak on the cross-correlation function that corresponds with travel time. \( \sigma_0 = 100 \text{kPa}, f_{\text{trans}} = 30 \text{kHz}, R_d = 5.63 \) and \( \lambda/d_{\text{so}} = 6.40 \).
Figure 5.39: Comparison of normalised transmitted signals (dashed) and normalised received signals (solid) transmitted with a single period sine pulse at different frequencies in the frequency domain (a) 7kHz ($\sigma_0 = 100$ kPa, $R_d = 1.31$ and $\lambda/d_0 = 27.4$), (b) 15kHz ($\sigma_0 = 100$ kPa, $R_d = 2.81$ and $\lambda/d_0 = 12.8$), (c) 20kHz ($\sigma_0 = 100$ kPa, $R_d = 3.75$ and $\lambda/d_0 = 9.60$), (d) 30kHz ($\sigma_0 = 100$ kPa, $R_d = 5.63$ and $\lambda/d_0 = 6.40$).
Figure 5.40: Comparison of normalised transmitted signals (dashed) and normalised received signals (solid) transmitted with different waveshapes in the frequency domain (a) single sine pulse, (b) single triangular pulse, (c) single sine pulse with a 270° phase angle, (d) single square pulse. $\sigma_0 = 100\,\text{kPa}$, $f_{\text{trans}} = 20\,\text{kHz}$, $R_d = 3.75$ and $\lambda/d_{50} = 9.60$.

Figure 5.41: Comparison of transmitted signals (dashed) and received signals (solid) transmitted with a single period sine pulse at different frequencies in the frequency domain (a) 7kHz ($\sigma_0 = 100\,\text{kPa}$, $R_d = 1.31$ and $\lambda/d_{50} = 27.4$), (b) 15kHz ($\sigma_0 = 100\,\text{kPa}$, $R_d = 2.81$ and $\lambda/d_{50} = 12.8$), (c) 20kHz ($\sigma_0 = 100\,\text{kPa}$, $R_d = 3.75$ and $\lambda/d_{50} = 9.60$), (d) 30kHz ($\sigma_0 = 100\,\text{kPa}$, $R_d = 5.63$ and $\lambda/d_{50} = 6.40$).
Figure 5.42: Comparison of transmitted signals (dashed) and received signals (solid) transmitted with different waveshapes in the frequency domain (a) single sine pulse, (b) single triangular pulse, (c) single sine pulse with a 270° phase angle, (d) single square pulse. $\sigma_0 = 100\text{kPa}$, $f_{trans} = 20\text{kHz}$, $R_d = 3.75$ and $\lambda/d_50 = 9.60$.

Figure 5.43: The effect of different transmitted frequencies on amplitude in both the time domain (top) and frequency domain (bottom). The following frequencies are used: 7kHz ($\sigma_0 = 100\text{kPa}$, $R_d = 1.31$ and $\lambda/d_50 = 27.4$), 12.621kHz ($\sigma_0 = 100\text{kPa}$, $R_d = 2.37$ and $\lambda/d_50 = 15.21$), 15kHz ($\sigma_0 = 100\text{kPa}$, $R_d = 2.81$ and $\lambda/d_50 = 12.8$), 20kHz ($\sigma_0 = 100\text{kPa}$, $R_d = 3.75$ and $\lambda/d_50 = 9.60$), 30kHz ($\sigma_0 = 100\text{kPa}$, $R_d = 5.63$ and $\lambda/d_50 = 6.40$).
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Figure 5.45: Comparison of transmitted signals (dashed) and received signals (solid) transmitted with a single period sine pulse at different signal lengths in the time domain - 7kHz (\( \sigma_0 = 100\text{kPa}, R_d = 1.31 \) and \( \lambda/d_{50} = 27.4 \)).
Figure 5.46: Comparison of transmitted signals (dashed) and received signals (solid) transmitted with a single period sine pulse at different signal lengths in the frequency domain - 7kHz ($\sigma_0 = 100$kPa, $R_d = 1.31$ and $\lambda/d_{50} = 27.4$).

Figure 5.47: Comparison of normalised transmitted signals (dashed) and normalised received signals (solid) transmitted with different frequencies in the frequency domain (top) 400kHz ($\sigma_0 = 100$kPa, $R_d = 7.73$ and $\lambda/d_{50} = 1.29$) and (bottom) 800kHz ($\sigma_0 = 100$kPa, $R_d = 15.45$ and $\lambda/d_{50} = 0.65$). Simulations carried out on the prototype sample.
Figure 5.48: Normalised amplitude versus frequency for the production sample at different confining pressures. Top - transmitted sine pulses, bottom - received sine pulses. ($\sigma_0 = 100\text{kPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 5.63$ and $\lambda/d_{50} = 6.40$; $\sigma_0 = 200\text{kPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 5.01$ and $\lambda/d_{50} = 7.18$; $\sigma_0 = 300\text{kPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 4.69$ and $\lambda/d_{50} = 7.68$; $\sigma_0 = 500\text{kPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 4.30$ and $\lambda/d_{50} = 8.37$; $\sigma_0 = 750\text{kPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 4.02$ and $\lambda/d_{50} = 8.95$; $\sigma_0 = 1\text{MPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 3.83$ and $\lambda/d_{50} = 9.39$).

Figure 5.49: Stacked phase versus frequency for the production sample. $\sigma_0 = 100\text{kPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 5.63$ and $\lambda/d_{50} = 6.40$. 

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Figure 5.50: Time-domain contour plot of position versus time where the contours are coloured by the incremental displacement in the y-direction.  \( \sigma_0 = 100 \text{kPa}, f_{\text{trans}} = 30 \text{kHz}, R_d = 5.63 \) and \( \lambda/d_M = 6.40 \).

Figure 5.51: Time-domain surface plot of position versus time where the peaks are measured by the displacement in the y-direction.  \( \sigma_0 = 100 \text{kPa}, f_{\text{trans}} = 30 \text{kHz}, R_d = 5.63 \) and \( \lambda/d_M = 6.40 \).
Figure 5.52: The decrease in maximum velocity squared of particle as a function of the particle’s position along the propagation axis. The dashed line is a line with a slope inversely proportional to the position squared. $\sigma_0 = 100\text{kPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 5.63$ and $\lambda/d_{\text{eo}} = 6.40$.

Figure 5.53: Plot of frequency versus position coloured by amplitude. Black indicates higher amplitude values than white. $\sigma_0 = 100\text{kPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 5.63$ and $\lambda/d_{\text{eo}} = 6.40$. 
Figure 5.54: A schematic of the process used to obtain a two-dimensional fast Fourier transform (2D FFT) of a pulse wave propagating through the sample.

Figure 5.55: Plot of angular velocity versus wavenumber (inverse of the wavelength) coloured by the magnitude of the $y$-velocity. Black indicates higher wave energy than white. $\sigma_0 = 100$ kPa, $f_{\text{trans}} = 30$ kHz, $R_d = 5.63$ and $\lambda/d_{\sigma_0} = 6.40$. 
Figure 5.56: Plot of angular velocity versus wavenumber (inverse of the wavelength) coloured by the magnitude of the y-velocity. The transmitted signal was a sine pulse that was repeated ten times. Black indicates higher wave energy than white. $\sigma_0 = 100\text{kPa}$, $f_{trans} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_{30} = 6.40$.

Figure 5.57: Plot of angular velocity versus wavenumber (inverse of the wavelength) coloured by the magnitude of the y-velocity. The signal length considered is 1ms longer in the time domain compared with the signal analysed in Figure 5.55. Black indicates higher wave energy than white. $\sigma_0 = 100\text{kPa}$, $f_{trans} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_{30} = 6.40$. 
Figure 5.58: Sample shear modulus, $G_{xy}$, versus isotropic confining stress, $\sigma_0$, obtained using different travel time determination techniques and effective medium theory, EMT.

Figure 5.59: Received signals from the bender (shear wave) test and extender (compressional wave) test plotted against time. Bender: $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/\Delta y_0 = 6.40$, Extender: $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 3.92$ and $\lambda/\Delta y_0 = 9.18$. 
Figure 5.60: Representative particle stresses plotted for time points (d) and (i) during the bender test wave propagation (plan view). The cross-section through the packing is at mid-way along z-axis. $\sigma_0 = 100\text{kPa}$, $f_{trans} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_0 = 6.40$.

Figure 5.61: Representative particle stresses plotted for time points (d) and (i) during the extender test wave propagation (plan view). The cross-section through the packing is at mid-way along z-axis. $\sigma_0 = 100\text{kPa}$, $f_{trans} = 30\text{kHz}$, $R_d = 3.92$ and $\lambda/d_0 = 9.18$. 
Figure 5.62: Received signals (y-displacement) from the plane wave test and point source wave test plotted against time. Plane wave: $\sigma_0 = 300\text{kPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 4.69$ and $\lambda/d_0 = 7.68$, Point source: $\sigma_0 = 300\text{kPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 4.69$ and $\lambda/d_0 = 7.68$.

Figure 5.63: Individual particle velocity vectors (x & y components) scaled by magnitude considering x and y components of velocity only. The sample is confined at $300\text{kPa}$ with standard flexible boundaries. View is a plan view of a 5mm thick cross-section through the sample. Only particle velocities less than or equal to 10mm/s magnitude are plotted to prevent larger velocities from "clouding" the system response. $\sigma_0 = 300\text{kPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 4.69$ and $\lambda/d_0 = 7.68$. 
Figure 5.64: Surface plot of a plane wave propagating through the production sample confined at 300kPa with standard flexible boundaries. The plot is created using a column of particles between the transmitter and receiver and is coloured by the amplitude of the waves. $\sigma_0 = 300\text{kPa}$, $f_{trans} = 30\text{kHz}$, $R_d = 4.69$ and $\lambda/d_{so} = 7.68$. 
Figure 5.65: Schematic of different boundary conditions implemented on the sample.

Figure 5.66: Four small-scale single contact test exploring how wall-ball contacts differ from ball-ball contacts and how different ball-ball contact simulations behave.
Figure 5.67: Results of the four small-scale single contact tests showing that the ball-wall contact behaves differently to all ball-ball contacts and that all ball-ball contacts behave similarly.

Figure 5.68: Schematic of periodic boundary condition logic from O’Sullivan (2011).
Figure 5.69: Received signals (y-displacement) from the bender tests for samples confined with flexible boundaries, rigid wall boundaries and periodic boundaries plotted against time. \( \sigma_0 = 100\text{kPa}, f_{trans} = 30\text{kHz}, R_d = 5.63 \) and \( \lambda/d_{50} = 6.40 \).

Figure 5.70: Representative particle stresses plotted for time points (d) and (l) during wave propagation through a sample with rigid wall boundaries (plan view). The cross-section through the packing is at mid-way along z-axis. \( \sigma_0 = 100\text{kPa}, f_{trans} = 30\text{kHz}, R_d = 5.63 \) and \( \lambda/d_{50} = 6.40 \).
Figure 5.71: Representative particle stresses plotted for time points (d) and (l) during wave propagation through a sample with periodic boundaries (plan view). The cross-section through the packing is at mid-way along z-axis. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 5.63$ and $\lambda/d_{50} = 6.40$.

$g = 10\text{m/s}$

Figure 5.72: Layout of a small-scale test examining the effect of the critical viscous damping ratio on a single contact system.
Figure 5.73: Contact force versus time results for a small-scale test examining the effect of the critical viscous damping ratio on a single contact system. The horizontal black line represents the static solution to the particle in contact with the wall under gravity loading where \( g = 10 \text{m/s} \).

Figure 5.74: Influence of \( \beta \) on contact stiffness where the new contact stiffness is equal to the old contact stiffness multiplied by the \( \lambda \) factor.
Figure 5.75: Received signal versus time for a plane wave propagating through the production sample confined at 300kPa with flexible boundaries. The values of $\beta$ refer to the critical viscous damping ratios at the contacts which include at least one membrane particle. $\sigma_0 = 300\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 4.69$ and $\lambda/d_{so} = 7.68$.

Figure 5.76: Individual particle velocity vectors (x & y components) scaled by magnitude considering x and y components of velocity only. The sample is confined at 100kPa with absorbing flexible boundaries. View is a plan view of a 5mm thick cross-section through the sample. Only particle velocities less than or equal to 10mm/s magnitude are plotted to prevent larger velocities from "clouding" the system response. $\sigma_0 = 300\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 4.69$ and $\lambda/d_{so} = 7.68$. 
Figure 5.77: Surface plot of a plane wave propagating through the production sample confined at 300kPa with absorbing flexible boundaries. The plot is created using a column of particles between the transmitter and receiver and is coloured by the amplitude of the waves. $\sigma_0 = 300\text{kPa}, f_\text{trans} = 30\text{kHz}, R_d = 4.69$ and $\lambda/d_{50} = 7.68$.

Figure 5.78: Received signal versus time for a plane wave propagating through the production sample confined at 300kPa with wall boundaries. The values of $\beta$ refer to the critical viscous damping ratios at the contacts which include a wall element. $\sigma_0 = 300\text{kPa}, f_\text{trans} = 30\text{kHz}, R_d = 4.64$ and $\lambda/d_{50} = 7.76$. 
Figure 5.79: Received signals (y-displacement) from the bender tests for samples with the HM contact model, CM contact model and HMD contact model plotted against time. HM: $\sigma_0 = 100$ kPa, $f_{\text{trans}} = 30$ kHz, $R_d = 5.63$ and $\lambda/d_{50} = 6.40$, CM: $\sigma_0 = 100$ kPa, $f_{\text{trans}} = 30$ kHz, $R_d = 8.22$ and $\lambda/d_{50} = 4.38$, HMD: $\sigma_0 = 100$ kPa, $f_{\text{trans}} = 30$ kHz, $R_d = 6.41$ and $\lambda/d_{50} = 5.62$.

Figure 5.80: Representative particle stresses plotted for time points (d) and (l) during wave propagation through a sample with the CM contact model (plan view). The cross-section through the packing is at mid-way along z-axis. $\sigma_0 = 100$ kPa, $f_{\text{trans}} = 30$ kHz, $R_d = 8.22$ and $\lambda/d_{50} = 4.38$. 
Figure 5.81: Representative particle stresses plotted for time points (d) and (l) during wave propagation through a sample with the HMD contact model (plan view). The cross-section through the packing is at mid-way along z-axis. \( \sigma_0 = 100\text{kPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 6.41 \) and \( \lambda/d_{30} = 5.62 \).

Figure 5.82: Sample shear modulus, \( G \), versus isotropic confining stress, \( \sigma_0 \), obtained for samples with different interparticle contact models using the two-dimensional fast Fourier transform travel time determination technique.
Figure 5.83: Sample shear modulus, $G$, versus isotropic confining stress, $\sigma_0$, obtained for samples with different interparticle contact models using the two-dimensional fast Fourier transform travel time determination technique. Two slopes are calculated for Cavarretta-Mindlin contact model. The first considering the stress range 100kPa-300kPa and the second considering the stress range 500kPa-1MPa.

Figure 5.84: Results from stress probes carried out on the sample confined at 100kPa, 500kPa and 1MPa are compared with the results from wave propagation tests. The two-dimensional fast Fourier transform was used to calculate the wave speeds. Two measurement regions were used to record stress and strain values in the stress probe tests: the whole sample and the measurement sphere.
## 5.10 Tables

### Table 5.1: Production sample properties.

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<td>16.67x10(^9) [Pa]</td>
</tr>
<tr>
<td>Particle Poisson’s Ratio ([\nu])</td>
<td>0.20 [-]</td>
</tr>
<tr>
<td>Viscous Damping at Contacts</td>
<td>0.10 [-] (reducing to 0.01 [-] for BE test)</td>
</tr>
<tr>
<td>No. of Particles</td>
<td>81,576 [-]</td>
</tr>
<tr>
<td>Frequency of the Sine Wave</td>
<td>30.0 [kHz]</td>
</tr>
<tr>
<td>Transmitter Amplitude</td>
<td>0.000125 [mm]</td>
</tr>
<tr>
<td>Travel Distance ([d])</td>
<td>91.50 [mm]</td>
</tr>
</tbody>
</table>

### Table 5.2: A reference second order stiffness tensor showing the position of some of the fourth order tensor components. Subscripts 1 = \( x \), 2 = \( y \) and 3 = \( z \).

\[
\begin{pmatrix}
\sigma_{xx} & C_{1111} & C_{1122} & C_{1133} \\
\sigma_{yy} & C_{2211} & C_{2222} & C_{2233} \\
\sigma_{zz} & C_{3311} & C_{3322} & C_{3333} \\
\tau_{yz} & C_{2323} & C_{3131} & C_{3333} \\
\tau_{zx} & C_{1212} & C_{1222} & C_{1233} \\
\tau_{xy} & C_{3131} & C_{3121} & C_{3131}
\end{pmatrix}

\begin{pmatrix}
\epsilon_{xx} \\
\epsilon_{yy} \\
\epsilon_{zz} \\
\gamma_{yz} \\
\gamma_{zx} \\
\gamma_{xy}
\end{pmatrix} = \mathbf{C} \begin{pmatrix}
\sigma_{xx} \\
\sigma_{yy} \\
\sigma_{zz} \\
\tau_{yz} \\
\tau_{zx} \\
\tau_{xy}
\end{pmatrix}

### Table 5.3: The values corresponding to the positions on Table 5.2 calculated for the production sample confined at 100kPa using PVD.

\[
\begin{pmatrix}
592.81 & 190.84 & 22.46 & 0 & 0 & 0 \\
190.84 & 592.81 & 22.46 & 0 & 0 & 0 \\
22.46 & 22.46 & 763.38 & 0 & 0 & 0 \\
0 & 0 & 0 & 591.19 & 0 & 0 \\
0 & 0 & 0 & 0 & 381.70 & 0 \\
0 & 0 & 0 & 0 & 0 & 338.65
\end{pmatrix}
\]
Table 5.4: Production sample $G_{\text{max}}$ values calculated using different time-domain travel time determination techniques for different frequency sine pulses.

<table>
<thead>
<tr>
<th>Sine Pulses</th>
<th>$G_{\text{max}}$ [MPa] from Different Travel Time Determination Techniques</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frequency – [kHz]</td>
<td>First Local Minimum</td>
</tr>
<tr>
<td>7</td>
<td>365.28</td>
</tr>
<tr>
<td>15</td>
<td>414.37</td>
</tr>
<tr>
<td>20</td>
<td>441.43</td>
</tr>
<tr>
<td>30</td>
<td>458.65</td>
</tr>
</tbody>
</table>

Table 5.5: Production sample $G_{\text{max}}$ values calculated using different time-domain travel time determination techniques for different wave shape pulses at a frequency of 20kHz. The square wave is frequency independent.

<table>
<thead>
<tr>
<th>Wave shape</th>
<th>$G_{\text{max}}$ [MPa] from Different Travel Time Determination Techniques</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frequency – 20kHz</td>
<td>First Local Minimum</td>
</tr>
<tr>
<td>Sine</td>
<td>441.43</td>
</tr>
<tr>
<td>Triangular</td>
<td>391.40</td>
</tr>
<tr>
<td>Sine + 270° phase</td>
<td>375.01</td>
</tr>
<tr>
<td>Square</td>
<td>389.29</td>
</tr>
</tbody>
</table>

Table 5.6: Production sample $G_{\text{max}}$ values calculated using different frequency-domain travel time determination techniques for different frequency sine pulses.

<table>
<thead>
<tr>
<th>Sine Pulses</th>
<th>$G_{\text{max}}$ [MPa] from Different Travel Time Determination Techniques</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frequency – [kHz]</td>
<td>Phase vs. Frequency</td>
</tr>
<tr>
<td>7</td>
<td>14.11</td>
</tr>
<tr>
<td>15</td>
<td>51.08</td>
</tr>
<tr>
<td>20</td>
<td>92.41</td>
</tr>
<tr>
<td>30</td>
<td>203.86</td>
</tr>
</tbody>
</table>

Table 5.7: Production sample $G_{\text{max}}$ values calculated using different frequency-domain travel time determination techniques for different wave shape pulses at a frequency of 20kHz. The square wave is frequency independent.

<table>
<thead>
<tr>
<th>Wave shape</th>
<th>$G_{\text{max}}$ [MPa] from Different Travel Time Determination Techniques</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frequency – 20kHz</td>
<td>Phase vs. Frequency</td>
</tr>
<tr>
<td>Sine</td>
<td>92.42</td>
</tr>
<tr>
<td>Triangular</td>
<td>103.30</td>
</tr>
<tr>
<td>Sine + 270° phase</td>
<td>88.11</td>
</tr>
<tr>
<td>Square</td>
<td>22.14</td>
</tr>
</tbody>
</table>
6 Randomly packed sample

6.1 Introduction

Real soil is not a material made up of uniformly sized grains on a regular packing. As shown in the triaxial example in Chapter 3 the stress-deformation response can be quite different for regularly packed DEM simulations compared to real soil. Randomly packed samples can further understanding of granular material beyond what is obtainable from regularly packed samples. Shaebani et al. (2012) have previously studied the effect of grainscale polydispersity on the micromechanics of granular materials. Increasing the width of the particle-size distribution was found to influence the response of the packing to weak external perturbations. The deviation of measured macroscopic quantities from the average packing properties increases with increasing width of the particle-size distribution. Mouraille (2009) examined the effect of polydispersity on wave propagation through granular material and found that results, in both time and frequency domains, were influenced by polydispersity. Randomly packed samples are more comparable with the laboratory tests on granular material. Sample structure or fabric can be quantified in a numerical sample and its effect on wave propagation and on sample stiffness can be measured. Section 6.2 introduces the sample and Section 6.3 illustrates the wave propagation mechanism through this sample. Section 6.4 outlines the analytical solutions to the wave speed; Section 6.5 details the analysis of the received signal to determine wave arrival time and Section 6.6 discuss the effect of varying sample properties on the stiffness measured. Throughout these Sections comparisons will be made with the laboratory work carried out at the University of Bristol on the same material.

6.2 Sample preparation and initial properties

6.2.1 Pluviation

The randomly packed sample considered in the current study is illustrated in Figure 6.1. To create the sample, a loose cloud of particles was created and the particles were allowed to fall under gravity into a rigid wall container. As it was not known how high a sample would be after pluviation a sufficiently high number of particles were created to ensure it was above the desired final height of the sample. The target sample size was 100mm$^3$ measuring
100mm in each of the three principal directions. Allowing a loose cloud of many particles to fall under gravity is a computationally expensive and time-consuming process. Granular LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) is an open-source DEM code that can be parallelised and Dr. George Marketos pluviated a sample containing 80,000 particles using the high performance computing cluster (CX1) in Imperial College London. The particles that were pluviated were similar to those used in Chapter 5 but the particles were of polydisperse size and the properties are listed on Table 6.1. Once the sample had reached a quasi-static state Dr. Marketos was able to provide the ball and contact data for the random sample he had created and this information was inputted into a PFC3D programme. 80,000 particles produced a sample size that was greater than 100mm in the z – direction (vertical direction) so if any part of a sphere was above 100mm it was removed. This resulted in a sample containing 64,136 spheres and Figure 6.2 plots a histogram of the particle size before and after this removal process to show that spheres of all sizes were removed in approximately equal measure and spheres of a particular size did not accumulate at the top or bottom of the sample during the pluviation process. The sample had been pluviated into a rigid, frictionless wall container and the dimensions of this container were fixed. The contact data allowed the existing tangential forces between the particles to be transferred directly from Granular LAMMPS to PFC3D preventing any change in fabric in the sample. The DEM sample was the same size as the laboratory sample, approximately 100mm³, and the samples are compared in Table 6.2. The fabric tensor on Table 6.3 shows the DEM sample to be cross-anisotropic (i.e. isotropic in the horizontal plane) and that there was no variation in fabric tensor with variation in confining pressure. This illustrated that the sample fabric was not disturbed by increasing confining pressure. The DEM sample was less dense than the laboratory sample. This implies that the stiffness, G, of the DEM sample should be less than the stiffness of the laboratory sample.

Close to the rigid wall boundaries some crystallisation was induced and the void ratios where higher than in the central region. The crystallisation was evident in the contact force rose diagrams in Figure 6.3 (a) and (c) which include all particles. There are peaks along the horizontal and vertical axes which indicated the presence of a simple cubic lattice. If the particles contacting the walls were removed the contact force rose diagrams did not have these peaks (Figure 6.3 (b) and (d)). A histogram of the connectivity of the particles in the sample is plotted in Figure 6.4 and indicated an average connectivity of approximately 5.5. A few particles had connectivity of 10 but as there were not many particles with high
connectivity the overall sample does not appear to be attaining a lattice. The sample was further examined using a statistical analysis tool called the radial (pair) distribution function, \( g(r) \). This is defined as the probability of finding the centre of a particle inside an annulus of internal radius \( r \) and thickness \( dr \) with centre at a randomly selected particle. It has previously been used to analyse a two-dimensional DEM simulation by Yazdchi (2012) and Pyrz (1994). From Ripley (1979) it is mathematically defined as:

\[
g(r) = \frac{1}{4\pi r^2} \frac{dK(r)}{dr} \tag{6.1}
\]

\[
K(r) = \frac{V}{N^2} \sum_{k=1}^{N} I_k(r) \tag{6.2}
\]

where \( K(r) \) is a second-order intensity function, also known as Ripley’s function and \( I_k(r) \) is defined as the number of centres of particles that lie within a sphere of radius \( r \) about an arbitrarily chosen particle and \( N \) is the number of particles in the observation volume, \( V \).

Figure 6.5 plots the results of the radial (pair) distribution function for this randomly packed sample. A truly random Poisson point distribution of particle centres would have a value of \( g(r) \) equal to 1.0 at all positions. As after the initial peak the value for this sample remained at approximately 1.0 this sample was deemed to be sufficiently randomly packed. The initial peak was because a large number of particles were suddenly detected once the distance increased to a particle diameter. These analyses indicate that crystallisation was not pervasive throughout the sample; rather it was limited to the boundary regions.

The variation in void ratio in the sample was measured by dividing the sample into different horizontal and vertical sections. The vertical void ratio variation is plotted on Figure 6.6 and as expected the top horizontal section was much less dense (i.e. had a higher void ratio) than the rest of the sample due to pluviation. The bottom horizontal section had a slightly higher void ratio than the rest of the sample due to the effect of the wall boundaries on the sample packing. The rigid walls mean that the sample packed less efficiently than if they had landed on a particle bed. The void ratio variation over different vertical sections is plotted on Figure 6.7 and the sides of the sample were found to be less dense than the rest of the sample due to the effect of the rigid wall boundaries as outlined above. The boundary condition effects outlined here agreed with the previous observations on Figure 6.3 using contact force rose diagrams. This was also previously observed in DEM simulations carried out by Marketos & Bolton (2010) who examined the effect of flat boundaries.
6.2.2 Achieving a stress state

The desired confining pressures were reached using servo-controlled frictionless walls. Initially after pluviation the top layers of particles were less dense than the rest of the sample. Therefore the top wall (cap) was moved vertically down, while the other walls were held in place, until percolation occurred. As defined in O’Sullivan (2011) the percolation threshold is the threshold between a situation where the contact network bridges the entire sample and can transmit the applied boundary stresses across the sample. Then all walls were moved using the same servo-controlled algorithm as was used in Section 5.2.4. A gain factor, which controlled the speed of the walls, of 0.2 was used in the servo-controlled compression. The damping used during this stage was viscous damping with a critical viscous damping ratio of 0.1.

6.2.3 Boundary conditions

Once the desired confining pressure was reached the six face wall elements were removed. Twelve infinitely thin “line3d” wall elements were installed at the sample edges. Any particles that came into contact with the “line3d” wall elements were fixed in space to provide some rigidity to the edges of the sample. This models the physical cubical cell’s aluminium frame that supported the cushions.

After removal of the wall elements the confining pressure was maintained using a flexible boundary that is conceptually similar to the work in Chapter 5 but has some refinements to account for the random packing. The algorithm, which largely follows the work of Cheung (2010), isolated the outermost particles and checked whether there was a particle that could block the virtual membrane acting on this particle. If this was not the case the particle was included as a membrane particle. On each face the outermost particle centroids were used to create two-dimensional Voronoi diagrams. The Voronoi polygons represented the area closest to a particular particle centroid. These areas were multiplied by the desired confining pressure to determine a force that was applied to the particle. The force was directed along one of the principle axes towards the centre of the sample. Figure 6.1 shows the resultant sample where the particles are coloured by the applied force. The particles along the edges and at the corners had a higher applied force as they interacted with two or three virtual membranes. Figure 6.8 compares the applied stress to the membrane boundaries with the stresses measured in the central measurement sphere region of the sample. After some initial fluctuations the measurement sphere stresses and applied stresses agreed to approximately
Further details about this flexible boundary algorithm can be found in Cheung & O’Sullivan (2008) and Cheung (2010).

### 6.2.4 Creating a stress wave

To simulate a bender element test a single particle was displaced to produce a stress wave that travels through the sample and a single particle was used as a receiver, i.e. the approach used in Chapter 5 was adopted here. Figure 6.9 shows a cross-section of the sample illustrating the position of the transmitting particle and receiving particle. For most of the simulations the input wave was a single period sine pulse, however some other signals were used, as discussed below. The displacement amplitude of the transmitter was 1μm, although this was varied in a parametric study, and the frequency was usually 15kHz but this too was varied in a parametric study. Similar to Chapter 5 an amplitude was chosen that was not influencing the packing of the sample but also was observable over the fluctuations in particle velocities in the quasi-static state. An example received signal for a DEM simulation is shown in Figure 6.10 and is compared with a laboratory signal in the same plot. The two signals were observed to be remarkably similar up to approximately 0.75ms. The arrival was seen to occur around the same time and the frequencies of the oscillations were close. After 0.75ms the laboratory signal showed some higher frequency components that produced a jagged received signal compared to the DEM signal. The shear wave velocity of both the laboratory and the DEM sample were measured using characteristic methods on the received signal. The shear wave speed propagating through the laboratory sample was found to be approximately 360m/s while the shear wave speed propagating through the DEM sample was found to be approximately 320m/s. The wave speeds measured for both samples is similar in magnitude and the difference in void ratio in Table 6.2 shows that as the laboratory sample had a lower void ratio than the DEM sample the wave speed is expected to be higher. A void ratio correction function can be applied to the results such as the one outlined in Hardin & Richart (1963):

\[
f(e) = \frac{(2.17 - e)^2}{1 + e}
\]

6.3

For the laboratory sample \(f(e) = 1.35\) and for the DEM sample \(f(e) = 1.27\). The shear wave speeds corrected for void ratio are \(V_S = 267\text{m/s}\) for the laboratory sample and \(V_S = 252\text{m/s}\) for the DEM sample.
6.2.5 Preserving the elasticity of the sample

In principle, during the bender element test, the displacement is sufficiently small that the behaviour is assumed to be elastic. In a laboratory test it is difficult to confirm that the system remains elastic, this is not the case for the DEM simulations. Figure 6.11 presents two measures of plasticity occurring in the DEM sample during the wave propagation that produced the received signal shown in Figure 6.10 (a). There were small changes in average coordination number and there were some contacts that started to slide. The 8,000 contacts that started sliding represent approximately 4.5% of the total number of contacts in the sample. It was assumed that the sample’s elasticity and packing would not be affected significantly by these changes in coordination number and number of sliding contacts.

6.2.6 Effect of transmitter connectivity on wave propagation

The connectivity of the transmitter was found to influence the stress wave that was produced with higher amplitude signals being produced by particles with a higher connectivity. This was found when signals were propagated in different directions as different transmitters were used. It is mentioned here as it influenced the stress wave that was created. Figure 6.12 shows relationship between the connectivity of the transmitter particle and the sum of the kinetic energies, both translational and rotational, of all the particles in the sample during wave propagation. The transmitter particles that had higher connectivity values led to higher peaks on the kinetic energy plot. Differences in kinetic energy between particles of the same connectivity highlighted the effect of local packing on the transmitter. Figure 6.13 isolates the particle used for y-direction transmission and the fabric tensor shows that it had more contacts in the x-direction so the kinetic energy produced when it was displaced in that direction was higher than when it was displaced in the other directions. This finding illustrated that the placement of the bender element in a laboratory sample will influence the wave that propagates through the system. A bender element that has a good connection with the soil particles surrounding it will produce relatively higher amplitude signals than a bender element that has a poor connection with the soil particles.

6.3 Wave propagation through the sample

The propagation of the waves through the sample was visualised using various techniques including many of those that worked well for the regularly packed sample in Chapter 5. The
methods utilised were individual particle velocity vectors, individual particle translational velocities, relative representative particle shear stresses and relative particle kinetic energies.

6.3.1 Individual particle velocity vectors

On Figure 6.14 the individual velocity vectors are plotted on a plan view of the simulation. The velocity vectors only considered the x and y components to indicate direction and the magnitude was calculated using these two components only. As before, each arrow illustrated the motion of one particle, and the arrow direction matched with the velocity vector orientation, while the length matched with the magnitude. The slice of the sample was 5mm thick and was located mid-way along the z-axis. Only particle velocity vectors that had a magnitude less than 0.5mm/s were plotted to reduce the clouding of the simulation response due to the large velocities near the transmitter. On time point (a) the movement of the transmitter created a lobe in the sample that was observed and the highest magnitude velocity vectors were located near the transmitter. The spherical shear wave lobe became evident by time points (b) and (c) and was seen to move through the system towards the receiver. At time points (b) and (c) there was obviously an interaction between the wave and the flexible boundaries and complicated reflected waves were produced that travel diagonally from the edge towards the centre of the sample. There had already been movement of the receiver particle and this initial movement was due to an effect of the wave interaction with the flexible boundaries that was observed on time point (c).

By time point (d) the shear wave lobe arrived at the receiver. Time point (d) appeared to be almost coincident with the point of first local minimum on the received signal. The complicated waves resulting from the interference of reflections were observed on time points (e) and (f). An interesting observation from the final time points was that all the higher particle velocities appeared “trapped” at the transmitter end of the sample. The higher velocity components coincided with higher frequency waves so this indicated that the sample was acting as a frequency filter similar to the samples explored by Lawney & Luding (2013) and mentioned in Chapter 2. This observation will be explored in more detail in the frequency domain analysis.

An elevation view of the simulation on Figure 6.15 plots the velocity vectors during the wave propagation in the xy-plane and clearly indicates the spherical nature of the shear wave lobe. The shear wave lobe appeared to arrive at a time close to time point (d) in agreement with the
previous plan view plots. The frequency filtering noted previously was observed in elevation view.

### 6.3.2 Particle translational velocities

The same simulation and time interval is considered in Figure 6.16, however in this case the particles are coloured by the y-component of their particle velocity vectors. Lighter coloured particles had a high positive y-velocity component and darker coloured particles had a high negative y-velocity component. The plot is a plan view of the simulation through a cross-section mid-way along the z-axis of the sample. Time-point (a) shows the initial disturbance that was created by the movement of the transmitter particle. Time-points (c) to (e) illustrate the shear wave component as a circular wave propagating towards the receiver. The reflected waves were not easily seen in this visualisation in comparison with Figure 6.14 as they contained significant x-direction velocity components. Frequency filtering was observed as the higher y-velocity components remain trapped at the transmitter end of the sample.

Figure 6.17 plots the relative particle y-velocity components for time point (d) at a higher colour resolution. The initial shear wave lobes were found to be more clearly observed at this colour resolution. The arrival of the true shear wave was found to have not occurred by time point (d) based on these micromechanical data. There was a lot of noise following the initial shear wave lobes and reflections were not clearly observable when only individual particle y-velocity components were considered. This was because the x-components of the velocity vectors were relatively large.

### 6.3.3 Representative particle shear stresses

Again considering the same simulation and time interval, the representative particle shear stresses are plotted in Figure 6.18 and were calculated using the method outlined in Chapter 5. The lighter coloured particles have a high positive representative particle shear stress and the darker coloured particles have a high negative representative particle shear stress. The plan view is a cross-section mid-way along the z-axis of the sample. Alternating light and dark regions indicating peaks and troughs on the shear wave propagating through the system were observed in Figure 6.18 during time-points (b) to (e). The higher relative particle shear stresses were trapped by the frequency filtering of the medium.

Figure 6.19 plots the representative particle shear stresses for time point (d) at a higher resolution. As in Figure 6.17 two clear initial shear wave lobes were observed propagating
through the system, although they were noisier in this plot compared to the particle y-velocities. It was hard to determine on Figure 6.19 whether the true shear wave had arrived at the sample because of the noise. There were a lot of random fluctuations following the initial shear wave lobes and no clear reflections could be observed.

### 6.3.4 Particle kinetic energies

The kinetic energy of each individual particle is plotted relative to the initial state on Figure 6.20. The kinetic energy is calculated from the particle’s translational and rotational velocities. The plan view is a cross-section mid-way along the z-axis of the sample. Lighter particles have higher kinetic energies than darker particles. The shear wave lobes propagated as regions of higher kinetic energy. Reflected waves were observed to initiate around time-point (c) and travelled towards the receiver in time-points (d) to (f). Relative kinetic energies were found to be the clearest way of observing the reflected waves propagating in the sample.

Figure 6.21 plots the relative particle kinetic energies for time point (d) at a higher colour resolution. Similarly to Figure 6.17 and Figure 6.19 the first shear wave lobes were clearly visible and similar to Figure 6.17 true shear wave arrival was seen to have not occurred by this time point. There were complex waves following these initial two lobes and they were not clearly observed using any of the methods or colour resolutions. Reflections were clearly observed propagating on one side of the sample diagonally towards the receiver. Reflections were not as clearly observed on the other side of the sample.

### 6.4 Analytical solutions

**Effective medium theory**

Effective medium theory (EMT) was used to predict the stiffness of a random, isotropic packing of monosized granular material as outlined in Chapters 2, 4 and 5. The theory cannot provide an accurate stiffness value for the sample considered here as it had an anisotropic packing and polydisperse particles; however, it provided an estimate for comparison with other methods. EMT provided a single value of shear modulus ($G$) and a single value of Young’s modulus ($E$) that were not dependent on the direction considered. The equation for shear modulus is as follows:
The values were dependent on the sample confining pressure, \( P \), average coordination number, \( C_p \), and porosity, \( n \), and on the particle shear modulus, \( G_{\text{particle}} \), and Poisson’s ratio, \( \nu_{\text{particle}} \). The equation can be found in the work of Duffaut et al. (2010) and Chang et al. (1991). The stress dependency of the sample shear modulus is a power law relationship with confining pressure of 1/3 just as with the regular packing. The relationship between \( G \) and \( E \) and the confining pressure is plotted on Figure 6.22 for different values of confining pressures. As expected a power law relationship close to 1/3 was observed; however the magnitudes of the elastic moduli predicted by EMT should be greater than those measured in simulation as the sample considered was not isotropic and the particles were polydisperse. The EMT analytical solution assumes that the randomly packed particles were of equal size and that the sample was isotropic.

**Near-field effect**

The arrival of the near-field effect was predicted using the equations in Sanchez-Salinero et al. (1986) for a random sample. This was carried out on the regular packing in Chapter 5. The Sanchez-Salinero solution created a Green’s function that was convoluted with the fast Fourier transform of the transmitted signal to produce a received signal that was inversely fast Fourier transformed to the time domain. The Green’s function was composed of four parts: the near-field shear wave component, the near-field compressional wave component, the far-field shear wave component and the far-field compressional wave component. To calculate each of these components the compressional wave speed and shear wave speed were measured using the two-dimensional fast Fourier transform and the density and travel distance were measured. The other parameters inputted were input wave period, input wave force amplitude and sample Poisson’s ratio. The signal produced using the equations in Sanchez-Salinero et al. (1986) was plotted with the recorded signal on Figure 6.23. The signal was created with zero material damping as the DEM simulation had a low value of viscous damping. The first deviation of the recorded signal from the zero-line corresponded with the arrival of the near-field component as predicted by the analytical solution. This shows that the near-field effect clouded the arrival of the true shear wave.
6.5 Determining the travel time

6.5.1 Analysis of the received signal

The received signal produced in the DEM analysis was analysed using time and frequency domain methods similar to those used previously in Chapters 4 and 5. Some of these same analysis techniques were used on the results for laboratory samples provided by the University of Bristol. The DEM input signals were single sine pulses with frequencies of 7kHz, 15kHz, 20kHz and 30kHz. The signals were compared in the time domain in Figure 6.24 where arrival times are similar in all simulations. As the transmitted frequency increased the amplitude of the received signals decreased. This provided evidence of frequency filtering.

The propagating waves were examined using the micromechanical data. The wave transmitted by 7kHz and the wave transmitted at 30kHz were chosen for a comparison as they were the limits of this parametric study. Figure 6.25 and Figure 6.26 plot individual velocity vectors considering the x and y components of velocity only. A 5mm thick slice was taken through the sample mid-way along the z-axis and all particle velocity vectors that had a magnitude less than 0.5mm/s were plotted. The larger velocities were omitted as they clouded the observation of the wave propagating through the system. Figure 6.25 plots the velocity vectors for a transmitted frequency of 7kHz and Figure 6.26 plots the velocity vectors for a transmitted frequency of 30kHz. It is clear that the velocity vectors were much larger in Figure 6.25 compared to Figure 6.26, especially at the receiver end of the sample. This indicates that the received signal was of a larger amplitude for the signal transmitted at 7kHz than for the signal transmitted at 30kHz. There was no evidence of frequency filtering in the sample when the transmitted frequency was 7kHz as there was little or no amplitude propagated at frequencies above the maximum frequency of 15kHz. In contrast frequency filtering was clearly observed in Figure 6.26 as the larger velocity components remained trapped at the transmitter end of the sample. The velocity vectors that reached the receiver were much smaller than those trapped at the transmitter end and this indicated that the received signal was greatly attenuated.

The DEM signals were compared to laboratory signals propagated at different frequencies. Lab signals were propagated at 7kHz, 10kHz, 15kHz and 20kHz and are compared in Figure 6.27. The properties of the laboratory sample was isotropically confined at a pressure of
100kPa and a void ratio of 0.67 (Hamlin (2014)). All waves appeared to arrive at similar times as in the DEM simulations and the initial oscillations were unaffected by the increasing transmitting frequency. As the transmitting frequency increased the latter part of the received signal was seen to respond with a higher frequency oscillation. This was different to what was observed in Figure 6.24 for the DEM data.

**Characteristic points**

A number of characteristic points were considered on the received signal which may correspond to the arrival of the shear wave at the receiver. Two of these points are illustrated on Figure 6.28 which are the first arrival as the first zero crossing of the received signal and the peak-peak method, utilising the first peak. Referring to Figure 6.29 other methods considered were the point of first local minimum on the received signal, the first point where the first derivative of the received signal equals zero and the second point where the second derivative of the received signal equals zero (point of first inflection). The signal decomposition method which was outlined in Chapter 4 was also used in this parametric study. The arrival times for all frequencies considered were determined using each of these methods, as listed on Table 6.4. Comparing the calculated arrival times, the first zero-crossing and the peak-peak methods have standard deviations less than 5MPa was approximately 4% of the mean value of $G_{xy}$ from all the methods and frequencies considered here. However, previously in Chapter 5 both these methods were shown to be dependent on the frequency of the sine wave. The point of first zero-crossing generally agreed with the arrival of the shear wave visualised using the micromechanical data in Section 6.3. The other characteristic points considered seem to give less reliable estimates of the arrival time.

**Cross-correlation**

Cross-correlation was applied similarly to Chapter 5 using the method outlined in Mohsin & Airey (2003) and Yang & Gu (2013) where a peak on the cross-correlation function near to the first-zero crossing or first local minimum was picked as the arrival of the shear wave. This is illustrated on Figure 6.30 for a wave recorded in the DEM simulation. The standard deviation of the moduli calculated using this method was greater than some of the characteristic point methods at approximately 8.4% of the mean value of $G_{xy}$ (Table 6.4).

**Amplitude versus frequency plots**

The signals of different transmitted frequencies were compared in the frequency domain in Figure 6.31 on normalised amplitude plots. The single sine pulse that was inputted has a
frequency domain spectrum that has an initial large peak followed by continuing smaller peaks. The initial peak in the transmitted signal occurs at the transmitted frequency and the spectrum shows that the signal has significant amplitudes occurring at frequencies up to twice the inputted frequency. The 7kHz transmitted signal contained significant amplitudes at frequency components up to 14kHz and the corresponding received signal contained amplitudes at frequency components up to 14kHz as well. When the transmitted frequency rose above 7kHz, frequency filtering was observed as the received signal did not contain the higher frequency components that were transmitted. The received signal did not contain frequencies above approximately 15kHz regardless of the frequency of the transmitter signal. If the signal transmitted at 30kHz is considered, it is clear that the magnitude of amplitude transmitted at frequencies below the threshold frequency of 15kHz is relatively small and this will affect the amplitude of the received signal. The observation of lower amplitude oscillations on the time domain plot noted above can be linked to the frequency effects. The oscillations on the received signal in the time domain were less when the transmitted signal frequency increased.

Figure 6.32 plots non-normalised amplitude versus frequency for the same signals as above. The reduction in amplitude with increasing frequency was clearly visible. As the transmitting frequency increased the inputted amplitude was spread over higher frequencies. As these frequencies were susceptible to filtering the associated amplitudes did not reach the receiver particle.

The higher frequency response was observed in laboratory signals from Hamlin (2014) in Figure 6.33 where the signals are compared in the frequency domain using normalised amplitude versus frequency. As the transmitted frequency increased the amplitude of the received wave component at approximately 30kHz also increased. Again this was not observed in the DEM data in Figure 6.31. In both the simulations and the laboratory tests, there was a definite peak at a lower frequency that did not change as transmitted frequency increased. This peak appeared to be at approximately 7kHz. After this peak the amplitude component was observed to drop towards zero before rising again when higher transmitted frequencies, i.e. 15kHz and 20kHz, were used. Figure 6.34 plots non-normalised amplitude versus frequency for the same signals as Figure 6.33. The reduction in amplitude with increasing frequency was clearly visible. As the transmitting frequency increased the inputted amplitude was spread over higher frequencies. As these frequencies were susceptible to filtering the associated amplitudes may not have reached the receiver particle.
In Figure 6.31 and Figure 6.32 there was a local maximum peak in amplitude observed at approximately 1.456kHz on the frequency axis. This peak was a global maximum peak for signals transmitted with frequencies of 15kHz, 20kHz and 30kHz. A signal was propagated at a transmitted frequency of 1.456kHz to observe any effects of resonance on the system. Figure 6.35 compares the results from this test with waves transmitted at the other frequencies in the time and frequency domains. The amplitude of the received signals was much greater when the transmitted frequency was 1.456kHz and the frequency of oscillations was much lower. On the frequency domain plot the received signal was observed to oscillate at a frequency that was quite similar to the transmitted frequency. On the top plot the received signal appears to arrive at a similar arrival time compared with the signals resulting from different transmitter frequencies. The speed of the wave, calculated using 2D FFT method, was 297.87m/s which is a little faster than the speed of the wave calculated for the lower transmitter frequencies where 7kHz – 274.36m/s, 15kHz – 269.70m/s, 20kHz – 276.70m/s and 30kHz – 277.61m/s.

The number of oscillations in the transmitted signal influenced the response in the time and frequency domains (Figure 6.36). Both signals appeared to arrive at a similar time and the amplitude of the received signal resulting from the ten pulse transmitted signal was similar to the amplitude of the received signal resulting from the single pulse transmitted signal. This differs from the response of the regularly packed sample where there was an increase in amplitude when the transmitted signal was cycled over ten cycles. In the frequency domain the transmitted pulse that was cycled ten times was a narrower peak over the transmitted frequency. The maximum peak was still at a frequency of approximately 1.44 kHz providing robust evidence that there is a fundamental sample mode at that frequency. There was also a local maximum at the transmitted frequency of 15kHz. Unlike in the case of the regularly packed sample this was not the global maximum.

The amplitude versus frequency plots for transmitted signals (top) and received signals (bottom) are shown on Figure 6.37. The signals were transmitted through samples under different isotropic confining pressures. The threshold frequency which was previously observed to be approximately 15kHz under a confining pressure of 100kPa was observed to increase with increasing confining pressure. When the sample was confined at 1MPa the threshold frequency was approximately 22kHz. The effect of confining pressure on frequency filtering was not observed in previous regularly packed simulations in Chapter 5.
Phase versus frequency plots

The plots of stacked phase versus frequency were created similarly to Chapter 5 utilising the method in Greening & Nash (2004). The slope of this plot (Figure 6.38), divided by \(2\pi\), is a value for the arrival time of the shear wave. The plot was more non-linear than the plot created in Chapter 5. This indicates that more dispersion was occurring in the randomly packed sample than in the regularly packed sample. The phase velocities were calculated using the secant slope of this line. The group velocities were calculated by averaging the tangent slopes of the line. As in Chapter 5 the phase velocities were favoured as the group velocities were more scattered. In Table 6.5 the range of values calculated using this method was much lower than the range of values calculated using other methods in Table 6.4 and Table 6.5. In Chapter 5 this method was also found to be inaccurate compared with all the other methods used.

6.5.2 Temporal – spatial analysis of system

Time-domain contour plots

The time domain contour plots were created using the individual particle y-velocity components along a column of particles between the transmitter and receiver. On Figure 6.39 the plot is of position versus time and is coloured by the y-velocity of the particles. A number of contour slopes were seen on Figure 6.39 which corresponded to the speeds of waves propagating through the system. The initial contour slopes are steeper than the following contour slopes and indicated the near-field effect propagating through the system. The subsequent contour slopes appeared to have a similar slope value. The values of the contour slopes gave a value of shear wave speed. The results from this method are summarised on Table 6.4. The propagating wave was visualised on a three-dimensional surface plot on Figure 6.40 where a number of propagating shear waves travelled through the sample as indicated as peaks and troughs on the surface plot. The reflections clouded the shear wave propagation at later time points. The standard deviation of the \(G_{xy}\) values is similar to the standard deviation of the \(G_{xy}\) values calculated using the cross-correlation method. The reduction in the magnitude of the propagating kinetic energy was further highlighted by Figure 6.41 which shows the non-linear reduction in particle velocities squared as the wave travelled through the system. The dots indicate the positions of the particles. The square of the particle velocities is analogous to their kinetic energy, \(KE\), and the relationship is \(KE \propto 1/r^{4.28}\) where \(r\) is the position of the particle along the propagation.
axis. This differs from the relationship for regularly packed simulations in Chapter 5 where \( KE \alpha 1/r^{2.15} \). The dashed line on Figure 6.41 is the theoretical relationship of \( KE \alpha 1/r^2 \) and the numerical result is observed to have a steeper slope than the theoretical line. The steeper decrease in propagating kinetic energy must be linked to the increased disorder in the sample packing.

**Frequency versus position plots**

Frequency versus position plots coloured by the amplitude of the displacement are illustrated on Figure 6.42 for the same sample under different confining pressures, (a) 100kPa, (b) 500kPa and (c) 1MPa. In all cases the highest frequencies that existed near the transmitter were filtered and the receiver contained a frequency spectrum that was narrower. As confining pressure increased the threshold frequency increased as well. The threshold frequency was raised throughout the whole sample as was seen in Figure 6.42. The threshold frequency for 100kPa was approximately 15kHz, for 500kPa was approximately 17kHz and for 1MPa was approximately 22kHz.

**Two-dimensional fast Fourier transform plots**

A two-dimensional fast Fourier transform is illustrated on Figure 6.43 where angular velocity \( \omega \) is plotted against wavenumber \( k \). The angular velocity is equal to \( 2\pi f \) where \( f \) is the frequency and wavenumber is equal to \( 2\pi/\lambda \) where \( \lambda \) is the wavelength. The plot is coloured by the amplitude of the Fourier coefficients of the wave at a given angular velocity and wavenumber. Darker regions had higher amplitude associated with them than lighter regions. The slope of a best fit line through the darker region in Figure 6.43 gave a value of wave speed. The two-dimensional fast Fourier transform was carried out on a large number of the particles between the transmitter and receiver to measure a sample-scale response. A number of particles in a yz-plane were selected at each discrete point in the x-direction. The y-velocities of these particles were used as inputs. The sample stiffness calculated from two-dimensional fast Fourier transform plots was compared for waves transmitted at different frequencies in Table 6.4. The standard deviation of these stiffness values was very small.

The effect of signal length in the time domain on the results of this method was considered. Figure 6.44 plots the two-dimensional fast Fourier transform of angular velocity against wavenumber. As the transmitted wave of frequency 15kHz \( (\omega = 94.248 \times 10^3 \text{rad/s}) \) was cycled continuously for ten cycles there is a dark band on Figure 6.44 at this angular velocity. Along this dark band a darker region is observed at a wavenumber of 375.3rad/m and if the
angular velocity was divided by this wavenumber the resulting wave speed was 248.36m/s. This was close to the value calculated for a single sine pulse, 267.70m/s.

6.5.3 Comparison of different methods

The results from different travel time determination techniques for the calculation of $G_{xy}$ and the results from the effective medium theory (EMT) analytical solution for $G$ were compared and are plotted over different confining pressures on Figure 6.45. Compared to the regular packed simulation, effective medium theory greatly over predicted the stiffness of the randomly packed sample. Many of the methods appeared clustered around the same values of $G_{xy}$ at each confining pressure; however, the phase versus frequency method consistently gave values much lower than any other method. The values calculated for $G_{xy}$ using the point where first derivative equals zero and the point of first local minimum were found to lie between the EMT values and the clustered values from other methods. Regarding the relationship between $G_{xy}$ and confining pressure, which will be termed alpha, EMT produced a relationship close to the expected value of $1/3$. Peak-peak, cross-correlation and the contour plot methods produced higher values of alpha that were greater than 0.4 while first zero crossing, the two-dimensional fast Fourier transform, the point of first local minimum, the first derivative equal to zero and the second derivative equal to zero produced a relationship closer to $1/3$. The phase versus frequency results produced a relationship that was much lower at alpha equal to 0.18. Comparing the techniques using both Table 6.4 and Table 6.5 the two-dimensional fast Fourier transform technique was observed to give results with the least scatter amongst the methods considered.

6.6 Stiffness of the sample

The stiffness of the randomly packed sample was predicted to be influenced by the fabric tensor. The fabric tensor, on Table 6.3, illustrates that the sample was cross-anisotropic. Wave propagation tests and stress probes were used to evaluate the stiffness of the sample in different directions and across different shear planes. Two travel time determination techniques were used to calculate wave travel time or wave speed. They were the time domain cross-correlation method and the frequency domain two-dimensional fast Fourier transform. Attempts were made to quantify the effect of the connectivity and local packing around the transmitter and receiver particles on the waves that propagate through the sample. It was possible that this could affect the results from wave interpretation techniques. As
confining pressures increased the sample coordination number increased with a power law relationship of 0.019. This is plotted on Figure 6.46 where the coordination number, $CN$, is

$$CN = \frac{2N^C}{N^P}$$

6.5

where $N^C$ is the number of contacts and $N^P$ is the number of particles.

6.6.1 Compressional wave propagation

Compressional waves were propagated through the sample to determine the values of constrained moduli in each of the three principal directions. $M_x$, $M_y$ and $M_z$ were calculated for samples isotropically confined at 100kPa, 300kPa, 500kPa, 750kPa and 1MPa. The compressional wave was produced by displacing the particle in the direction which the wave was going to propagate. For example, to measure $M_x$ the transmitting particle was moved in the x-direction and the speed of the wave propagating in the x-direction was measured.

Received signals

The received signals for each of the three directions are plotted at three different confining pressures on Figure 6.47. As the confining pressure increased the signals were seen to arrive sooner and also to be of higher amplitude. The amplitudes of the waves propagating in the x and z direction were similar at approximately $5.0 \times 10^{-5}$mm; however, the amplitude of the waves propagating in the y-direction were almost twice as large at approximately $1.0 \times 10^{-4}$mm. This was due to the connectivity of the transmitting particle in y-direction being twice the value of the transmitting particles in the x- and z-directions as shown on Figure 6.12. There was not a large difference in the arrival times that were observable on the plots but as the waves were travelling along paths of different lengths the difference would become more apparent in later analysis.

Micromechanics

Figure 6.48, Figure 6.49 and Figure 6.50 plot the compressional waves propagating in the x-, y- and z-directions respectively. These plots were created similarly to Figure 6.14 except that in the case of the z-direction compressional wave the velocity components used to create the plot are the y and z components. The compressional wave appeared to arrive around time point (c) in all cases. The compressional wave was also observed to be the first wave to arrive at the receiver particle. There was evidence of some frequency filtering at time point
(f) as the higher velocities appear trapped at the transmitter end of the samples. The velocity vectors plotted for the wave propagating in the y-direction were larger than the velocity vectors plotted for the waves propagating in the x- and z-directions. This was due to the increased kinetic energy in the sample because of the increased connectivity of the transmitter particle when the y-direction was considered. This shows how increased transmitter connectivity led to more energy inputted into the sample. This caused more movement of the particles across the whole sample and ultimately an increased movement of the receiver particle.

**Constrained moduli \((M_i)\) versus confining pressure**

The compressional wave velocities were calculated using two-dimensional fast Fourier transform plots as outlined in Section 6.5.2. The number of particles considered to create plots had to be increased to avoid local packing effects around the transmitter and receiver particles. The wave velocities were used to calculate the constrained moduli in each direction and the relationship of these moduli values with confining pressure is plotted on Figure 6.51. The value of \(M_z\) was shown to be slightly greater than the values of \(M_x\) and \(M_y\) at the isotropic confining pressures considered here and the slope of the best-fit line in log-log space was higher for \(M_z\) than for \(M_x\) and \(M_y\). The independence of \(M_z\) was expected based on the cross-anisotropy of the fabric tensor on Table 6.3.

Values for constrained moduli were calculated using the cross-correlation method and the results are plotted on Figure 6.52. On this plot the value of \(M_y\) was observed to be above \(M_x\) and \(M_z\) and this was not expected. It was possible that the cross-correlation method was affected by the higher connectivity of the transmitting particle in the y-direction. As the two-dimensional fast Fourier transform plots gave a more sample wide response to the wave when more particles were included in the column of particles between the transmitter and receiver it was possible to avoid local packing effects with this method.

**6.6.2 Shear wave propagation**

Shear waves were propagated in different planes to measure the values of the shear moduli, \(G_{ij}\). All possible shear planes were measured for the sample confined at 100kPa to check if the sample was cross-anisotropic. The shear planes were \(G_{xy}, G_{yx}, G_{yz}, G_{zy}, G_{xz}\) and \(G_{zx}\). Based on these findings only three shear planes were measured for the further confining pressures (300kPa, 500kPa, 750kPa and 1MPa).
Received signals

The received signals for three different shear planes at three different confining pressures are illustrated on Figure 6.53. The shear moduli measured here were $G_{xy}$, $G_{yz}$ and $G_{zx}$ and the confining pressures examined were 100kPa, 500kPa and 1MPa. The amplitudes of all waves increased as the confining pressure increased. Similarly to the previous compressional wave analysis the amplitude of the waves propagating in the y-direction, at $6.0 \times 10^{-5}\text{mm}$, were larger than for either the x- or z-directions as both these directions had similar amplitude at $2.5 \times 10^{-5}\text{mm}$. There did not appear to be a large difference in arrival times on Figure 6.53 but, as these waves propagated along different travel paths, differences may become apparent in later analysis.

Micromechanics

Figure 6.54 and Figure 6.55 plot the individual velocity vectors for the waves propagating in the yz-plane and zx-plane and these were compared with Figure 6.14 which plots the individual velocity vectors for the xy-plane. The same criteria that were used to create the plot on Figure 6.14 were used to create the other plots for waves travelling on different planes. The shear wave appeared to arrive between time points (d) and (e) in all three cases. The shear wave was not the first wave to arrive as there were some initial fluctuations on the received trace before true shear wave arrival. These initial fluctuations indicated the near-field effect. It appeared to be related to movements around the boundary particles. There was evidence of some frequency filtering at time point (f) as the higher velocities appeared trapped at the transmitter end of the samples. The velocity vectors plotted for the wave propagating in the yz-plane were larger than the velocity vectors plotted for the waves propagating in the xy-plane and zx-plane. This was due to the increased kinetic energy in the sample because of the increased connectivity of the transmitter particle when the y-direction was considered.

Shear moduli ($G_{ij}$) versus confining pressure

The shear moduli are calculated for the sample confined at 100kPa to check if the sample was cross-anisotropic. These values are given with the values of constrained moduli on Table 6.6. They were measured using wave propagation tests as outlined above and two interpretation techniques were used, namely two-dimensional fast Fourier transforms (a frequency domain method) and cross-correlation (a time domain method). The two-dimensional fast Fourier transforms indicates that the sample was, at least partially, cross-anisotropic with $G_{xy} = G_{yx}$,
$G_{yz} = G_{zy}$ and $G_{xz} = G_{zx}$, while the constrained moduli indicated $M_x = M_y \neq M_z$. However, $G_{yz} \neq G_{xz}$ and $G_{xy} \neq G_{zx}$ as would be expected in a truly cross-anisotropic material. The directions x and y equalled h and z equalled v so that $G_{hv} = G_{vh}$ if the material was truly cross-anisotropic. The cross-correlation results did not indicate these trends, however, as $M_y$ was the largest constrained modulus value it was questioned to what degree the local packing of the transmitters and receivers were influencing the results.

For the subsequent confining pressures the values of $G_{xy}, G_{yz}$ and $G_{zx}$ were measured using the two-dimensional fast Fourier transform plots and cross-correlation. The resulting $G_{ij}$ values were plotted on log-log plots against confining pressure. When results were calculated using two-dimensional fast Fourier transforms, plotted on Figure 6.56, $G_{yz}$ was found to be consistently higher than $G_{xy}$ and $G_{zx}$, however, all values were reasonably close indicating that the sample was not strongly anisotropic. The slopes of the best-fit lines were close to the expected Hertzian response which is $1/3$. The results calculated using cross-correlation are plotted on Figure 6.57 and a different trend to the two-dimensional fast Fourier transform plots was found. Here $G_{zx}$ was consistently the largest value and the slopes of the best-fit lines were larger than the plot on Figure 6.56. Due to the disparity in the results for constrained moduli calculated using cross-correlation and fabric tensor the values of $G_{ij}$ calculated using this method may not be accurate.

### 6.6.3 Stress probe results

Stress probe tests were carried out on the sample to determine their elastic moduli independently to the wave propagation tests at different confining pressures. The stress probes were applied to the flexible bounded samples by increasing the stress applied to the sample in each of the three principal directions by 10% of the isotropic confining pressure. The confining pressures chosen for analysis were 100kPa, 500kPa and 1MPa. The change in axial stress and change in axial strain were measured allowing a Young’s moduli ($E_i$) to be calculated for each of the directions that the probe was carried out, i.e. x-, y- and z-direction. Poisson’s ratios ($v_{ij}$) were measured for the probes in the x- or y-directions as the xy-plane was isotropic. The shear modulus ($G_{xy}$) in the plane of isotropy could be calculated using the equation below:

$$G_{xy} = \frac{E_x}{2(1 + v_{xy})}$$
Two measurement regions were considered in each sample: the whole sample and the measurement sphere which had a centre at the centre of the sample and a diameter that was 80% of the sample length.

The resulting Young’s moduli from the stress probes were plotted against confining pressure on Figure 6.58. The value of Young’s modulus in the z-direction lay above the values of Young’s modulus in the x- and y-directions at both 500kPa and 1MPa but not at 100kPa for the measurement sphere region. There was more scatter among the stress probe values of Young’s modulus compared with the constrained modulus values calculated using wave propagation simulations and the two-dimensional fast Fourier transform interpretation method. The exponent relationship between Young’s modulus and confining pressure (alpha) was found to be between 0.34 and 0.48. The expected alpha was 1/3 due to the Hertz-Mindlin contact model. The Poisson’s ratios calculated from probes in the x- or y-directions are given on Table 6.7. The measurement sphere results showed a bit of scatter with a minimum value equal to 0.15 and a maximum value of 0.34. The whole sample results were not very scattered if results at 500kPa were omitted; however these results were much lower than the mean of the other values (0.14). By comparison the results were approximately zero for Poisson’s ratios calculated when the sample was confined at 500kPa. The magnitudes of the Young’s moduli calculated from the stress probes was similar to the magnitudes of the constrained moduli calculated from the wave propagation tests as the values of Poisson’s ratios were small. The shear moduli calculated using Equation 6.6 were compared with the shear moduli from using wave propagation tests calculated using the two-dimensional fast Fourier transform on Figure 6.59. The magnitudes of the $G$ values are similar at 500kPa and 1MPa but differ at 100kPa with the measurement sphere region stress probe value of $G_{xy}$ significantly lower than all other values. If that individual value is discarded then the agreement among the results is quite good. The alpha value for relating shear modulus with confining pressure was found to be between 0.33 and 0.44 for all tests except for the values of $G_{xy}$ calculating using the particles lying within the measurement sphere region. The value for alpha here is 0.54 which is higher than the other tests.

6.6.4 Effect of reversing wave propagation direction

Received signal
A shear wave was propagated in the xy-plane in the negative x-direction, i.e. from the previously used x-direction receiver to the x-direction transmitter. The purpose was to
investigate the effect of the path direction of the wave propagation through the sample. The received signal from this test was compared with the received signal from the original test in the positive x-direction in the time-domain. They are illustrated on Figure 6.60 and it was observed that when the propagation direction was reversed the amplitude of the received signal increased. This was because the positive x-direction transmitter had a connectivity of 4 while the negative x-direction transmitter had a connectivity of 5. As outlined previously increasing the connectivity of the transmitter increases the amplitude of the propagating shear waves and consequently increases the amplitude of the received signal. The shape of the received signals was also different reflecting the influence of the local packings of particles around the transmitters.

When the signals were compared in the frequency domain on Figure 6.61 the increased amplitude when the signal propagation direction was reversed was confirmed. The maximum “threshold” frequency appeared to occur in a similar place in both samples indicating that this was a sample response rather than propagation path dependent.

The wave speeds for both tests were calculated using the two-dimensional fast Fourier transform and cross-correlation. The speed of the wave propagating in the positive x-direction was 269.70m/s and the speed of the wave propagating in the negative x-direction was 267.95m/s using the two-dimensional fast Fourier transform. These wave speeds match well and showed that the shear stiffness in the xy-plane was the same regardless of propagation direction. Using cross-correlation the speeds calculated were 253.28m/s and 248.32m/s for the positive and negative x-directions respectively. The match between these speeds was not as good indicating that they may be influenced by the local packings around the receivers and the amount of kinetic energy that was inputted by the transmitter particle.

Micromechanics

On Figure 6.62 the individual velocity vectors are plotted of the simulation on a plan view of the wave propagating in the negative x-direction, i.e. the reversal of the propagation direction. The velocity vectors only considered the x and y components for direction and the magnitude was calculated using these two components only. The slice of the sample was 5mm thick and was located mid-way along the z-axis. Only particle velocity vectors that had a magnitude less than 0.5mm/s were plotted to reduce the clouding of the simulation response due to the large velocities near the transmitter. This plot was compared with Figure 6.14 for a wave propagating in the positive x-direction. On time point (a) the movement of the
transmitter created a lobe in the sample that was observed and the highest magnitude velocity vectors were located near the transmitter. The circular shear wave lobe was formed on time points (b) and (c) and was seen to move through the system towards the receiver. The wave interacted with the flexible boundaries during these time points and complicated reflected waves were produced that travel diagonally from the edge towards the centre of the sample. The magnitudes of the velocity vectors were larger due to the higher connectivity of this transmitter particle. The wave appeared to arrive between time points (d) and (e) and there was evidence of frequency filtering as some large amplitude waves were trapped at the transmitter end of the sample at time point (f).

6.6.5 Effect of wall boundaries

Received signal
A shear wave was propagated through a sample confined with wall boundaries to investigate the effect of boundary conditions on the sample. This can be related to the parametric study on boundary conditions carried out in Chapter 5. The wave was propagated in the xy-plane in the positive x-direction. Figure 6.63 compares the received signal obtained from the flexible bounded sample with a signal obtained from the wall bounded sample. The amplitudes of each wave were observed to be similar but the shape of the received signal from the wall bounded sample was quite different. The receiver in the rigidly bounded sample was permanently offset by the arrival of the shear wave indicating a local plastic response. Rearrangement of the packing due to the application of flexible boundaries led to the differences in the movement of the receiver particle as the local packing around the receiver was now different.

In the frequency domain comparison of the two signals illustrated on Figure 6.64 there was a large amplitude component observed near zero on the frequency axis for the wave propagating through the wall bounded sample. This was the result of the offset in the received signal observed on Figure 6.63. Otherwise the amplitudes of the frequencies present in the wave were similar to the amplitudes of the frequencies propagating through the flexible bounded sample. Frequency filtering was observed to occur at similar frequencies in the wall bounded sample than in the flexible bounded sample. The maximum frequency observed in the wall sample was approximately 15.66kHz and in the flexible bounded sample it was 15.78kHz. This was not expected but will be discussed in relation to the wave speeds below.
The speeds of the shear waves propagating through the sample were calculated using the two-dimensional fast Fourier transform and cross-correlation methods. The wave speeds calculated using the two-dimensional fast Fourier transform were found to be 269.70 m/s and 253.67 m/s for the flexible bounded sample and the wall bounded sample respectively. Using cross-correlation the speeds were found to be 253.28 m/s and 255.18 m/s. The system wide response was less stiff when wall boundaries were used while there was little or no effect on the relationship between the transmitted and received signals as indicated by cross-correlation. It could be that the wall boundaries have affected the entire system response, measured by the two-dimensional fast Fourier transform, but not the relationship between transmitted and received signal, measured by cross-correlation. This confirmed the frequency domain plots on Figure 6.64 that showed frequency filtering occurring at lower frequencies in the wall bounded sample than in the flexible bounded sample. There was little or no variation in shear wave speed in the regularly packed sample.

**Micromechanics**

On Figure 6.65 the individual velocity vectors are plotted of the simulation on a plane view of the wall bounded simulation. The velocity vectors only considered the x and y components for direction and the magnitude was calculated using these two components only. The slice of the sample was 5 mm thick and was located mid-way along the z-axis. Only particle velocity vectors that had a magnitude less than 0.5 mm/s were plotted to reduce the clouding of the simulation response due to the large velocities near the transmitter. This plot was compared with Figure 6.14 for a wave propagating in the flexible bounded simulation. On time point (a) the movement of the transmitter created a lobe in the sample that was observed and the highest magnitude velocity vectors were located near the transmitter. As the wave propagated through the system it was observed to be very different to Figure 6.14 and appeared to be more similar to the compressional wave behaviour on Figure 6.48. The compressional wave may have been caused by reflections off the wall boundary at the transmitter end of the sample. It made it very hard to discern any shear waves propagating through the sample. The compressional wave appeared to arrive between time points (c) and (d).
6.6.6 Effect of force-driven transmitter

Received signal

A force-driven simulation was carried out to compare with the results of previous displacement-driven simulations. A shear wave was propagated in the xy-plane in the positive x-direction. The out-of-balance forces acting on the transmitter particle during a displacement-driven simulation were calculated and the y-component of this force was used as transmitter force amplitude for the force-driven simulation. The boundary conditions were the flexible boundary conditions. The resulting transmitted and received signals are plotted on Figure 6.66 for the displacement-driven and force-driven simulations. The amplitudes were plotted as displacement. The difference in transmitted amplitude and shape between the two signals was immediately apparent. The force-driven simulation produced a lop-sided signal and a permanent offset in the position of the transmitter. The amplitude of the force-driven simulation in terms of displacement was larger than the displacement-driven simulation. The received signals in both cases were quite similar, particularly in the shape of the oscillations. The only difference was in the amplitude of the signals. The force-driven simulation had a larger amplitude received signal than the displacement-driven simulation due to the larger amplitude transmitter signal in the force-driven simulation.

Comparing the signals in the frequency domain on Figure 6.67 confirms the observations made in the time domain. Large amplitude near zero frequency on the transmitted signal indicates the permanent offset that can be seen on the Figure 6.66. The transmitted force-driven amplitude was found to be larger than the transmitted displacement-driven amplitude. The received amplitudes were found to be similar except that the force-driven received amplitude, at 2.74x10^-5mm, was larger than the displacement-driven received amplitude, at 7.72x10^-6mm. The second peak on the received force-driven amplitude plot was found to be larger relative to the neighbouring peaks than the second peak on the received displacement-driven amplitude. The frequencies were observed to be filtered similarly with both types of input, highlighting that frequency filtering is a system wide response. The maximum frequency observed in the displacement-driven simulation was 15.78kHz and in the force-driven simulation was 15.55kHz.

The wave speeds for the force-driven simulation and the displacement-driven simulation were calculated using the two-dimensional fast Fourier transform method and the cross-correlation method. The speeds calculated using the two-dimensional fast Fourier transform
method were 269.70m/s and 279.56m/s for the displacement-driven and force-driven simulations respectively. The speeds calculated using cross-correlation were 253.28m/s and 264.82m/s. The variation in speeds was similar for both methods. The force-driven wave was faster than the displacement-driven simulation. The number of sliding contacts was examined in both simulations with the displacement-driven simulation on Figure 6.11 (b) and the force-driven simulation on Figure 6.68. The number of sliding contacts increased to a higher value on Figure 6.11 than on Figure 6.68 where the number of sliding contacts did overshoot 8,000 in the displacement-driven simulation while it remained below 8,000 in the force-driven simulation. There were approximately 1,000 more sliding contacts in the displacement-driven simulation compared to the force-driven simulation. This would lower the stiffness of the sample and this would have lowered the speed of the displacement-driven wave propagating through the sample.

Micromechanics
On Figure 6.69 the individual velocity vectors are plotted of the simulation on a plane view of the force-driven simulation. The velocity vectors only considered the x and y components for direction and the magnitude was calculated using these two components only. The slice of the sample was 5mm thick and was located mid-way along the z-axis. Only particle velocity vectors that had a magnitude less than 0.5mm/s were plotted to reduce the clouding of the simulation response due to the large velocities near the transmitter. This plot was compared with Figure 6.14 for the displacement-driven simulation. On time point (a) the movement of the transmitter created a lobe in the sample that was observed and the highest magnitude velocity vectors were located near the transmitter. The wave propagation through the sample was very similar to the displacement-driven simulation on Figure 6.14. Time points (b) and (c) illustrate a central shear wave lobe forming in the sample. The shear wave arrived between time points (d) and (e). The velocity vectors had larger amplitudes compared to the displacement-driven simulation due to the larger amplitude transmitted wave. Frequency filtering could be observed on time point (f) where many velocity vectors were trapped at the receiver end of the sample.

6.7 Conclusions
The preparation procedure followed in this research proved a number of points:
- It is possible to transfer large, pluviated samples from an open-source, parallelised code such as LAMMPS to a commercial code such as PFC3D provided the correct shear contact force data are transferred along with the particle positions and radii.
- The random sample appeared to be sufficiently heterogeneous on the basis of a number of statistical measures including contact force rose diagrams, average coordination number and the radial (pair) distribution function, although there was some latticing present at the boundaries.
- The received signal from the DEM simulation is directly comparable with the received signals from the laboratory tests and both display striking similarities. This is encouraging for the use of DEM simulations to model laboratory tests.

The propagation of the waves through the sample was readily visualised using:

- the individual particle velocity vectors,
- the particle velocity components in one direction,
- the representative particle shear stresses,
- the individual particle kinetic energies.

Analytical methods were implemented on the randomly packed sample with varying degree of success:

- Effective medium theory was found to over predict sample stiffness considerably and does not account for inherent anisotropy which is present in this sample due to its preparation method.
- The Sanchez-Salinero analytical solution for the near-field effect accurately predicted the arrival of the near-field effect when the shear wave speed calculated using the two-dimensional fast Fourier transform method was inputted.

Frequency filtering was observed in this sample. This was observed in a number of ways:

- The amplitude versus frequency plots show a maximum frequency or “threshold” frequency above which no frequencies propagate.
- This maximum frequency was observed to be a function of confining pressure. Theoretically this maximum frequency is a function of the interparticle contact stiffness so this explains the link to confining pressure.
The amplitude of the received signal was found to reduce as the transmitting frequency increased. This was found in the experimental work also. Increasing the frequency of the sine wave increases the amplitudes associated with frequencies above the maximum will frequency which will not propagate through though the sample.

Different travel time determination techniques were used and critically assessed in this research:

- The two-dimensional fast Fourier transform was found to be the most reliable of the methods after comparing results for waves transmitted at different frequencies.
- Waves were propagated in different directions and in different shear planes. Using the two-dimensional fast Fourier transform method the sample was found to be cross-anisotropic with $M_x = M_y \neq M_z$ and $G_{xy} = G_{yx} \neq G_{yz} = G_{zy} \neq G_{xz} = G_{zx}$.
- The relationship between elastic moduli and confining pressure was found to be approximately 1/3.

Parametric studies were carried out on the sample to investigate the effect of propagation direction, sample boundary conditions and the differences between a displacement-driven and force-driven transmitter:

- The direction of wave propagation along the same principal axis affected the shape and amplitude of the received signal but not the wave speed. This highlights the effect of connectivity and local packing around the transmitter and receiver.
- In general, the connectivity of the transmitter and local packing of the particle contacting the transmitter influence the kinetic energy inputted to the sample, the magnitude of the waves that propagated through the sample and the amplitude of the received signal that was recorded.
- The boundary conditions applied to the sample affected the amplitude and shape of the received signal, namely flexible and wall boundaries. They also appeared to affect the stiffness and caused frequency filtering to occur at different frequency values.
- Whether the wave was inputted by a displacement- or force-driven simulation affected the amplitude of the received signal but not the shape. The frequency filtering appeared to occur at similar values, although the force-driven wave caused
fewer sliding contacts in the sample. This had the effect of the shear wave speed measured from the force-driven simulation to be faster than the one measured from the displacement-driven simulation.
6.8 Figures

Figure 6.1: Layout of sample with particles coloured by applied force.

Figure 6.2: Histogram illustrating the normal distribution of particle sizes (top) before removal of particles above 100mm and (bottom) after removal of particles above 100mm.
Figure 6.3: Contact force rose diagrams for contacts acting in (a) the xy-plane including boundary particles, (b) the xz-plane including boundary particles, (c) the xy-plane excluding boundary particles and (d) the xz-plane excluding boundary particles. Sectors are coloured by factor which multiplied by overall mean contact force gives the local mean contact force in that sector. The yz-plane is identical to the xz-plane.
Figure 6.4: Histogram of particle connectivity before bender element test illustrating that the mean particle connectivity is approximately 5.5 and very few particles have no connectivity or very high connectivity, > 8.

Figure 6.5: Radial pair distribution function illustrating the likelihood of finding a particle located at a given distance from a particular particle. A relatively horizontal line following the initial peak indicates a randomly packed sample where there is an equal likelihood of finding a particle at any given distance.
Figure 6.6: Variation in sample void ratio over the z-direction. Void ratios are calculated based on the particles and parts of particles that lie within a certain section.

Figure 6.7: Variation in sample void ratio over the x-direction. Void ratios are calculated based on the particles and parts of particles that lie within a certain section.
Figure 6.8: Comparison between applied stresses to the flexible bounded sample and the internal measurement region stresses.

Figure 6.9: Layout of bender element test with single particle transmitter and single particle receiver.
Figure 6.10: A received signal for (a) the DEM simulation and (b) the randomly packed laboratory sample (University of Bristol). Both samples are of equal size and contain particles of similar size and material properties. DEM: $\sigma_0 = 100\text{kPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 3.65$ and $\lambda/d_{50} = 9.93$.

Figure 6.11: Measures of plasticity (a) global average coordination number, (b) sliding contacts, occurring in the sample during the bender element test. $\sigma_0 = 100\text{kPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 3.65$ and $\lambda/d_{50} = 9.93$. 

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Figure 6.12: Effect of transmitter connectivity on the amount of kinetic energy generated during the wave propagation simulation. (x-direction – $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 3.53$ and $\lambda/d_{50} = 9.93$; y-direction – $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 3.65$ and $\lambda/d_{50} = 9.93$; z-direction – $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 3.64$ and $\lambda/d_{50} = 9.93$).

Figure 6.13: Effect of local fabric tensor on the amount of kinetic energy generated during the wave propagation simulation in the y-direction. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 3.65$ and $\lambda/d_{50} = 9.93$. 
Figure 6.14: Individual particle velocity vectors (x & y components) scaled by magnitude considering x and y components of velocity only. View is a plan view of a 5mm thick cross-section through the sample. Only particle velocities less than or equal to 0.5mm/s magnitude are plotted to prevent larger velocities from "clouding" the system response. \( \sigma_0 = 100\text{kPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 3.53 \) and \( \lambda/d_0 = 9.93 \).

Figure 6.15: Individual particle velocity vectors (x & z components) scaled by magnitude considering x and z components of velocity only. View is an elevation view of a 5mm thick cross-section through the sample. Only particle velocities less than or equal to 0.5mm/s magnitude are plotted to prevent larger velocities from "clouding" the system response. \( \sigma_0 = 100\text{kPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 3.53 \) and \( \lambda/d_0 = 9.93 \).
Figure 6.16: Relative particle y-velocity component illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along z-axis. $\sigma_0 = 100\text{kPa}, f_{trans} = 15\text{kHz}, R_d = 3.53$ and $\lambda/d_{50} = 9.93$.

Figure 6.17: Relative particle y-velocity component illustrating wave propagation through the sample at time point (d) at a higher colour resolution (plan view). The cross-section through the packing is at mid-way along z-axis. $\sigma_0 = 100\text{kPa}, f_{trans} = 15\text{kHz}, R_d = 3.53$ and $\lambda/d_{50} = 9.93$. 

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Figure 6.18: Relative representative particle shear stresses (average of $\sigma_{xy}$ and $\sigma_{yx}$) illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along z-axis. $\sigma_0 = 100\text{ kPa}, f_{\text{trans}} = 15\text{ kHz}, R_d = 3.53$ and $\lambda/d_{\text{eq}} = 9.93$.

Figure 6.19: Relative representative particle shear stresses (average of $\sigma_{xy}$ and $\sigma_{yx}$) illustrating wave propagation through the sample at time point (d) at a higher colour resolution (plan view). The cross-section through the packing is at mid-way along z-axis. $\sigma_0 = 100\text{ kPa}, f_{\text{trans}} = 15\text{ kHz}, R_d = 3.53$ and $\lambda/d_{\text{eq}} = 9.93$. 
Figure 6.20: Relative particle kinetic energies (sum of translational and rotational) illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along z-axis. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 3.53$ and $\lambda/d_0 = 9.93$.

Figure 6.21: Relative particle kinetic energies (sum of translational and rotational) illustrating wave propagation through the sample at time point (d) at a higher colour resolution (plan view). The cross-section through the packing is at mid-way along z-axis. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 3.53$ and $\lambda/d_0 = 9.93$. 
Figure 6.22: Calculated values of Young's modulus in the x-direction ($E_x$) and shear modulus in the xy-plane ($G_{xy}$) for different confining pressures using effective medium theory (EMT).

Figure 6.23: A recorded signal from a numerical bender element test compared with the result from the Sanchez-Salinero equations. The Sanchez-Salinero solution is scaled by $2 \times 10^6$ so that it can be observable with the recorded signal. Recorded signal: $\sigma_0 = 100$ kPa, $f_{\text{trans}} = 15$ kHz, $R_y = 3.53$ and $\lambda/d_{\text{ho}} = 9.93$. 
Figure 6.24: Comparison of transmitted signals (dashed) and received signals (solid) transmitted at different frequencies in the time domain (a) 7kHz ($\sigma_0 = 100\text{kPa}, R_d = 1.70$ and $\lambda/d_{so} = 21.27$), (b) 15kHz ($\sigma_0 = 100\text{kPa}, R_d = 3.53$ and $\lambda/d_{so} = 9.93$), (c) 20kHz ($\sigma_0 = 100\text{kPa}, R_d = 4.85$ and $\lambda/d_{so} = 7.45$), (d) 30kHz ($\sigma_0 = 100\text{kPa}, R_d = 7.28$ and $\lambda/d_{so} = 4.96$).

Figure 6.25: Individual particle velocity vectors (x & y components) scaled by magnitude considering x and y components of velocity only. View is a plan view of a 5mm thick cross-section through the sample. Transmitted signal frequency is 7kHz. Only particle velocities less than or equal to 0.5mm/s magnitude are plotted to prevent larger velocities from "clouding" the system response. $\sigma_0 = 100\text{kPa}, f_{trans} = 7\text{kHz}, R_d = 1.70$ and $\lambda/d_{so} = 21.27$. 
Figure 6.26: Individual particle velocity vectors (x & y components) scaled by magnitude considering x and y components of velocity only. View is a plan view of a 5mm thick cross-section through the sample. Transmitted signal frequency is 30kHz. Only particle velocities less than or equal to 0.5mm/s magnitude are plotted to prevent larger velocities from "clouding" the system response. $\sigma_0 = 100kPa$, $f_{trans} = 30kHz$, $R_d = 7.28$ and $\lambda/d_{iso} = 4.96$.

Figure 6.27: Comparison of transmitted signals (dashed) and received signals (solid) transmitted at different frequencies in the time domain from the laboratory tests (a) 7kHz, (b) 10kHz, (c) 15kHz, (d) 20kHz.
Travel time determination techniques

\[ V_S = \frac{d}{t_{\text{arr}}} \]
\[ d = \text{travel distance} \]
\[ t_{\text{arr}} = \text{travel time} \]

\[ G = \rho V_S^2 \]

Figure 6.28: Two time-domain travel time determination methods. Peak-peak is from the peak on the transmitted signal to the first peak on the received signal. First arrival is from the start of the transmitted signal to the point of first zero-crossing on the received signal. Received signal: \( \sigma_0 = 100\,\text{kPa}, f_{\text{trans}} = 15\,\text{kHz}, R_d = 3.53 \) and \( \lambda / d_{50} = 9.93 \).

Figure 6.29: Locations of characteristic arrival times on a typical numerical received signal. \( \sigma_0 = 100\,\text{kPa}, f_{\text{trans}} = 15\,\text{kHz}, R_d = 3.53 \) and \( \lambda / d_{50} = 9.93 \).
Figure 6.30: Cross-correlation function, received signal and transmitted signal plotted on normalised amplitude versus time plot. Red arrow indicates the peak on the cross-correlation function that corresponds with travel time. $\sigma_0 = 100\text{kPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 3.53$ and $\lambda/d_{50} = 9.93$.

Figure 6.31: Comparison of normalised transmitted signals (dashed) and normalised received signals (solid) transmitted at different frequencies in the frequency domain (a) 7kHz ($\sigma_0 = 100\text{kPa}, R_d = 1.70$ and $\lambda/d_{50} = 21.27$), (b) 15kHz ($\sigma_0 = 100\text{kPa}, R_d = 3.53$ and $\lambda/d_{50} = 9.93$), (c) 20kHz ($\sigma_0 = 100\text{kPa}, R_d = 4.85$ and $\lambda/d_{50} = 7.45$), (d) 30kHz ($\sigma_0 = 100\text{kPa}, R_d = 7.28$ and $\lambda/d_{50} = 4.96$).
Figure 6.32: Comparison of transmitted signals (dashed) and received signals (solid) transmitted at different frequencies in the frequency domain (a) 7kHz ($\sigma_0 = 100\text{kPa}$, $R_d = 1.70$ and $\lambda/d_{50} = 21.27$), (b) 15kHz ($\sigma_0 = 100\text{kPa}$, $R_d = 3.53$ and $\lambda/d_{50} = 9.93$), (c) 20kHz ($\sigma_0 = 100\text{kPa}$, $R_d = 4.85$ and $\lambda/d_{50} = 7.45$), (d) 30kHz ($\sigma_0 = 100\text{kPa}$, $R_d = 7.28$ and $\lambda/d_{50} = 4.96$).

Figure 6.33: Comparison of normalised transmitted signals (dashed) and normalised received signals (solid) transmitted at different frequencies in the frequency domain from the laboratory tests (a) 7kHz, (b) 10kHz, (c) 15kHz, (d) 20kHz.
Figure 6.34: Comparison of transmitted signals (dashed) and received signals (solid) transmitted at different frequencies in the frequency domain from the laboratory tests (a) 7kHz, (b) 10kHz, (c) 15kHz, (d) 20kHz.

Figure 6.35: Top – time domain plot and bottom – frequency domain plot of the received and transmitted signals for the following frequencies: 1.456kHz ($\sigma_0 = 100kPa$, $R_d = 0.34$ and $\lambda/d_{so} = 102.27$), 7kHz ($\sigma_0 = 100kPa$, $R_d = 1.70$ and $\lambda/d_{so} = 21.27$), 15kHz ($\sigma_0 = 100kPa$, $R_d = 3.53$ and $\lambda/d_{so} = 9.93$), 20kHz ($\sigma_0 = 100kPa$, $R_d = 4.85$ and $\lambda/d_{so} = 7.45$) and 30kHz ($\sigma_0 = 100kPa$, $R_d = 7.28$ and $\lambda/d_{so} = 4.96$).
Figure 6.36: Comparison of single pulse and ten pulses in top - time domain and bottom - frequency domain. $\sigma_0 = 100\text{kPa}, f_{trans} = 15\text{kHz}, R_d = 3.53$ and $\lambda/d_0 = 9.93$.

Figure 6.37: Normalised amplitude versus frequency for the sample at different confining pressures. Top - transmitted sine pulses, bottom - received sine pulses. ($\sigma_0 = 100\text{kPa}, f_{trans} = 15\text{kHz}, R_d = 3.53$ and $\lambda/d_0 = 9.93$; $\sigma_0 = 300\text{kPa}, f_{trans} = 15\text{kHz}, R_d = 2.91$ and $\lambda/d_0 = 12.03$; $\sigma_0 = 500\text{kPa}, f_{trans} = 15\text{kHz}, R_d = 2.67$ and $\lambda/d_0 = 13.10$; $\sigma_0 = 750\text{kPa}, f_{trans} = 15\text{kHz}, R_d = 2.49$ and $\lambda/d_0 = 14.05$; $\sigma_0 = 1\text{MPa}, f_{trans} = 15\text{kHz}, R_d = 2.36$ and $\lambda/d_0 = 14.78$).
Figure 6.38: Stacked phase versus frequency for the sample confined at 100kPa. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 3.53$ and $\lambda/d_0 = 9.93$.

Figure 6.39: Time-domain contour plot of position versus time where the contours are coloured by the displacement in the y-direction. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 3.53$ and $\lambda/d_0 = 9.93$. 
Figure 6.40: Time-domain surface plot of position versus time where the peaks are measured by the velocity in the y-direction. \( \sigma_0 = 100\text{kPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 3.53 \) and \( \lambda/d_{50} = 9.93 \).

Figure 6.41: Reduction in velocity magnitude squared as a function of particle position along the propagation axis. The dashed line is a line with a slope inversely proportional to the position. \( \sigma_0 = 100\text{kPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 3.53 \) and \( \lambda/d_{50} = 9.93 \).
Figure 6.42: Plot of frequency versus position coloured by amplitude for different confining pressures (a) 100kPa, (b) 500kPa, (c) 1MPa. Black indicates higher amplitude values than white. ($\sigma_0 = 100\text{kPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 3.53 \text{ and } \lambda/d_{50} = 9.93; \sigma_0 = 500\text{kPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 2.67 \text{ and } \lambda/d_{50} = 13.10; \sigma_0 = 1\text{MPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 2.36 \text{ and } \lambda/d_{50} = 14.78$).

Figure 6.43: Two-dimensional fast Fourier transform plot of angular velocity ($\omega$) versus wavenumber ($k$). The darker regions indicate more wave intensity associated with those particular angular velocities and wavenumbers. $\sigma_0 = 100\text{kPa}, f_{\text{trans}} = 30\text{kHz}, R_d = 7.05 \text{ and } \lambda/d_{50} = 4.96$. 
Figure 6.44: Plot of angular velocity versus wavenumber (inverse of the wavelength) coloured by the magnitude of the y-velocity. The transmitted signal was a sine pulse that was repeated ten times. Black indicates higher wave energy than white. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 3.53$ and $\lambda/d_{\text{to}} = 9.93$.

Figure 6.45: Comparison of different travel time determination techniques with effective medium theory (EMT) to calculate a value of $G_{xy}$ for the sample confined at 100kPa.
Figure 6.46: Variation in coordination number with confining pressure illustrated on a log-log plot.

Figure 6.47: Comparison of compressional waves propagating in different directions (x, y and z) through samples confined at different pressures (100kPa, 500kPa and 1000kPa).
Figure 6.48: Individual particle velocity vectors (x & y components) scaled by magnitude considering x and y components of velocity only. View is a plan view of a 5mm thick cross-section through the sample. Transmitted signal frequency is 15kHz. Only particle velocities less than or equal to 0.5mm/s magnitude are plotted to prevent larger velocities from "clouding" the system response. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 2.46$ and $\lambda/d_{50} = 14.21$.

Figure 6.49: Individual particle velocity vectors (x & y components) scaled by magnitude considering x and y components of velocity only. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 2.55$ and $\lambda/d_{50} = 14.21$. 

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Figure 6.50: Individual particle velocity vectors (y & z components) scaled by magnitude considering y and z components of velocity only. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 2.54$ and $\lambda/d_0 = 14.21$.

Figure 6.51: Comparison of constrained moduli, calculated using two-dimensional fast Fourier transforms, from compressional waves propagated in different directions. The confining pressures used were 100kPa, 300kPa, 500kPa, 750kPa and 1000kPa.
Figure 6.52: Comparison of constrained moduli, calculated using cross-correlation, from compressional waves propagated in different directions. The confining pressures used were 100kPa, 300kPa, 500kPa, 750kPa and 1000kPa.

Figure 6.53: Comparison of shear waves propagating in different planes (xy, yz and zx) through samples confined at different pressures (100kPa, 500kPa and 1000kPa).
Figure 6.54: Individual particle velocity vectors (y & z components) scaled by magnitude considering y and z components of velocity only. View is a plan view of a 5mm thick cross-section through the sample. Transmitted signal frequency is 15kHz. Only particle velocities less than or equal to 0.5mm/s magnitude are plotted to prevent larger velocities from "clouding" the system response. $\sigma_0 = 100kPa$, $f_{trans} = 15kHz$, $R_d = 3.65$ and $\lambda/d_{so} = 9.93$.

Figure 6.55: Individual particle velocity vectors (x & z components) scaled by magnitude considering x and z components of velocity only. $\sigma_0 = 100kPa$, $f_{trans} = 15kHz$, $R_d = 3.64$ and $\lambda/d_{so} = 9.93$. 
Figure 6.56: Comparison of shear moduli, calculated using two-dimensional fast Fourier transforms, from shear waves propagated in different directions. The confining pressures used were 100kPa, 300kPa, 500kPa, 750kPa and 1000kPa.

Figure 6.57: Comparison of shear moduli, calculated using cross-correlation, from shear waves propagated in different directions. The confining pressures used were 100kPa, 300kPa, 500kPa, 750kPa and 1000kPa.
Figure 6.58: Comparison of Young’s moduli ($E_i$) calculated from stress probe simulations. The two measurement regions considered were the entire sample and the central measurement sphere region.

Figure 6.59: Values of shear modulus ($G_{ij}$) calculated from the stress probe simulations compared with the shear modulus values calculated from the wave propagation simulation using the two-dimensional fast Fourier transform interpretation method. The two measurement regions considered were the entire sample and the central measurement sphere region.
Figure 6.60: Transmitted and received signals for shear waves propagating in the xy-plane in the positive x-direction (top) and negative x-direction (bottom). Time domain comparison. \( \sigma_0 = 100\text{kPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 3.53 \) and \( \lambda/d_0 = 9.93 \).

Figure 6.61: Transmitted and received signals for shear waves propagating in the xy-plane in the positive x-direction (top) and negative x-direction (bottom). Frequency domain comparison. \( \sigma_0 = 100\text{kPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 3.53 \) and \( \lambda/d_0 = 9.93 \).
Figure 6.62: Individual particle velocity vectors (x & y components) scaled by magnitude considering x and y components of velocity only. View is a plan view of a 5mm thick cross-section through the sample. Only particle velocities less than or equal to 0.5mm/s magnitude are plotted to prevent larger velocities from "clouding" the system response. $\sigma_0 = 100\text{kPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 3.53$ and $\lambda/d_0 = 9.93$.

Figure 6.63: Transmitted and received signals for shear waves propagating in the xy-plane with flexible boundaries (top) and wall boundaries (bottom). Time domain comparison. $\sigma_0 = 100\text{kPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 3.53$ and $\lambda/d_0 = 9.93$. The permanent offset in the bottom figure represents a local plastic response to the wave propagation.
Figure 6.64: Transmitted and received signals for shear waves propagating in the xy-plane with flexible boundaries (top) and wall boundaries (bottom). Flexible domain comparison. $\sigma_0 = 100\text{kPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 3.53$ and $\lambda/d_{50} = 9.93$.

Figure 6.65: Individual particle velocity vectors (x & y components) scaled by magnitude considering x and y components of velocity only. View is a plan view of a 5mm thick cross-section through the sample. Only particle velocities less than or equal to 0.5mm/s magnitude are plotted to prevent larger velocities from "clouding" the system response. $\sigma_0 = 100\text{kPa}, f_{\text{trans}} = 15\text{kHz}, R_d = 3.53$ and $\lambda/d_{50} = 9.93$. 
Figure 6.66: Transmitted and received signals for shear waves propagating in the xy-plane with displacement-driven transmitter (top) and force-driven transmitter (bottom). Time domain comparison. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 3.53$ and $\lambda/d_{50} = 9.93$.

Figure 6.67: Transmitted and received signals for shear waves propagating in the xy-plane with displacement-driven transmitter (top) and force-driven transmitter (bottom). Frequency domain comparison. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 3.53$ and $\lambda/d_{50} = 9.93$. 
Figure 6.68: Sliding contacts occurring in the sample during the force-driven simulation. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 3.65$ and $\lambda/d_0 = 9.93$.

Figure 6.69: Individual particle velocity vectors ($x$ & $y$ components) scaled by magnitude considering $x$ and $y$ components of velocity only. View is a plan view of a 5mm thick cross-section through the sample. Only particle velocities less than or equal to 0.5mm/s magnitude are plotted to prevent larger velocities from "clouding" the system response. $\sigma_0 = 100\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 3.53$ and $\lambda/d_0 = 9.93$. 
### 6.9 Tables

Table 6.1: Sample properties.

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<th>Property</th>
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<th>LAB</th>
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<td>Mean Particle Size</td>
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<tr>
<td>Particle Density [$\rho$]</td>
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</tr>
<tr>
<td>Interparticle Friction [$\mu$]</td>
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</tr>
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<td>Contact Model</td>
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</tr>
<tr>
<td>Particle Shear Modulus [G]</td>
<td>16.67x10^9 [Pa]</td>
<td></td>
</tr>
<tr>
<td>Particle Poisson’s Ratio [$\nu$]</td>
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<td></td>
</tr>
<tr>
<td>Viscous Damping at Contacts</td>
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<td></td>
</tr>
<tr>
<td>No. of Particles</td>
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<td></td>
</tr>
<tr>
<td>Frequency of the Sine Wave</td>
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<td>Transmitter Amplitude</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>y direction: 9.21x10^{-2} [m]</td>
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</tr>
<tr>
<td></td>
<td>z direction: 9.17x10^{-2} [m]</td>
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Table 6.2: Comparisons between DEM sample and laboratory sample.

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<tr>
<th>Property</th>
<th>DEM</th>
<th>LAB</th>
</tr>
</thead>
<tbody>
<tr>
<td>Preparation</td>
<td>Dry pluviation</td>
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</tr>
<tr>
<td>Volume [m^3]</td>
<td>~1x10^{-3}</td>
<td></td>
</tr>
<tr>
<td>Void Ratio [-]</td>
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<td>0.67</td>
</tr>
<tr>
<td>Mass [kg]</td>
<td>1.27</td>
<td>1.30</td>
</tr>
</tbody>
</table>
Table 6.3: Fabric tensor measured for the DEM sample at different confining pressures.

<table>
<thead>
<tr>
<th></th>
<th>100kPa</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.33</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>0.00</td>
<td>0.33</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>0.00</td>
<td>0.00</td>
<td>0.34</td>
</tr>
<tr>
<td>300kPa</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.33</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>0.00</td>
<td>0.33</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>0.00</td>
<td>0.00</td>
<td>0.34</td>
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<tr>
<td>500kPa</td>
<td></td>
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<td></td>
</tr>
<tr>
<td></td>
<td>0.33</td>
<td>0.00</td>
<td>0.00</td>
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<tr>
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<td>0.00</td>
<td>0.33</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>0.00</td>
<td>0.00</td>
<td>0.34</td>
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<tr>
<td>750kPa</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td></td>
<td>0.33</td>
<td>0.00</td>
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<td></td>
<td>0.00</td>
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<tr>
<td></td>
<td>0.00</td>
<td>0.00</td>
<td>0.34</td>
</tr>
<tr>
<td>1000kPa</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.33</td>
<td>0.00</td>
<td>0.00</td>
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<tr>
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</tr>
<tr>
<td></td>
<td>0.00</td>
<td>0.00</td>
<td>0.34</td>
</tr>
</tbody>
</table>
Table 6.4: Sample $G_{\text{max}}$ values calculated using different time-domain travel time determination techniques for different frequency sine pulses.

<table>
<thead>
<tr>
<th>Sine Pulses</th>
<th>$G_{\text{max}}$ [MPa] from Different Travel Time Determination Techniques</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frequency - [kHz]</td>
<td>First Local Minimum</td>
</tr>
<tr>
<td>7</td>
<td>121.77</td>
</tr>
<tr>
<td>15</td>
<td>136.99</td>
</tr>
<tr>
<td>20</td>
<td>134.36</td>
</tr>
<tr>
<td>30</td>
<td>132.84</td>
</tr>
<tr>
<td>Std Dev</td>
<td>6.70</td>
</tr>
</tbody>
</table>

Table 6.5: Sample $G_{\text{max}}$ values calculated using different frequency-domain travel time determination techniques for different frequency sine pulses.

<table>
<thead>
<tr>
<th>Sine Pulses</th>
<th>$G_{\text{max}}$ [MPa] from Different Travel Time Determination Techniques</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frequency - [kHz]</td>
<td>Phase vs. Frequency</td>
</tr>
<tr>
<td>7</td>
<td>7.30</td>
</tr>
<tr>
<td>15</td>
<td>15.55</td>
</tr>
<tr>
<td>20</td>
<td>10.51</td>
</tr>
<tr>
<td>30</td>
<td>10.51</td>
</tr>
<tr>
<td>Std Dev</td>
<td>3.41</td>
</tr>
</tbody>
</table>
Table 6.6: Measured values of constrained moduli, $M_i$, and shear moduli, $G_{ij}$, for the sample confined at 100kPa using wave propagation tests. Two wave interpretation techniques are used namely, two-dimensional fast Fourier transform plots and cross-correlation.

<table>
<thead>
<tr>
<th>Moduli calculated for sample confined at 100kPa</th>
<th>Two-dimensional fast Fourier transform plots</th>
<th>Cross-correlation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M_x$</td>
<td>261.25 MPa</td>
<td>221.79 MPa</td>
</tr>
<tr>
<td>$M_y$</td>
<td>260.95 MPa</td>
<td>253.16 MPa</td>
</tr>
<tr>
<td>$M_z$</td>
<td>263.97 MPa</td>
<td>216.85 MPa</td>
</tr>
<tr>
<td>$G_{xy}$</td>
<td>96.74 MPa</td>
<td>85.32 MPa</td>
</tr>
<tr>
<td>$G_{yx}$</td>
<td>98.83 MPa</td>
<td>101.74 MPa</td>
</tr>
<tr>
<td>$G_{yz}$</td>
<td>103.66 MPa</td>
<td>89.02 MPa</td>
</tr>
<tr>
<td>$G_{zy}$</td>
<td>104.97 MPa</td>
<td>87.36 MPa</td>
</tr>
<tr>
<td>$G_{xz}$</td>
<td>100.52 MPa</td>
<td>90.56 MPa</td>
</tr>
<tr>
<td>$G_{zx}$</td>
<td>99.91 MPa</td>
<td>97.95 MPa</td>
</tr>
</tbody>
</table>

Table 6.7: Poisson’s ratios calculated from stress probes on the randomly packed sample confined at different isotropic confining pressures. The xy-plane was found to be isotropic so the Poisson’s ratios were calculated in that plane only.

<table>
<thead>
<tr>
<th>Confining Pressure – [kPa]</th>
<th>Poisson’s Ratio – [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Whole Sample</td>
</tr>
<tr>
<td></td>
<td>$\nu_{xy}$</td>
</tr>
<tr>
<td>100</td>
<td>0.15</td>
</tr>
<tr>
<td>500</td>
<td>0.02</td>
</tr>
<tr>
<td>1000</td>
<td>0.15</td>
</tr>
</tbody>
</table>
7 Stress-induced anisotropy

7.1 Introduction

This Chapter describes two series of simulations that were carried out under anisotropic confining stress conditions. Two samples were considered; the regularly packed sample outlined in Chapter 5 (81,576 particles) and the randomly packed sample outlined in Chapter 6 (64,136 particles). For both samples, the initial isotropic confining pressure was 300kPa and the mean confining pressure was maintained close to this value. In the parametric study, the major principal stress was specified to increase from 300kPa to 375kPa, the minor principal stress was specified to decrease from 300kPa to 225kPa and the intermediate principal stress was specified to remain constant at 300kPa. Wave propagation tests to measure stiffness were carried out at 25kPa intervals. The tolerances associated with the stress control procedure used were finite and so the actual stresses deviated somewhat from the target values. The tolerance in the variation of these stresses was ±2.50%. The simulations on the regularly packed sample were created with the aid of Mr. Philip Vautier who carried out an MEng research project on wave propagation through anisotropically compressed samples, Vautier (2012).

7.2 Regularly packed sample

7.2.1 Sample preparation and initial properties

The sample properties are outlined in Table 7.1. In all cases the servo-controlled wall system described in Chapter 5 was used to compress the sample to the required confining pressures. The data given on Table 7.2 show that the fabric tensor does not change with increasing degree of induced stress anisotropy. This is to be expected for the stable, lattice packing considered here. Figure 7.1 illustrates the sample and Table 7.3 outlines the three anisotropic stress cases that were specified (± 2.5%) and the variation of the stresses in each of the principal directions. The stress states that were reached using this algorithm were measured by examining the stresses acting on the wall elements and examining the stress tensors of the particles (Table 7.4). The value of mean stress, $p'$, is included on Table 7.4 to show that there was some variation in mean stress as the anisotropic confining pressures were reached. The sample underwent volumetric straining ($\Delta \varepsilon_{vol}$) with Cases 1 and 2 exhibiting consistent
contractive behaviour. For Case 3, for one stress increment the sample contracted while the sample dilated for the other two stress increments. The representative stress tensors for the particles are illustrated on Table 7.5 and \( p' \) is included with \( \Delta \varepsilon_{vol} \). The variation in \( p' \) caused a variation in volumetric strain in the sample and this affected the stiffness that were measured to a small extent. Due to the small magnitude in variation of \( p' \) the effect of the variation on stiffness was not considered in further analysis. The wall boundaries were replaced by flexible boundaries prior to simulating the bender element test and there was a fluctuation in the stress applied so the system was cycled to allow it to equilibrate. After cycling, the ball stress and strain tensors were used to measure the sample stress and strain change from the same point in the isotropic case, i.e. when the isotropic flexible boundary was applied. Table 7.6 summarises the stresses in each of the principal directions, the mean stress and the change in volumetric strain reached after cycling with the flexible boundary conditions applied.

The wave was input using the single-particle approach described in Chapter 5 and as illustrated in Figure 7.2. Particles were chosen on different faces and displaced in different directions to measure different shear moduli and a summary of the planes used is provided in Figure 7.3.

7.2.2 Particle-scale analysis

An example received signal under increasing stress in the direction of propagation (\( \sigma_{prop} \)) is shown on Figure 7.4 for waves propagating in the xy-plane. The signal was transmitted at 30kHz and is a single sine pulse. As \( \sigma_{prop} \) increased the travel time of the wave was observed to reduce. This was observed more clearly on Figure 7.5 which zooms in on the first zero-crossing. \( G_{xy} \) increased as the stress applied to the x-direction increased in agreement with previous observations by Roesler (1979). The different combinations of changes in \( \sigma_{prop} \), stress in the direction of oscillation (\( \sigma_{osc} \)) and stress in the third direction (\( \sigma_{third} \)) will be explored in Section 7.2.3.

The micromechanical interpretation methods documented in Chapters 5 and 6 were used to investigate whether the propagating wave front changed shape as the applied stress became increasingly anisotropic. In addition individual particle kinetic energies were used for further visualisation.
**Individual particle velocity vectors**

Figure 7.6 illustrates the velocity vectors for the regularly packed sample isotropically confined at 294.60kPa. The plots were generated using the approach used in Chapter 5 (e.g. Figure 5.14). Figure 7.7 plots the velocity vectors when the confining pressure in the propagating direction, $x$, was increased by 73.85kPa and the confining pressure in the oscillating direction, $y$, was kept constant and the stress in the third direction was reduced by 73.08kPa. The wave was plotted using an identical method to the previous plot. It is hard to discern any differences between the propagating waves as the approximate 75kPa change in stress appeared to not affect the wave propagation mechanism. There is, however, a reduction in the amplitude of the propagating signal with an approximate 75kPa change in stress. The received signal plotted in the centre of the figure appeared to arrive slightly earlier in the anisotropically stressed sample than in the isotropically stressed sample.

**Individual particle rotational velocities**

The isotropic confining pressure case is illustrated on Figure 7.8 where $\sigma_x = \sigma_y = 295.64$ kPa and $\sigma_z = 292.58$ kPa. Figure 7.9 plots the individual particle rotational velocities for the anisotropic stress case with $\sigma_x = 369.49$ kPa, $\sigma_y = 295.62$ kPa and $\sigma_z = 219.50$ kPa. No change in the wave propagation mechanism was noted but the received signal appeared to arrive earlier in this plot compared to the arrival in Figure 7.8. This was similar to the previous observation regarding the individual velocity vectors, Figure 7.7, although no change in amplitude was observed.

**Individual particle kinetic energies**

The isotropic confining pressure case is illustrated on Figure 7.10 while Figure 7.11 plots the individual particle kinetic energies for the anisotropic stress case. There was no change in the wave propagation mechanism except for a small reduction in the propagating wave and the received signal appeared to arrive earlier in this plot compared to the arrival in Figure 7.10.

### 7.2.3 Analysis of the received signal

To determine the shear wave velocity the received signals were firstly considered, i.e. the data that would be available in a physical test are used. An increase in $\sigma_{prop}$ was expected to produce the largest changes in wave speed and the objective was to establish whether both methods capture this trend. A change in $\sigma_{osc}$ was also expected to affect the wave speed; however, changing $\sigma_{third}$, i.e. normal to the shear plane, was predicted to have a limited effect.
The following cases were considered. Case A: increasing $\sigma_{\text{prop}}$, keeping $\sigma_{\text{osc}}$ constant and decreasing $\sigma_{\text{third}}$; Case B: keeping $\sigma_{\text{prop}}$ constant, decreasing $\sigma_{\text{osc}}$ and increasing $\sigma_{\text{third}}$ and Case C: decreasing $\sigma_{\text{prop}}$, increasing $\sigma_{\text{osc}}$ and keeping $\sigma_{\text{third}}$ constant. These same classifications are used when discussing the stiffness of the sample later in Section 6.6.

**Case A: $\sigma_{\text{prop}}$ increasing, $\sigma_{\text{osc}}$ constant and $\sigma_{\text{third}}$ decreasing**

The received signals from the Case A simulations for each of the shear planes, $G_{xy}$, $G_{yz}$ and $G_{zx}$ are plotted in the time domain on Figure 7.12. The received signals were plotted at a smaller scale than the transmitted signal scale. The earlier parts of the received signal (< 2.2x10^{-4}s) exhibit little sensitivity to the stress anisotropy. However, the amplitude of the later parts of the signals was noticeably affected by the changes in $\sigma_{\text{prop}}$ with the amplitude reducing as $\sigma_{\text{prop}}$ increased.

Figure 7.13 zooms in on the first zero-crossing point in Figure 7.12 to examine the effect of increasing $\sigma_{\text{prop}}$ more closely. The first-zero crossing occurred progressively earlier on the received signal as $\sigma_{\text{prop}}$ increased, showing that the wave speed increased with $\sigma_{\text{prop}}$, which agrees with the literature. The difference in arrival time was larger in the yz-shear plane (-0.027x10^{-4}s) and zx-shear plane (-0.030x10^{-4}s) compared to the xy-shear plane (-0.015x10^{-4}s).

The data presented in Figure 7.12 and Figure 7.13 are considered in the frequency domain in Figure 7.14 and the shapes of the transmitted and received spectra are clearly similar for waves propagating in all shear planes. In all cases there is a zero frequency offset, and there are two local maxima at frequencies of between 10kHz and 20kHz and between 20kHz and 30kHz while at frequencies above 40kHz the amplitudes are very small. As was observed in Figure 7.12 the amplitude of the received signals was affected by the degree of anisotropy of the applied stress. As the stress anisotropy increased the amplitudes of the received signals decreased across all frequencies. The maximum peak amplitude on the xy-plane plots decreased from 7.241x10^{-8}mm to 5.712x10^{-8}mm. On the yz-plane the peak decreased from 7.939x10^{-8}mm to 6.487x10^{-8}mm while on the zx-plane the peak decreased from 7.823x10^{-8}mm to 5.747x10^{-8}mm. The anisotropic confining pressures affected the propagating wave modes as illustrated by the location of the peaks in these plots. The two largest peaks shifted in their location on the frequency axis by approximately -100Hz to -500Hz and, as summarised on Table 7.7 the locations of both peaks in all three planes decreased as $\sigma_{\text{prop}}$ increased, $\sigma_{\text{osc}}$ stayed constant and $\sigma_{\text{third}}$ decreased.
Case B: $\sigma_{\text{prop}}$ constant, $\sigma_{\text{osc}}$ decreasing and $\sigma_{\text{third}}$ increasing

Figure 7.15 plots the received signals for the three shear planes considered here for the Case B simulations. It is hard to discern a difference in arrival time at this scale. The amplitudes of the signals appeared to increase as the degree of induced anisotropy increased. The $V_{xy}$ received signal at $\sigma_p = 295.66\, \text{kPa}$, $\sigma_o = 221.78\, \text{kPa}$ and $\sigma_t = 365.62\, \text{kPa}$ was offset compared to the other simulations. This offset may be due to increased particle sliding due to the application of anisotropic stresses to the system.

Figure 7.16 zooms in on the first zero-crossing points for the data presented on Figure 7.15 to better observe changes in the arrival time due to increasingly anisotropic confining pressure. As $\sigma_{\text{osc}}$ decreased the arrival time was progressively later in the simulation. This shows that $\sigma_{\text{osc}}$ influences the stiffness of the system when $\sigma_{\text{prop}}$ was held constant. In the $xy$-plane the difference in arrival time was $0.071 \times 10^{-4}$s, in the $yz$-plane the difference in arrival time was $0.033 \times 10^{-4}$s and in the $zx$-plane the difference was $0.030 \times 10^{-4}$s.

The frequency domain plots for these signals are illustrated on Figure 7.17 and these plots confirm some of the earlier observations noted in relation to Figure 7.15. The magnitudes of the data in the frequency domain increased with increasingly anisotropic confining pressures across the range of frequencies considered. The amplitudes in the $xy$-plane increased from $7.192 \times 10^{-8}$mm to $1.033 \times 10^{-7}$mm, in the $yz$-plane they increased from $7.986 \times 10^{-8}$mm to $9.144 \times 10^{-8}$mm and in the $zx$-plane they increased from $7.823 \times 10^{-8}$mm to $9.066 \times 10^{-8}$mm. The propagating wave modes were affected as illustrated by the location of the peaks in these plots. The two largest peaks shift in their location on the frequency axis and as summarised on Table 7.7 both peaks in all three planes decreased as $\sigma_{\text{prop}}$ stayed constant, $\sigma_{\text{osc}}$ decreased and $\sigma_{\text{third}}$ increased by between 20Hz and 650Hz.

Case C: $\sigma_{\text{prop}}$ decreasing, $\sigma_{\text{osc}}$ increasing and $\sigma_{\text{third}}$ Constant

The Case A and Case B simulations considered $\sigma_{\text{prop}}$ and $\sigma_{\text{osc}}$ separately, Case C considers the combined effect of simultaneous variation of $\sigma_{\text{prop}}$ and $\sigma_{\text{osc}}$. $\sigma_{\text{prop}}$ was decreased in approximately 25kPa increments while $\sigma_{\text{osc}}$ was increased in approximately 25kPa increments and $\sigma_{\text{third}}$ was kept constant at approximately 300kPa. Figure 7.18 plots the received signals in each of the three shear planes: $G_{xy}$, $G_{yz}$ and $G_{zx}$ in the time domain. There was less variation in wave amplitude compared to the variation of $\sigma_{\text{prop}}$ summarised in Case A. However, for the final stress increment considered for the $yz$-plane the wave appeared to be offset compared to the other stress cases in that plane.
Figure 7.19 zooms in on the data around first zero-crossing on Figure 7.18 and shows that the arrival times decreased as the degree of anisotropy increased. Comparing Figure 7.13 and Figure 7.18 it is clear that $\sigma_{\text{prop}}$ was more influential on shear stiffness than $\sigma_{\text{osc}}$. The arrival time decreased in the xy-plane by $0.015 \times 10^{-4}$ s, by $0.093 \times 10^{-4}$ s in the yz-plane and by $0.028 \times 10^{-4}$ s in the zx-plane.

The frequency domain plots on Figure 7.20 agree with much of the observations on Figure 7.18. There were very small reductions in the amplitudes at the peaks on the frequency domain plot as the degree of induced anisotropy; however, $V_{yz}$ behaved differently to all other signals when $\sigma_x = 295.66$ kPa, $\sigma_y = 221.78$ kPa and $\sigma_z = 365.62$ kPa. If this signal is discarded then the amplitudes of the received signals reduced as the degree of anisotropy increased. In the xy-plane the amplitude reduced from $7.126 \times 10^{-8}$ mm to $6.611 \times 10^{-8}$ mm, in the yz-plane the amplitude reduced from $7.939 \times 10^{-8}$ mm to $7.467 \times 10^{-8}$ mm and in the zx-plane the amplitude reduced from $7.850 \times 10^{-8}$ mm to $7.145 \times 10^{-8}$ mm. The propagating wave modes were affected as illustrated by the location of the peaks in these plots. The two largest peak locations are summarised on Table 7.7 and both peaks in all three planes slightly increased, although it was not as obvious as in the previous anisotropic cases (by between 150 Hz and 250 Hz).

### 7.2.4 Stiffness of the sample

The shear wave arrival time was calculated both by cross-correlation and by using the 2D FFT method. The resultant stiffness values can be used to assess overall trends in the variation of the sample response.

**Case A: $\sigma_{\text{prop}}$ increasing, $\sigma_{\text{osc}}$ constant and $\sigma_{\text{third}}$ decreasing**

Referring Figure 7.21 (a), it is clear that the values of shear moduli in each of the three shear planes, $G_{xy}$, $G_{yz}$ and $G_{zx}$, increase with increasing $\sigma_{\text{prop}}$. This was observed with both cross-correlation and the 2D FFT. Moduli calculated using cross-correlation were lower than moduli calculated using the two-dimensional fast Fourier transform method. In fact the cross-correlation moduli were always lower than the 2D FFT moduli for all the simulations in Cases A, B and C considered here. Although the stiffness values generally increase, some of the data such as $G_{yz}$ calculated using cross-correlation show an initial drop in stiffness before consistently increasing.
**Case B: \( \sigma_{prop} \) constant, \( \sigma_{osc} \) decreasing and \( \sigma_{third} \) increasing**

Figure 7.21 (b) shows that as \( \sigma_{osc} \) decreased the stiffness of the sample decreased in each of the three shear planes. This was true for both the cross-correlation method and the 2D FFT. The moduli are plotted against \( \sigma_{osc} \).

**Case C: \( \sigma_{prop} \) decreasing, \( \sigma_{osc} \) increasing and \( \sigma_{third} \) constant**

Figure 7.21 (c) shows that the values of shear moduli against the values of \( \sigma_{prop} \). The values of shear moduli were observed to decrease with decreasing \( \sigma_{prop} \). Using the same data, Figure 7.21 (d) shows that the values of shear moduli decreased for the Case C simulations even though the values of \( \sigma_{osc} \) increased. This proved that \( \sigma_{prop} \) had a larger effect on the values of moduli than \( \sigma_{osc} \).

**Summary plots for each shear plane**

Summary plots were examined for each shear plane where the values of \( G_{ij} \) are plotted as circles on a two-dimensional plane with x-axis as stress in direction of propagation and y-axis as stress in direction of oscillation. The circles are centred on the values of stress in direction of propagation and stress in direction of oscillation when the wave propagation test was carried out. Figure 7.22 (a) plots the summary of the response of \( G_{xy} \) to changes in \( \sigma_{prop} \) and changes in \( \sigma_{osc} \) while Figure 7.22 (b) considers \( G_{yz} \) and Figure 7.22 (c) considers \( G_{zx} \). In all three shear planes when \( \sigma_{prop} \) increased and \( \sigma_{osc} \) remained constant the value of \( G \) increased.

When \( \sigma_{osc} \) decreased and \( \sigma_{prop} \) remained constant the value of \( G \) decreased. A more interesting case was when both stresses changed simultaneously with \( \sigma_{prop} \) decreasing and \( \sigma_{osc} \) increasing. In all three shear planes it was observed that the values of \( G \) decreased but did not decrease to the lowest magnitude observed when only \( \sigma_{osc} \) was decreased. The values of \( G \) were clearly affected by the increase in \( \sigma_{osc} \); however, the overall trend remained a decrease in stiffness. Gu et al. (2013) considered a mean stress equal to the average of the propagation stress and oscillation stress, \( \sigma_{m} = (\sigma_{prop} + \sigma_{osc})/2 \). The current study shows that \( G \) varied even when there was no change in \( \sigma_{m} \). Simply using a scalar stress value is not an accurate way of accounting for simultaneous changes in \( \sigma_{prop} \) and \( \sigma_{osc} \). In general it appeared that the values of \( G \) were lowest in the xy-plane, higher in the yz-plane and highest in the zx-plane. This agrees with the measured values in the isotropic case that was outlined in Chapter 5 proving the cubic anisotropy of the stiffness.
7.3 Randomly packed sample

7.3.1 Sample preparation and initial properties

The randomly packed sample, prepared using simulated pluviation, was inherently cross-anisotropic in the vertical direction. By anisotropically compressing the randomly packed sample the combination of inherent and induced anisotropy could be investigated. The properties of the randomly packed sample are summarised in Table 7.8 and Figure 7.23 illustrates the sample. The sample investigated was initially isotropically compressed to approximately 300kPa.

The stress states considered here are summarized on Table 7.9. As before, these were target stresses and the finite tolerance used in the stress control process (± 2.50%) meant that they were not exactly matched. In each case the stress was increased by approximately 25kPa in the major principal direction, kept at approximately 300kPa in the intermediate principal direction and reduced by approximately 25kPa in the minor principal direction. The loading regime was similar to the simulations carried out on the regularly packed simulation outlined earlier in this Chapter; however only two of the load cases were examined here. The two cases considered here were the case with stress in the x-direction increasing, stress in the y-direction constant, stress in the z-direction decreasing; and stress in the x-direction constant, stress in the y-direction decreasing and stress in the z-direction increasing.

The data presented in Table 7.10 show the sample is cross-anisotropic and that the anisotropic stress cases affect the sample fabric. This differs from what was observed for the regularly packed sample as there is no longer a highly stable, lattice packing.

It took a long time to anisotropically compress the sample due to the random packing of the sample which allowed the particles to move and caused fluctuations in the sample stress. The computer used was a HP Z800 workstation with two Intel X5687 3.60GHz processors, 32GB of RAM and a 64 bit operating system. The time taken to reach an anisotropic confining pressure was approximately four months. Once the required anisotropic confining pressure was reached the walls were removed and the flexible boundary conditions were applied. These boundary conditions were identical to those outlined in more detail in Chapter 6; however, each direction had a different applied stress in this case dependent on the stress case simulated. The number of cycles required to reduce particle velocities to a quasi-static state was reduced due to the extended time taken to get to the anisotropic stress state.
The stress states that were reached using this algorithm were measured by examining the stresses acting on the wall elements and examining the stress tensors of the particles in the sample. The stresses acting on the walls are illustrated on Table 7.11 and the value of mean stress, $p'$, is included to show that there was some variation in mean stress as the anisotropic confining pressures were reached. The sample also underwent volumetric straining ($\Delta \varepsilon_{\text{vol}}$) with Case 1 and Case 2 both exhibiting contractive and dilative behaviour as included on Table 7.11. The representative stress tensors for the particles are illustrated on Table 7.12 and $p'$ is included with $\Delta \varepsilon_{\text{vol}}$. The variation in $p'$ caused a variation in volumetric strain in the sample and this affected the stiffness that were measured. Due to the small magnitude in variation of $p'$ the effect of the variation on stiffness was not considered in further analysis. Table 7.13 shows the stresses that were reached after cycling using the ball stress tensors to calculate the sample stress tensor.

The wave was input using the single particle approach described in Chapter 6 and as illustrated on Figure 7.24. Particles were chosen on different faces and displaced in different directions to measure different compressional moduli and shear moduli. A summary of the directions and planes used is provided in Figure 7.25.

### 7.3.2 Particle-scale analysis

Example received signals for two different stresses in the direction of propagation ($\sigma_{\text{prop}}$) are shown on Figure 7.26 for waves propagating in the $xy$-plane. The single sine pulse signal was transmitted at 15kHz and the amplitude was 1$\mu$m. The travel time of the wave was lower for the higher $\sigma_{\text{prop}}$ value. The resultant increase in $G_{xy}$ as the stress applied to the $x$-direction increased is in agreement with previous observations by Roesler (1979) and predicted by the Hardin & Blandford (1989) analytical method. The amplitude of the received signal was observed to reduce as the degree of anisotropy increased. The different combinations of changes in $\sigma_{\text{prop}}$, stress in the direction of oscillation ($\sigma_{\text{osc}}$) and stress in the third direction ($\sigma_{\text{third}}$) will be explored in Section 7.3.4. There is no need to zoom in to observe changes in arrival time as was the case for the lattice packed sample considered earlier in this Chapter, as the changes in stress produced a change in stiffness that was visibly large enough to affect arrival time.

**Individual particle velocity vectors**

Figure 7.27 illustrates the velocity vectors for the randomly packed sample isotropically confined at approximately 300kPa the plots were generated using the approach outlined in
Chapter 6, e.g. Figure 6.14. Figure 7.28 is equivalent to Figure 7.27, but it plots the velocity vectors when the confining pressure in the propagating direction, x, was increased by 37.70kPa and the confining pressure in the oscillating direction, y, was kept constant and the stress in the third direction was reduced by 31.72kPa. Comparing Figure 7.28 with Figure 7.27, there is a reduction in the magnitude of the velocity vectors indicating that the propagating waves have reduced in amplitude. The received signal plotted in the centre of the figure arrived slightly earlier in the anisotropically stressed sample than in the isotropically stressed sample.

**Individual particle kinetic energies**

The plots of individual particle kinetic energies, the sum of translational and rotational kinetic energies are given in Figure 7.29 for the isotropic case and Figure 7.30 for the anisotropic case. In comparison with the isotropic case illustrated on Figure 7.29, the received signal appeared to arrive earlier in the simulation with an anisotropic stress state (Figure 7.30). The propagating waves were found to reduce in amplitude as the magnitude of the particle kinetic energies is reduced. This was similar to the previous observation regarding the individual velocity vectors (Figure 7.28).

**7.3.3 Analysis of the received signal**

**Constrained modulus, \( M \)**

Figure 7.31 shows the extender element test data in the time domain for increasing values of \( \sigma_{\text{prop}} \). The point of first zero-crossing arrived sooner on the time axis for both \( V_{xx} \) (top) and \( V_{zz} \) (bottom) as \( \sigma_{\text{prop}} \) increased. The amplitudes of the received signals increased as \( \sigma_{\text{prop}} \) increased and to maintain \( p' \) at approximately 300kPa the stress in one of the orthogonal directions was reduced by the same amount. Figure 7.32 presents the results in the frequency domain. It appears that the peaks occur at increasingly higher frequencies as \( \sigma_{\text{prop}} \) increased and this is confirmed in Table 7.14 where they rise by 150Hz to 200Hz. However, the amplitudes of the received signals did not vary in a consistent way; \( V_{xx} \) appeared to decrease in amplitude as the degree of anisotropy increased and \( V_{zz} \) appeared to increase in amplitude as the degree of anisotropy increased. \( V_{xx} \) went from a maximum amplitude peak of 5.99x10^{-7} mm to 3.90x10^{-7} mm while \( V_{zz} \) went from a maximum peak of 3.72x10^{-7} mm to 5.53x10^{-7} mm.

On Figure 7.33 the time domain data for the extender test cases where \( \sigma_{\text{prop}} \) remained constant are presented and the speed of wave propagation did not measurably change in the time-
domain. The stress in one of the orthogonal directions increased while the other decreased to maintain \( p' \) at approximately 300kPa. The point of first zero-crossing arrived at similar times on the time axis for both \( V_{xx} \) (top) and \( V_{yy} \) (bottom). The amplitudes of the received signals also remained similar as \( \sigma_{prop} \) remained constant. Figure 7.34 presents the results in the frequency domain. Both the location of the peaks on the frequency axis, confirmed on Table 7.14, and their values on the amplitude axis appear to remain similar as the degree of anisotropy increased. The change was limited to frequencies between 50Hz and 100Hz. The amplitude peak on \( V_{xx} \) went from 6.09x10^{-7} mm to 6.04x10^{-7} mm, dropping to 4.94x10^{-7} mm for the second stress increment. \( V_{zz} \) increased from 6.58x10^{-7} mm to 7.48x10^{-7} mm.

As \( \sigma_{prop} \) decreased, the arrival time increased and the speed of wave propagation decreased. Figure 7.35 shows the effect of decreasing \( \sigma_{prop} \) in the time-domain while one of the stresses in an orthogonal direction increased to keep the \( p' \) value constant. The point of first zero-crossing arrived later on the time axis for both \( V_{yy} \) (top) and \( V_{zz} \) (bottom) as \( \sigma_{prop} \) decreased. The amplitudes of the received signals increased as \( \sigma_{prop} \) decreased. Figure 7.36 plots the results in the frequency domain. Referring to Table 7.14 the frequencies associated with the peaks in the frequency domain plots decreased systematically; while the amplitudes of the peaks also decreased. The frequencies decreased by between 100Hz and 300Hz. The peak amplitude on \( V_{yy} \) decreased from 6.50x10^{-7} mm to 4.65x10^{-7} mm while \( V_{zz} \) decreased from a peak of 3.74x10^{-7} mm to 1.16x10^{-7} mm.

Shear modulus, \( G \)

As \( \sigma_{prop} \) increased, \( \sigma_{osc} \) remained constant and \( \sigma_{third} \) decreased, the arrival time decreased and the speed of wave propagation increased (Figure 7.37). The point of first zero-crossing arrived sooner on the time axis for both \( V_{xy} \) (top) and \( V_{zx} \) (bottom). The amplitudes of the received signals decreased as \( \sigma_{prop} \) increased. Figure 7.38 presents the results in the frequency domain. It appears that the peaks occur at similar frequencies as the degree of stress anisotropy is increased. However, the amplitudes of the received signals vary with \( V_{xy} \) appearing to decrease in amplitude as the degree of anisotropy increased and \( V_{zx} \) appearing to increase in amplitude as the degree of anisotropy increased. \( V_{xy} \) decreased from 3.41x10^{-7} mm to 1.90x10^{-7} mm and \( V_{zx} \) increased from 1.50x10^{-7} mm to 2.92x10^{-7} mm. The peaks on the frequency domain are summarised on Table 7.15 and there was an increase between 200Hz and 600Hz. Figure 7.39 plots an empirical cumulative distribution function of the kinetic
energies. There was a clear increase in the kinetic energies in the sample as the degree of anisotropy increased.

As $\sigma_{\text{prop}}$ remained approximately constant, $\sigma_{\text{osc}}$ decreased and $\sigma_{\text{third}}$ increased the speed of wave propagation decreased as can be seen in the time domain plot in Figure 7.40. The point of first zero-crossing arrived later on the time axis for both $V_{xy}$ (top) and $V_{yz}$ (bottom). The amplitudes of the received signals increased as $\sigma_{\text{osc}}$ decreased. Referring to the frequency domain data on Figure 7.41, it appears that the peaks occur at similar frequencies as the degree of stress anisotropy is increased. However, the amplitudes of the received signals vary and there is no discernible pattern in the variation. The maximum peak on $V_{xy}$ increases from $3.42 \times 10^{-7}$ mm to $9.82 \times 10^{-7}$ mm before falling to $5.40 \times 10^{-7}$ mm. The maximum peak on $V_{xz}$ increases from $6.69 \times 10^{-7}$ mm 8.39$ \times 10^{-7}$ mm before falling to $7.55 \times 10^{-7}$ mm. The location of the maximum peak also varies with increasing degree of stress-induced anisotropy. The locations of peaks on the frequency domain are summarised on Table 7.15 and the change in the peak location was very scattered. The kinetic energy presented in Figure 7.42 indicates little change with increasing anisotropy as $\sigma_{\text{prop}}$ remained constant.

Referring to the time domain plot in Figure 7.43 it is evident that as $\sigma_{\text{prop}}$ decreased, $\sigma_{\text{osc}}$ increased and $\sigma_{\text{third}}$ remained constant any changes in arrival time or wave speed were hard to discern. The point of first zero-crossing did not appear to change and the amplitudes of the received signals remained relatively similar as the degree of stress anisotropy changed. In the frequency domain (Figure 7.44), it appears that the peaks occur at similar frequencies as the degree of stress anisotropy is increased. The peak amplitude on $V_{yz}$ varied between $6.67 \times 10^{-7}$ mm and $6.47 \times 10^{-7}$ mm and the peak amplitude on $V_{zx}$ decreased from $1.50 \times 10^{-7}$ mm to $4.92 \times 10^{-8}$ mm. The locations of the peaks on the frequency domain are summarised on Table 7.15 and there was generally a change of less than 100Hz in the peak location. The representative kinetic energy data presented on Figure 7.45 showed a clear decrease in the kinetic energies in the sample as the degree of anisotropy increased.

7.3.4 Stiffness of the sample

In order to quantify the stiffness, the wave speeds were calculated using the 2D FFT method. As outlined in Chapter 6 this method was the most reliable.
**Constrained modulus, $M$**

The first case investigated was the case with $\sigma_{\text{prop}}$ increasing while a stress in the orthogonal direction decreased to maintain constant $p'$. Figure 7.46 (a) illustrates that increasing $\sigma_{\text{prop}}$ increases the magnitude of both $M_x$ and $M_z$. The ratio of $M_z/M_x$ increases from 1.01 in the isotropic case to 1.03 at the highest degree of anisotropy.

Considering the case where $\sigma_{\text{prop}}$ remained constant while the two orthogonal stresses were varied, Figure 7.46 (b) illustrates that there is little variance in $M$ values for each direction as $\sigma_{\text{prop}}$ does not vary significantly. There is a 3% variance in $M_x$ and a 5.5% variance in $M_y$.

Referring to Figure 7.46 (c) it is clear that both $M_y$ and $M_z$ decrease with increasing degree of anisotropy. The ratio of $M_z/M_y$ changes from 1.01 to 0.71 illustrating that the induced stress anisotropy has the effect of breaking down the inherent anisotropy where $M_z > M_y$ in this case. As $\sigma_{\text{prop}}$ in the $z$-direction is reduced the stiffness in that direction decreases rapidly. This is the effect of the stress-induced anisotropy on the sample where $M_y$ became greater than $M_z$.

**Shear modulus, $G$**

The first loading case considered here is $\sigma_{\text{prop}}$ increasing, $\sigma_{\text{osc}}$ constant and $\sigma_{\text{third}}$ decreasing as illustrated on Figure 7.47 (a). In this case, the value of shear modulus in the $xy$- and $zx$-planes increased although in the $xy$-plane this increase was not monotonic as the peak value of $G_{xy}$ was not coincident with the largest degree of stress anisotropy. The ratio $G_{xy}/G_{zx}$ increased from 1.02 to 1.09 before decreasing to 1.05.

The second loading case considered here is $\sigma_{\text{prop}}$ constant, $\sigma_{\text{osc}}$ decreasing and $\sigma_{\text{third}}$ increasing as illustrated on Figure 7.47 (b). The $xy$- and $yz$-planes are considered in this investigation and in both cases the values of shear moduli decrease but not monotonically. $G_{xy}$ and $G_{yz}$ both increase at the initial degree of anisotropy before decreasing after. The ratio $G_{yz}/G_{xy}$ increases from 1.04 to 1.08 as the degree of anisotropy increases.

The final case considered was $\sigma_{\text{prop}}$ decreasing, $\sigma_{\text{osc}}$ increasing and $\sigma_{\text{third}}$ constant. The values of shear moduli in the $yz$- and $zx$-planes are plotted against $\sigma_{\text{prop}}$ on Figure 7.47 (c) and against $\sigma_{\text{osc}}$ on Figure 7.47 (d). The values of shear moduli do not appear to change much and $G_{yz}$ remains larger in magnitude than $G_{zx}$. In the $yz$-shear plane the value of shear modulus decreases with decreasing $\sigma_{\text{prop}}$ from 152.1MPa to 152MPa which is a very small decrease. In the $zx$-shear plane the value of shear modulus increases from 142.7MPa to 143.5MPa.
which is a 0.5% increase. These tiny increases indicate that as $\sigma_{\text{prop}}$ is decreasing and $\sigma_{\text{osc}}$ is increasing there is little or no overall change in the stiffness of the sample. This contrasts with the observations in Section 6.6 for the regular sample where $\sigma_{\text{prop}}$ influences the stiffness more than $\sigma_{\text{osc}}$. This implies that $\sigma_m = \frac{1}{2}(\sigma_{\text{prop}} + \sigma_{\text{osc}})$ might be a good measure of to account for simultaneous changes in the values of $\sigma_{\text{prop}}$ and $\sigma_{\text{osc}}$ applied to the randomly packed sample.

Shear plane summary plots
A summary plot for $G_{xy}$ is presented in Figure 7.48 (a) where the effect of $\sigma_{\text{prop}}$ increasing and $\sigma_{\text{osc}}$ decreasing is illustrated. $G_{xy}$ increases as $\sigma_{\text{prop}}$ increases and decreases as $\sigma_{\text{osc}}$ decreases. The combined effect of both $\sigma_{\text{prop}}$ and $\sigma_{\text{osc}}$ changing is not investigated. On Figure 7.48 (b) the summary plot for $G_{yz}$ is presented where the cases examined are $\sigma_{\text{osc}}$ decreasing and the combined effect of decreasing $\sigma_{\text{prop}}$ and increasing $\sigma_{\text{osc}}$. As $\sigma_{\text{osc}}$ decreases the value of $G_{yz}$ decreases and has $\sigma_{\text{osc}}$ and $\sigma_{\text{prop}}$ change simultaneously the value of $G_{yz}$ appears to not vary. The final summary plot is for $G_{zx}$ and the cases illustrated on Figure 7.48 (c) are increasing $\sigma_{\text{prop}}$ and the combined effect of decreasing $\sigma_{\text{prop}}$ and increasing $\sigma_{\text{osc}}$. As $\sigma_{\text{prop}}$ increases the value of $G_{zx}$ increases as illustrated by the colour and size of the circles. As both $\sigma_{\text{prop}}$ and $\sigma_{\text{osc}}$ change simultaneously there is little or no change in $G_{zx}$. The change in $G$ when $\sigma_{\text{prop}}$ was decreased and $\sigma_{\text{osc}}$ was increased was predicted when the stress-compliance matrix, $\Sigma$, presented in Hardin & Blandford (1989) was considered. The value associated with shear modulus when the major principal stress increased and minor principal stress decreased is $(\sigma_3'\sigma_1')^{n/2}$ and this value changes as $\sigma_1'$ increases and $\sigma_3'$ decreases, $n$ is 1/3 due to Hertzian contact mechanics. This value will influence the $G$ value that is calculated from Hardin & Blandford theory. This links with the changes in $G$ that were observed in the summary plots.

7.4 Conclusions
Regularly packed sample

- Stress-induced anisotropy and particle-scale measurements are interlinked. For this lattice packing the fabric tensor did not change with changes in stress and so $G_{zx}$ remained larger than $G_{yz}$ which in turn was larger than $G_{xy}$.
- The effect of induced stress anisotropy was difficult to observe in particle scale visualisations of the waves propagating through the system.
• Analysis of the data in the time domain indicated that stress-induced anisotropy affected both wave speed and amplitude. When $\sigma_{\text{prop}}$ increased while $\sigma_{\text{osc}}$ remained constant and $\sigma_{\text{third}}$ decreased, the wave speed increased and the amplitude decreased. When $\sigma_{\text{prop}}$ remained constant, as $\sigma_{\text{osc}}$ decreased and $\sigma_{\text{third}}$ increased, the wave speed decreased and the amplitude increased. When $\sigma_{\text{prop}}$ decreased, as $\sigma_{\text{osc}}$ increased and $\sigma_{\text{third}}$ remained constant there was little change in amplitude and the wave speed decreased.

• In the frequency domain, stress-induced anisotropy affected both the amplitude and the location of peaks on the amplitude versus frequency plots. When $\sigma_{\text{prop}}$ was increased, while $\sigma_{\text{osc}}$ remained constant and $\sigma_{\text{third}}$ decreased, the location of the peaks on the frequency axis decreased and the amplitude decreased. When $\sigma_{\text{prop}}$ remained constant, while $\sigma_{\text{osc}}$ decreased and $\sigma_{\text{third}}$ increased the location of the peaks decreased and the amplitude increased. When $\sigma_{\text{prop}}$ decreased, while $\sigma_{\text{osc}}$ increased and $\sigma_{\text{third}}$ remained constant there was little change in amplitude and little change in the location of the peaks, although there was a slight increase.

• The stiffness calculated from wave speeds measured using cross-correlation were found to be lower than the wave speeds calculated using 2DFFT. When $\sigma_{\text{prop}}$ increased, $\sigma_{\text{osc}}$ remained constant and $\sigma_{\text{third}}$ decreased the stiffness increased. When $\sigma_{\text{prop}}$ remained constant, $\sigma_{\text{osc}}$ decreased and $\sigma_{\text{third}}$ increased the stiffness decreased. When $\sigma_{\text{prop}}$ decreased, $\sigma_{\text{osc}}$ increased and $\sigma_{\text{third}}$ remained constant the stiffness decreased but there was an influence from the increasing $\sigma_{\text{osc}}$.

• The summary plots confirmed the inherent cubic-anisotropy found in wave propagation tests on the isotropically confined sample as was noted in Chapter 5.

• $\sigma_m = \frac{1}{2}(\sigma_{\text{prop}} + \sigma_{\text{osc}})$, proposed by Yu & Richart (1984) and used by Gu et al. (2013), was found to be a poor way of accounting for simultaneous changes in both $\sigma_{\text{prop}}$ and $\sigma_{\text{osc}}$ as in these tests $\sigma_m$ would not change as the degree of anisotropy changed and there was a change in the value of $G$ measured.

Randomly packed sample

• The influence of stress-induced anisotropy on the fabric of the randomly packed sample was clearly observed. The changes in fabric changed the stiffness of the packing. This was clearly observed as $M_z$, which was greater than $M_y$ in the
isotropically confined case, became less than $M_y$ as the degree of stress-induced anisotropy.

- The amplitude of the wave was affected by the degree of stress anisotropy as observed in the received signal plots and particle-scale wave propagation plots. Unlike in the regularly packed simulation the changes to applied stress resulted in visible changes to the amplitude of the propagating wave in the randomly packed simulation.

- The stiffness of the sample was affected in a systematic way. Regarding the values of constrained modulus, $M$, the values increased with increasing $\sigma_{prop}$, decreased with decreasing $\sigma_{prop}$ and remained constant with constant $\sigma_{prop}$. The ratio of constrained moduli, such as $M_z/M_x$, changed as the degree of anisotropy increased.

- The values of $G$ were affected by $\sigma_{prop}$ and $\sigma_{osc}$. As $\sigma_{prop}$ increased the value of $G$ increased and as $\sigma_{osc}$ decreased the value of $G$ decreased. However, as both $\sigma_{prop}$ decreased and $\sigma_{osc}$ increased simultaneously there was little or no variation in $G$. Therefore, unlike in the regularly packed simulations, $\sigma_m = \frac{1}{2}(\sigma_{prop} + \sigma_{osc})$ may be more suitable for accounting for combined changes in $\sigma_{prop}$ and $\sigma_{osc}$. 
7.5 Figures

Figure 7.1: Layout of regularly packed sample with particles coloured by applied force.

Figure 7.2: Layout of bender element test with single particle transmitter and single particle receiver.

Figure 7.3: Summary of the propagation directions and oscillation directions for the wave propagation tests carried out on the regularly packed sample.
Figure 7.4: Transmitted and received signals for shear waves propagating in the xy-plane under increasingly anisotropic confining pressure. The direction of propagation is x and the direction of oscillation is y. $f_{\text{trans}} = 30\text{kHz}$, $R_d = 4.69$ and $\lambda/d_{50} = 7.68$.

Figure 7.5: Zoom in on the first zero-crossing on the received signals for shear waves propagating in the xy-plane under increasingly anisotropic confining pressure. $f_{\text{trans}} = 30\text{kHz}$, $R_d = 4.69$ and $\lambda/d_{50} = 7.68$. 
Figure 7.6: Individual particle velocity vectors (x & y components) scaled by magnitude considering x and y components of velocity only. View is a plan view of a 5mm thick cross-section through the sample. Only particle velocities less than or equal to 0.5mm/s magnitude are plotted to prevent larger velocities from "clouding" the system response. Time points (a) to (f) are shown in this plot. $\sigma_x = 295.64$ kPa, $\sigma_y = 295.64$ kPa, $\sigma_z = 292.58$ kPa, $f_{trans} = 30$ kHz, $R_d = 4.69$ and $\lambda/d_{50} = 7.68$.

Figure 7.7: Individual particle velocity vectors (x & y components) scaled by magnitude considering x and y components of velocity only. $\sigma_x = 369.49$ kPa, $\sigma_y = 295.62$ kPa, $\sigma_z = 219.50$ kPa, $f_{trans} = 30$ kHz, $R_d = 4.69$ and $\lambda/d_{50} = 7.68$. 
Figure 7.8: Relative particle rotations about the z-axis illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along z-axis. Time points (a) to (f) are shown in this plot. $\sigma_x = 295.64\text{kPa}$, $\sigma_y = 295.64\text{kPa}$, $\sigma_z = 292.58\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 4.69$ and $\lambda/d_{50} = 7.68$.

Figure 7.9: Relative particle rotations about the z-axis illustrating wave propagation through the sample (plan view). $\sigma_x = 369.49\text{kPa}$, $\sigma_y = 295.62\text{kPa}$, $\sigma_z = 219.50\text{kPa}$, $f_{\text{trans}} = 30\text{kHz}$, $R_d = 4.69$ and $\lambda/d_{50} = 7.68$. 
Figure 7.10: Particle kinetic energies, sum of translational and rotational, illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along z-axis. Time points (a) to (f) are shown in this plot. \( \sigma_x = 295.64\, \text{kPa}, \sigma_y = 295.64\, \text{kPa}, \sigma_z = 292.58\, \text{kPa}, f_{trans} = 30\, \text{kHz}, R_d = 4.69 \) and \( \lambda/d_{50} = 7.68 \).

Figure 7.11: Particle kinetic energies, sum of translational and rotational, illustrating wave propagation through the sample (plan view). \( \sigma_x = 369.49\, \text{kPa}, \sigma_y = 295.62\, \text{kPa}, \sigma_z = 219.50\, \text{kPa}, f_{trans} = 30\, \text{kHz}, R_d = 4.69 \) and \( \lambda/d_{50} = 7.68 \).
Figure 7.12: The effect of increasing the propagation stress, keeping the oscillation stress constant and decreasing the third stress for (a) $V_{xy}$ shear wave, (b) $V_{yz}$ shear wave and (c) $V_{zx}$ shear wave. Results are presented in the time domain. $f_{trans} = 30\text{kHz}$, $R_d = 4.69$ and $\lambda/d_{50} = 7.68$.

Figure 7.13: Zoom in on first zero-crossing to better illustrate the effect of increasing the propagation stress, keeping the oscillation stress constant and decreasing the third stress for (a) $V_{xy}$ shear wave, (b) $V_{yz}$ shear wave and (c) $V_{zx}$ shear wave. Results are presented in the time domain. $f_{trans} = 30\text{kHz}$, $R_d = 4.69$ and $\lambda/d_{50} = 7.68$. 

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Figure 7.14: The effect of increasing the propagation stress, keeping the oscillation stress constant and decreasing the third stress for (a) $V_{xy}$ shear wave, (b) $V_{yz}$ shear wave and (c) $V_{zx}$ shear wave. Results are presented in the frequency domain. $f_{trans} = 30\text{kHz}$, $R_d = 4.69$ and $\lambda/d_{50} = 7.68$.

Figure 7.15: The effect of keeping the propagation stress constant, decreasing the oscillation stress and increasing the third stress for (a) $V_{xy}$ shear wave, (b) $V_{yz}$ shear wave and (c) $V_{zx}$ shear wave. Results are presented in the time domain. $f_{trans} = 30\text{kHz}$, $R_d = 4.69$ and $\lambda/d_{50} = 7.68$. 
Figure 7.16: Zoom in on first zero-crossing to better illustrate the effect of keeping the propagation stress constant, decreasing the oscillation stress and increasing the third stress for (a) $V_{xy}$ shear wave, (b) $V_{yz}$ shear wave and (c) $V_{zx}$ shear wave. Results are presented in the time domain. $f_{trans} = 30$kHz, $R_d = 4.69$ and $\lambda/d_{50} = 7.68$.

Figure 7.17: The effect of keeping the propagation stress constant, decreasing the oscillation stress and increasing the third stress for (a) $V_{xy}$ shear wave, (b) $V_{yz}$ shear wave and (c) $V_{zx}$ shear wave. Results are presented in the frequency domain. $f_{trans} = 30$kHz, $R_d = 4.69$ and $\lambda/d_{50} = 7.68$. 
Figure 7.18: The effect of decreasing the propagation stress, increasing the oscillation stress and keeping the third stress constant for (a) \(V_{xy}\) shear wave, (b) \(V_{yz}\) shear wave and (c) \(V_{zx}\) shear wave. Results are presented in the time domain. \(f_{\text{trans}} = 30\,\text{kHz}, \beta_d = 4.69\) and \(\lambda/d_0 = 7.68\).

Figure 7.19: Zoom in on first zero-crossing to better illustrate the effect of decreasing the propagation stress, increasing the oscillation stress and keeping the third stress constant for (a) \(V_{xy}\) shear wave, (b) \(V_{yz}\) shear wave and (c) \(V_{zx}\) shear wave. Results are presented in the time domain. \(f_{\text{trans}} = 30\,\text{kHz}, \beta_d = 4.69\) and \(\lambda/d_0 = 7.68\).
Figure 7.20: The effect of decreasing the propagation stress, increasing the oscillation stress and keeping the third stress constant for (a) $V_{xy}$ shear wave, (b) $V_{yz}$ shear wave and (c) $V_{zx}$ shear wave. Results are presented in the frequency domain. $f_{trans} = 30\text{kHz}$, $R_d = 4.69$ and $\lambda/d_{dp} = 7.68$. 
Figure 7.21: (a) Variation in $G_{ij}$ with increasing propagation direction pressure; (b) variation in $G_{ij}$ with decreasing oscillation direction pressure; (c) variation in $G_{ij}$ with decreasing propagation direction pressure and increasing oscillation direction pressure. The variation in propagation direction pressure is isolated here; and (d) variation in $G_{ij}$ with decreasing propagation direction pressure and increasing oscillation direction pressure. The variation in oscillation direction pressure is isolated here. The values for wave speed were obtained using the cross-correlation (closed symbols) and two-dimensional fast Fourier transform (open symbols) travel time determination techniques. $f_{\text{trans}} = 30$ kHz, $R_d = 4.69$ and $\lambda/d_{\text{ho}} = 7.68$.

Figure 7.22: Summary of effect of propagation direction stress and oscillation direction stress on the value of (a) $G_{xy}$, (b) $G_{yz}$, and (c) $G_{zx}$. Wave speed measured using 2D FFT method. The circle radius increases with increasing $G_{ij}$ and the filled colour becomes darker as $G_{ij}$ increases.
Figure 7.23: Layout of randomly packed sample with particles coloured by applied force.

Figure 7.24: Layout of bender element test with single particle transmitter and single particle receiver.
Figure 7.25: Summary of the propagation directions and oscillation directions for the wave propagation tests carried out on the randomly packed sample.

Figure 7.26: Transmitted and received signals for shear waves propagating in the xy-plane under increasingly anisotropic confining pressure. The direction of propagation is x and the direction of oscillation is y. $f_{\text{trans}} = 15$kHz, $R_d = 2.91$ and $\lambda d_{so} = 12.03$. 
Figure 7.27: Individual particle velocity vectors (x & y components) scaled by magnitude considering x and y components of velocity only. View is a plan view of a 5mm thick cross-section through the sample. Only particle velocities less than or equal to 0.5mm/s magnitude are plotted to prevent larger velocities from "clouding" the system response. Time points (a) to (f) are shown in this plot. $\sigma_x = 272.36\text{kPa}$, $\sigma_y = 271.84\text{kPa}$, $\sigma_z = 277.53\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 2.91$ and $\lambda/d_{50} = 12.03$.

Figure 7.28: Individual particle velocity vectors (x & y components) scaled by magnitude considering x and y components of velocity only. $\sigma_x = 290.95\text{kPa}$, $\sigma_y = 271.55\text{kPa}$, $\sigma_z = 261.93\text{kPa}$, $f_{\text{trans}} = 15\text{kHz}$, $R_d = 2.91$ and $\lambda/d_{50} = 12.03$. 
Figure 7.29: Particle kinetic energies, sum of translational and rotational, illustrating wave propagation through the sample (plan view). The cross-section through the packing is at mid-way along z-axis. Time points (a) to (f) are shown in this plot. \( \sigma_x = 272.36 \text{kPa}, \sigma_y = 271.84 \text{kPa}, \sigma_z = 277.53 \text{kPa}, f_{\text{trans}} = 15 \text{kHz}, R_d = 2.91 \text{ and } \lambda/d_{50} = 12.03. \)

Figure 7.30: Particle kinetic energies, sum of translational and rotational, illustrating wave propagation through the sample (plan view). \( \sigma_x = 290.95 \text{kPa}, \sigma_y = 271.55 \text{kPa}, \sigma_z = 261.93 \text{kPa}, f_{\text{trans}} = 15 \text{kHz}, R_d = 2.91 \text{ and } \lambda/d_{50} = 12.03. \)
Figure 7.31: The effect of increasing the propagation stress (a) $V_{xx}$ compressional wave and (b) $V_{zz}$ compressional wave. Results are presented in the time domain. $f_{trans} = 15\text{kHz}$, $R_d = 2.91$ and $\lambda/d_{50} = 17.21$.

Figure 7.32: The effect of increasing the propagation stress (a) $V_{xx}$ compressional wave and (b) $V_{zz}$ compressional wave. Results are presented in the frequency domain. $f_{trans} = 15\text{kHz}$, $R_d = 2.91$ and $\lambda/d_{50} = 17.21$.  

$V_{xx} \quad V_{zz}$
Figure 7.33: The effect of keeping the propagation stress constant (a) $V_{xx}$ compressional wave and (b) $V_{yy}$ compressional wave. Results are presented in the time domain. $f_{trans} = 15$kHz, $R_d = 2.91$ and $\lambda/d_{50} = 17.21$.

Figure 7.34: The effect of keeping the propagation stress constant (a) $V_{xx}$ compressional wave and (b) $V_{yy}$ compressional wave. Results are presented in the frequency domain. $f_{trans} = 15$kHz, $R_d = 2.91$ and $\lambda/d_{50} = 17.21$. 
Figure 7.35: The effect of decreasing the propagation stress (a) $V_{yy}$ compressional wave and (b) $V_{zz}$ compressional wave. Results are presented in the time domain. $f_{trans} = 15\text{kHz}$, $R_d = 2.91$ and $\lambda/d_{50} = 17.21$.

Figure 7.36: The effect of decreasing the propagation stress (a) $V_{yy}$ compressional wave and (b) $V_{zz}$ compressional wave. Results are presented in the frequency domain. $f_{trans} = 15\text{kHz}$, $R_d = 2.91$ and $\lambda/d_{50} = 17.21$. 

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Figure 7.37: The effect of increasing the propagation stress, keeping the oscillation stress constant and decreasing the third stress for (a) $V_{xy}$ shear wave and (b) $V_{zx}$ shear wave. Results are presented in the time domain. $f_{trans} = 15\text{kHz}$, $R_d = 2.91$ and $\lambda/d_{50} = 12.03$.

Figure 7.38: The effect of increasing the propagation stress, keeping the oscillation stress constant and decreasing the third stress for (a) $V_{xy}$ shear wave and (b) $V_{zx}$ shear wave. Results are presented in the frequency domain. $f_{trans} = 15\text{kHz}$, $R_d = 2.91$ and $\lambda/d_{50} = 12.03$. 
Figure 7.39: A plot of the empirical cumulative distribution function of the kinetic energies calculated from the translational velocities of the particles. The waves propagating in the xy-plane were used for this analysis and the stress case used was $\sigma_{\text{prop}}$ increasing, $\sigma_{\text{osc}}$ constant and $\sigma_{\text{third}}$ decreasing.

Figure 7.40: The effect of keeping the propagation stress constant, decreasing the oscillation stress and increasing the third stress for (a) $V_{xy}$ shear wave and (b) $V_{yz}$ shear wave. Results are presented in the time domain. $f_{\text{trans}} = 15\text{kHz}$, $R_d = 2.91$ and $\lambda/d_{50} = 12.03$. 

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Figure 7.41: The effect of keeping the propagation stress constant, decreasing the oscillation stress and increasing the third stress for (a) $V_{xy}$ shear wave and (b) $V_{yz}$ shear wave. Results are presented in the frequency domain. $f_{\text{trans}} = 15\text{kHz}$, $R_d = 2.91$ and $\lambda/d_{xy} = 12.03$.

Figure 7.42: A plot of the empirical cumulative distribution function of the kinetic energies calculated from the translational velocities of the particles. The waves propagating in the xy-plane were used for this analysis and the stress case used was $\sigma_{\text{prop}}$ constant, $\sigma_{\text{osc}}$ decreasing and $\sigma_{\text{third}}$ increasing.
Figure 7.43: The effect of decreasing the propagation stress, increasing the oscillation stress and keeping the third stress constant for (a) $V_{xy}$ shear wave and (b) $V_{zx}$ shear wave. Results are presented in the time domain. $f_{trans}$ = 15kHz, $R_d$ = 2.91 and $\lambda/d_{0}$ = 12.03.

Figure 7.44: The effect of decreasing the propagation stress, increasing the oscillation stress and keeping the third stress constant for (a) $V_{yz}$ shear wave and (b) $V_{zx}$ shear wave. Results are presented in the frequency domain. $f_{trans}$ = 15kHz, $R_d$ = 2.91 and $\lambda/d_{0}$ = 12.03.
Figure 7.45: A plot of the empirical cumulative distribution function of the kinetic energies calculated from the translational velocities of the particles. The waves propagating in the yz-plane were used for this analysis and the stress case used was $\sigma_{\text{prop}}$ decreasing, $\sigma_{\text{osc}}$ increasing and $\sigma_{\text{hard}}$ constant.

Figure 7.46: Variation in $M_i$ with (a) increasing propagation direction pressure; (b) constant propagation direction pressure and (c) decreasing propagation direction pressure using the two-dimensional fast Fourier transform travel time determination technique.
Figure 7.47: Variation in $G_{ij}$ (a) with $\sigma_{\text{prop}}$ increasing, $\sigma_{\text{osc}}$ constant and $\sigma_{\text{blind}}$ decreasing; (b) with $\sigma_{\text{prop}}$ constant, $\sigma_{\text{osc}}$ decreasing and $\sigma_{\text{blind}}$ increasing; (c) with $\sigma_{\text{prop}}$ decreasing, $\sigma_{\text{osc}}$ increasing and $\sigma_{\text{blind}}$ constant and (d) with $\sigma_{\text{prop}}$ decreasing, $\sigma_{\text{osc}}$ increasing and $\sigma_{\text{blind}}$ constant using the two-dimensional fast Fourier transform travel time determination technique. $f_{\text{trans}} = 15\text{kHz}$, $R_d = 2.91$ and $\lambda/d_0 = 12.03$.

Figure 7.48: Summary of effect of propagation direction stress and oscillation direction stress on the value of (a) $G_{xy}$, (b) $G_{yz}$ and (c) $G_{zx}$. Wave speed measured using 2D FFT method. The circle radius increases with increasing $G_{ij}$ and the filled colour becomes darker as $G_{ij}$ increases.
### 7.6 Tables

Table 7.1: Regularly packed sample properties.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle Size</td>
<td>2.54 [mm]</td>
</tr>
<tr>
<td>Particle Density ([\rho])</td>
<td>2.23x10(^{-3}) [g/mm(^3)]</td>
</tr>
<tr>
<td>Interparticle Friction ([\mu])</td>
<td>0.088 [-]</td>
</tr>
<tr>
<td>Contact Model</td>
<td>Hertz-Mindlin</td>
</tr>
<tr>
<td></td>
<td>Cavarretta-Mindlin</td>
</tr>
<tr>
<td></td>
<td>Hertz-Mindlin-Deresiewicz</td>
</tr>
<tr>
<td>Particle Shear Modulus ([G])</td>
<td>16.67x10(^9) [Pa]</td>
</tr>
<tr>
<td>Particle Poisson’s Ratio ([v])</td>
<td>0.20 [-]</td>
</tr>
<tr>
<td>Viscous Damping at Contacts</td>
<td>0.10 [-] (reducing to 0.01 [-] for BE test)</td>
</tr>
<tr>
<td>No. of Particles</td>
<td>81,576 [-]</td>
</tr>
<tr>
<td>Frequency of the Sine Wave</td>
<td>30.0 [kHz]</td>
</tr>
<tr>
<td>Transmitter Amplitude</td>
<td>0.000125 [mm]</td>
</tr>
</tbody>
</table>
Table 7.2: The fabric tensor measured for the regularly packed sample confined isotropically at 300kPa and for the three increasingly anisotropic stress cases. The details of these cases are outlined in Table 7.3.

<table>
<thead>
<tr>
<th>Isotropic fabric tensor</th>
<th>Case 1 (a)</th>
<th>Case 2 (a)</th>
<th>Case 3 (a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.33</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.33</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.33</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Case 1 (b)</th>
<th>Case 2 (b)</th>
<th>Case 3 (b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.33 0.00 0.00 0.33 0.00 0.00 0.33 0.00 0.00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.00 0.33 0.00 0.00 0.33 0.00 0.00 0.33 0.00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.00 0.00 0.33 0.00 0.00 0.33 0.00 0.00 0.33</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Case 1 (c)</th>
<th>Case 2 (c)</th>
<th>Case 3 (c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.33 0.00 0.00 0.33 0.00 0.00 0.33 0.00 0.00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.00 0.33 0.00 0.00 0.33 0.00 0.00 0.33 0.00</td>
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<tr>
<td>0.00 0.00 0.33 0.00 0.00 0.33 0.00 0.00 0.33</td>
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<td></td>
</tr>
</tbody>
</table>
Table 7.3: Summary of the anisotropic stress cases applied to the regularly packed sample.

<table>
<thead>
<tr>
<th>Stress direction</th>
<th>$\sigma_x$ [kPa]</th>
<th>$\sigma_y$ [kPa]</th>
<th>$\sigma_z$ [kPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotropic</td>
<td>300</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>Case 1:</td>
<td>325</td>
<td>300</td>
<td>275</td>
</tr>
<tr>
<td></td>
<td>350</td>
<td>300</td>
<td>250</td>
</tr>
<tr>
<td></td>
<td>375</td>
<td>300</td>
<td>225</td>
</tr>
<tr>
<td>Case 2:</td>
<td>325</td>
<td>275</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>350</td>
<td>250</td>
<td>300</td>
</tr>
<tr>
<td></td>
<td>375</td>
<td>225</td>
<td>300</td>
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<tr>
<td>Case 3:</td>
<td>300</td>
<td>275</td>
<td>325</td>
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<td></td>
<td>300</td>
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<td>300</td>
<td>225</td>
<td>375</td>
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</table>
Table 7.4: Stress states reached and volumetric strain change measured using the stresses acting on the wall boundaries and the movement of the wall boundaries.

<table>
<thead>
<tr>
<th>Stress direction</th>
<th>$\sigma_x$ [kPa]</th>
<th>$\sigma_y$ [kPa]</th>
<th>$\sigma_z$ [kPa]</th>
<th>$p'$ [kPa]</th>
<th>$\Delta\varepsilon_{vol}$ [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotropic</td>
<td>292.50</td>
<td>292.50</td>
<td>292.55</td>
<td>292.52</td>
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</tr>
<tr>
<td>Case 1:</td>
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<td>307.05</td>
<td>281.87</td>
<td>305.44</td>
<td>3.40x10^{-5}</td>
</tr>
<tr>
<td></td>
<td>352.54</td>
<td>306.58</td>
<td>256.25</td>
<td>305.12</td>
<td>2.74x10^{-5}</td>
</tr>
<tr>
<td></td>
<td>377.90</td>
<td>306.73</td>
<td>230.62</td>
<td>305.08</td>
<td>1.83x10^{-5}</td>
</tr>
<tr>
<td>Case 2:</td>
<td>280.49</td>
<td>316.88</td>
<td>299.22</td>
<td>298.86</td>
<td>1.90x10^{-5}</td>
</tr>
<tr>
<td></td>
<td>256.20</td>
<td>341.25</td>
<td>301.09</td>
<td>299.51</td>
<td>1.52x10^{-5}</td>
</tr>
<tr>
<td></td>
<td>230.62</td>
<td>369.00</td>
<td>304.19</td>
<td>301.27</td>
<td>1.34x10^{-5}</td>
</tr>
<tr>
<td>Case 3:</td>
<td>292.65</td>
<td>268.45</td>
<td>316.88</td>
<td>292.66</td>
<td>-2.41x10^{-6}</td>
</tr>
<tr>
<td></td>
<td>306.51</td>
<td>256.25</td>
<td>342.45</td>
<td>301.74</td>
<td>1.80x10^{-5}</td>
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<td></td>
<td>293.97</td>
<td>223.13</td>
<td>365.63</td>
<td>294.24</td>
<td>-2.04x10^{-5}</td>
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</table>
Table 7.5: Stress states reached and volumetric strain change measured using the representative particle stress and strain tensors.

<table>
<thead>
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<th>Stress direction</th>
<th>$\sigma_x$ [kPa]</th>
<th>$\sigma_y$ [kPa]</th>
<th>$\sigma_z$ [kPa]</th>
<th>$p'$ [kPa]</th>
<th>$\Delta\varepsilon_{vol}$ [-]</th>
</tr>
</thead>
<tbody>
<tr>
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<td>285.01</td>
<td>285.09</td>
<td>285.04</td>
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<tr>
<td>Case 1:</td>
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<td>299.19</td>
<td>274.68</td>
<td>297.62</td>
<td>3.09x10^{-5}</td>
</tr>
<tr>
<td></td>
<td>352.54</td>
<td>306.59</td>
<td>256.25</td>
<td>305.13</td>
<td>2.27x10^{-5}</td>
</tr>
<tr>
<td></td>
<td>368.22</td>
<td>298.86</td>
<td>224.74</td>
<td>297.27</td>
<td>1.15x10^{-5}</td>
</tr>
<tr>
<td>Case 2:</td>
<td>273.31</td>
<td>308.76</td>
<td>291.59</td>
<td>291.22</td>
<td>1.63x10^{-5}</td>
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<td>256.21</td>
<td>341.25</td>
<td>301.09</td>
<td>299.52</td>
<td>1.51x10^{-5}</td>
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<tr>
<td></td>
<td>224.72</td>
<td>359.55</td>
<td>296.43</td>
<td>293.57</td>
<td>1.34x10^{-5}</td>
</tr>
<tr>
<td>Case 3:</td>
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<td>261.58</td>
<td>308.79</td>
<td>285.17</td>
<td>-9.39x10^{-8}</td>
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<td></td>
<td>298.65</td>
<td>249.68</td>
<td>333.71</td>
<td>294.01</td>
<td>2.03x10^{-5}</td>
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<tr>
<td></td>
<td>286.44</td>
<td>217.42</td>
<td>356.30</td>
<td>286.72</td>
<td>-1.47x10^{-5}</td>
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</table>
Table 7.6: Stress states reached and volumetric strain change measured using the representative particle stress and strain tensors. These measurements were taken after the flexible boundaries were applied and the system was allowed to equilibrate.

<table>
<thead>
<tr>
<th>Stress direction</th>
<th>$\sigma_x$ [kPa]</th>
<th>$\sigma_y$ [kPa]</th>
<th>$\sigma_z$ [kPa]</th>
<th>$p'$ [kPa]</th>
<th>$\Delta \varepsilon_{\text{vol}}$ [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotropic</td>
<td>295.64</td>
<td>295.64</td>
<td>292.58</td>
<td>294.6</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>(300)</td>
<td>(300)</td>
<td>(300)</td>
<td>(300)</td>
<td></td>
</tr>
<tr>
<td>Case 1:</td>
<td></td>
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<td></td>
<td></td>
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<tr>
<td>(a)</td>
<td>320.26</td>
<td>295.65</td>
<td>268.24</td>
<td>294.7</td>
<td>-3.55x10^{-6}</td>
</tr>
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<td></td>
<td>(325)</td>
<td>(300)</td>
<td>(275)</td>
<td>(300)</td>
<td></td>
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<tr>
<td>(b)</td>
<td>344.88</td>
<td>295.63</td>
<td>243.88</td>
<td>294.8</td>
<td>-1.10x10^{-5}</td>
</tr>
<tr>
<td></td>
<td>(350)</td>
<td>(300)</td>
<td>(250)</td>
<td>(300)</td>
<td></td>
</tr>
<tr>
<td>(c)</td>
<td>369.49</td>
<td>295.62</td>
<td>219.5</td>
<td>294.9</td>
<td>-2.20x10^{-5}</td>
</tr>
<tr>
<td></td>
<td>(375)</td>
<td>(300)</td>
<td>(225)</td>
<td>(300)</td>
<td></td>
</tr>
<tr>
<td>Case 2:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(a)</td>
<td>271.01</td>
<td>320.26</td>
<td>292.58</td>
<td>294.6</td>
<td>-9.52x10^{-7}</td>
</tr>
<tr>
<td></td>
<td>(275)</td>
<td>(325)</td>
<td>(300)</td>
<td>(300)</td>
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</tr>
<tr>
<td>(b)</td>
<td>246.38</td>
<td>344.88</td>
<td>292.57</td>
<td>294.6</td>
<td>-4.32x10^{-6}</td>
</tr>
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<td>(250)</td>
<td>(350)</td>
<td>(300)</td>
<td>(300)</td>
<td></td>
</tr>
<tr>
<td>(c)</td>
<td>221.76</td>
<td>369.52</td>
<td>292.59</td>
<td>294.6</td>
<td>-1.09x10^{-5}</td>
</tr>
<tr>
<td></td>
<td>(225)</td>
<td>(375)</td>
<td>(300)</td>
<td>(300)</td>
<td></td>
</tr>
<tr>
<td>Case 3:</td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>(a)</td>
<td>295.64</td>
<td>271.01</td>
<td>316.94</td>
<td>294.5</td>
<td>-5.64x10^{-7}</td>
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<td>(300)</td>
<td>(275)</td>
<td>(325)</td>
<td>(300)</td>
<td></td>
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<tr>
<td>(b)</td>
<td>295.65</td>
<td>246.41</td>
<td>341.29</td>
<td>294.5</td>
<td>-5.01x10^{-6}</td>
</tr>
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<td>(300)</td>
<td>(250)</td>
<td>(350)</td>
<td>(300)</td>
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<td>365.62</td>
<td>294.4</td>
<td>-1.98x10^{-5}</td>
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<td>(300)</td>
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<td>(375)</td>
<td>(300)</td>
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Table 7.7: The frequencies at which the first and second peaks occur on the amplitude versus frequency plots on Figure 7.14, Figure 7.17 and Figure 7.20.

<table>
<thead>
<tr>
<th>Frequency at which peaks occur [Hz]</th>
<th>xy-plane</th>
<th>yz-plane</th>
<th>zx-plane</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>1st Peak</td>
<td>2nd Peak</td>
<td>1st Peak</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: 0kPa, $\Delta \sigma_{\text{osc}}$: 0kPa, $\Delta \sigma_{\text{third}}$: 0kPa</td>
<td>14695.87</td>
<td>25448.94</td>
<td>15001.07</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: +25kPa, $\Delta \sigma_{\text{osc}}$: 0kPa, $\Delta \sigma_{\text{third}}$: -25kPa</td>
<td>14642.86</td>
<td>25714.29</td>
<td>15002.68</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: +50kPa, $\Delta \sigma_{\text{osc}}$: 0kPa, $\Delta \sigma_{\text{third}}$: -50kPa</td>
<td>14570.52</td>
<td>25231.88</td>
<td>14636.58</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: +75kPa, $\Delta \sigma_{\text{osc}}$: 0kPa, $\Delta \sigma_{\text{third}}$: -75kPa</td>
<td>14475.36</td>
<td>25067.08</td>
<td>14607.90</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: 0kPa, $\Delta \sigma_{\text{osc}}$: 0kPa, $\Delta \sigma_{\text{third}}$: 0kPa</td>
<td>14964.19</td>
<td>25652.90</td>
<td>15049.45</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: 0kPa, $\Delta \sigma_{\text{osc}}$: -25kPa, $\Delta \sigma_{\text{third}}$: +25kPa</td>
<td>14850.18</td>
<td>25369.83</td>
<td>14995.18</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: 0kPa, $\Delta \sigma_{\text{osc}}$: -50kPa, $\Delta \sigma_{\text{third}}$: +50kPa</td>
<td>14642.86</td>
<td>25000.00</td>
<td>14921.13</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: 0kPa, $\Delta \sigma_{\text{osc}}$: -75kPa, $\Delta \sigma_{\text{third}}$: +75kPa</td>
<td>14871.99</td>
<td>26557.13</td>
<td>14823.70</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: 0kPa, $\Delta \sigma_{\text{osc}}$: 0kPa, $\Delta \sigma_{\text{third}}$: 0kPa</td>
<td>14847.81</td>
<td>25453.39</td>
<td>15001.07</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: -25kPa, $\Delta \sigma_{\text{osc}}$: +25kPa, $\Delta \sigma_{\text{third}}$: 0kPa</td>
<td>14849.38</td>
<td>25809.65</td>
<td>15044.60</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: -50kPa, $\Delta \sigma_{\text{osc}}$: +50kPa, $\Delta \sigma_{\text{third}}$: 0kPa</td>
<td>14840.47</td>
<td>25794.14</td>
<td>15037.06</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: -75kPa, $\Delta \sigma_{\text{osc}}$: +75kPa, $\Delta \sigma_{\text{third}}$: 0kPa</td>
<td>15163.80</td>
<td>25743.20</td>
<td>15618.34</td>
</tr>
</tbody>
</table>
Table 7.8: Randomly packed sample properties.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean Particle Size</td>
<td>2.54 [mm]</td>
</tr>
<tr>
<td>Particle Density [( \rho )]</td>
<td>( 2.23 \times 10^{-3} ) [g/mm(^3)]</td>
</tr>
<tr>
<td>Interparticle Friction [( \mu )]</td>
<td>0.088 [-]</td>
</tr>
<tr>
<td>Contact Model</td>
<td>Hertz-Mindlin</td>
</tr>
<tr>
<td>Particle Shear Modulus [( G )]</td>
<td>( 16.67 \times 10^9 ) [Pa]</td>
</tr>
<tr>
<td>Particle Poisson’s Ratio [( \nu )]</td>
<td>0.20 [-]</td>
</tr>
<tr>
<td>Viscous Damping at Contacts</td>
<td>0.10 [-] (reducing to 0.01 [-] for BE test)</td>
</tr>
<tr>
<td>No. of Particles</td>
<td>64,136 [-]</td>
</tr>
<tr>
<td>Frequency of the Sine Wave</td>
<td>15.0 [kHz]</td>
</tr>
<tr>
<td>Transmitter Amplitude</td>
<td>1.0 [( \mu )m]</td>
</tr>
<tr>
<td>Travel Distance [( d )]</td>
<td>x direction: ( 8.89 \times 10^{-2} ) [m]</td>
</tr>
<tr>
<td></td>
<td>y direction: ( 9.21 \times 10^{-2} ) [m]</td>
</tr>
<tr>
<td></td>
<td>z direction: ( 9.17 \times 10^{-2} ) [m]</td>
</tr>
</tbody>
</table>

Table 7.9: Summary of the anisotropic stress cases applied to the randomly packed sample.

<table>
<thead>
<tr>
<th>Stress direction</th>
<th>( \sigma_x ) [kPa]</th>
<th>( \sigma_y ) [kPa]</th>
<th>( \sigma_z ) [kPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotropic</td>
<td>300</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>Case 1:</td>
<td>325</td>
<td>300</td>
<td>275</td>
</tr>
<tr>
<td></td>
<td>350</td>
<td>300</td>
<td>250</td>
</tr>
<tr>
<td>Case 2:</td>
<td>300</td>
<td>275</td>
<td>325</td>
</tr>
<tr>
<td></td>
<td>300</td>
<td>250</td>
<td>350</td>
</tr>
</tbody>
</table>
Table 7.10: The fabric tensor measured for the randomly packed sample confined isotropically at 300kPa and for the two increasingly anisotropic stress cases. The details of these cases are outlined in Table 7.9.

<table>
<thead>
<tr>
<th></th>
<th>Isotropic fabric tensor</th>
<th>Case 1 (a)</th>
<th>Case 2 (a)</th>
<th>Case 1 (b)</th>
<th>Case 2 (b)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.33 0.00 0.00</td>
<td>0.34 0.00 0.00</td>
<td>0.34 0.00 0.00</td>
<td>0.35 0.00 0.00</td>
<td>0.35 0.00 0.00</td>
</tr>
<tr>
<td></td>
<td>0.00 0.33 0.00</td>
<td>0.00 0.33 0.00</td>
<td>0.00 0.33 0.00</td>
<td>0.00 0.33 0.00</td>
<td>0.00 0.33 0.00</td>
</tr>
<tr>
<td></td>
<td>0.00 0.00 0.34</td>
<td>0.00 0.00 0.33</td>
<td>0.00 0.00 0.33</td>
<td>0.00 0.00 0.32</td>
<td>0.00 0.00 0.35</td>
</tr>
</tbody>
</table>

Table 7.11: Stress states reached measured using the stresses acting on the wall boundaries and the movement of the wall boundaries.

<table>
<thead>
<tr>
<th>Stress direction</th>
<th>$\sigma_x$ [kPa]</th>
<th>$\sigma_y$ [kPa]</th>
<th>$\sigma_z$ [kPa]</th>
<th>$p'$ [kPa]</th>
<th>$\Delta\varepsilon_{vol}$ [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotropic</td>
<td>296.13</td>
<td>295.02</td>
<td>306.20</td>
<td>299.12</td>
<td>0</td>
</tr>
<tr>
<td>Case 1:</td>
<td>316.88</td>
<td>294.82</td>
<td>280.25</td>
<td>297.32</td>
<td>-0.441x10^{-6}</td>
</tr>
<tr>
<td>Case 2:</td>
<td>293.77</td>
<td>281.32</td>
<td>316.88</td>
<td>297.32</td>
<td>-0.096x10^{-6}</td>
</tr>
<tr>
<td></td>
<td>295.03</td>
<td>251.22</td>
<td>341.25</td>
<td>295.83</td>
<td>3.520x10^{-3}</td>
</tr>
</tbody>
</table>
Table 7.12: Stress states reached measured using the representative particle stress and strain tensors.

<table>
<thead>
<tr>
<th>Stress direction</th>
<th>$\sigma_x$ [kPa]</th>
<th>$\sigma_y$ [kPa]</th>
<th>$\sigma_z$ [kPa]</th>
<th>$p'$ [kPa]</th>
<th>$\Delta\varepsilon_{vol}$ [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotropic</td>
<td>295.23</td>
<td>294.13</td>
<td>305.92</td>
<td>298.43</td>
<td>0</td>
</tr>
<tr>
<td>Case 1:</td>
<td>316.85</td>
<td>294.80</td>
<td>280.89</td>
<td>297.51</td>
<td>0.517x10^{-3}</td>
</tr>
<tr>
<td>Case 2:</td>
<td>293.75 295.01</td>
<td>281.31 251.22</td>
<td>317.51 341.87</td>
<td>297.52</td>
<td>-0.720x10^{-6} 0.399x10^{-3}</td>
</tr>
</tbody>
</table>
Table 7.13: Stress states reached and volumetric strain change measured using the representative particle stress and strain tensors. These measurements were taken after the flexible boundaries were applied and the system was allowed to equilibrate.

![Table 7.13](image)

Note: The values are represented in kPa and the strain change in percent. The `Δε_{vol}` refers to the volumetric strain change.
Table 7.14: The frequencies at which the first and second peaks occur on the amplitude versus frequency plots on Figure 7.32, Figure 7.34 and Figure 7.36.

<table>
<thead>
<tr>
<th>Frequency at which peaks occur [Hz]</th>
<th>x-direction</th>
<th>y-direction</th>
<th>z-direction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1(^{st}) Peak</td>
<td>2(^{nd}) Peak</td>
<td>1(^{st}) Peak</td>
</tr>
<tr>
<td>(\Delta \sigma_{\text{prop}}: 0\text{kPa})</td>
<td>6902</td>
<td>9128</td>
<td>N/A</td>
</tr>
<tr>
<td>(\Delta \sigma_{\text{prop}}: +25\text{kPa})</td>
<td>7109</td>
<td>9219</td>
<td>N/A</td>
</tr>
<tr>
<td>(\Delta \sigma_{\text{prop}}: +50\text{kPa})</td>
<td>7175</td>
<td>9493</td>
<td>N/A</td>
</tr>
<tr>
<td>(\Delta \sigma_{\text{prop}}: 0\text{kPa})</td>
<td>6919</td>
<td>9151</td>
<td>6932</td>
</tr>
<tr>
<td>(\Delta \sigma_{\text{prop}}: 0\text{kPa})</td>
<td>6889</td>
<td>9111</td>
<td>7044</td>
</tr>
<tr>
<td>(\Delta \sigma_{\text{prop}}: 0\text{kPa})</td>
<td>6721</td>
<td>9035</td>
<td>6444</td>
</tr>
<tr>
<td>(\Delta \sigma_{\text{prop}}: 0\text{kPa})</td>
<td>N/A</td>
<td>N/A</td>
<td>6975</td>
</tr>
<tr>
<td>(\Delta \sigma_{\text{prop}}: -25\text{kPa})</td>
<td>N/A</td>
<td>N/A</td>
<td>6944</td>
</tr>
<tr>
<td>(\Delta \sigma_{\text{prop}}: -50\text{kPa})</td>
<td>N/A</td>
<td>N/A</td>
<td>6776</td>
</tr>
</tbody>
</table>
Table 7.15: The frequencies at which the first and second peaks occur on the amplitude versus frequency plots on Figure 7.38, Figure 7.41 and Figure 7.44.

<table>
<thead>
<tr>
<th>Frequency at which peaks occur [Hz]</th>
<th>xy-plane</th>
<th></th>
<th>yz-plane</th>
<th></th>
<th>zx-plane</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1(^{st}) Peak</td>
<td>2(^{nd}) Peak</td>
<td>1(^{st}) Peak</td>
<td>2(^{nd}) Peak</td>
<td>1(^{st}) Peak</td>
<td>2(^{nd}) Peak</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: 0kPa, $\Delta \sigma_{\text{osc}}$: 0kPa, $\Delta \sigma_{\text{third}}$: 0kPa</td>
<td>1793</td>
<td>6387</td>
<td>N/A</td>
<td>N/A</td>
<td>2464</td>
<td>6160</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: +25kPa, $\Delta \sigma_{\text{osc}}$: 0kPa, $\Delta \sigma_{\text{third}}$: -25kPa</td>
<td>1565</td>
<td>6708</td>
<td>N/A</td>
<td>N/A</td>
<td>3360</td>
<td>6496</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: +50kPa, $\Delta \sigma_{\text{osc}}$: 0kPa, $\Delta \sigma_{\text{third}}$: -50kPa</td>
<td>2111</td>
<td>6777</td>
<td>N/A</td>
<td>N/A</td>
<td>2110</td>
<td>6554</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: 0kPa, $\Delta \sigma_{\text{osc}}$: 0kPa, $\Delta \sigma_{\text{third}}$: 0kPa</td>
<td>1800</td>
<td>6300</td>
<td>1789</td>
<td>6261</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: 0kPa, $\Delta \sigma_{\text{osc}}$: -25kPa, $\Delta \sigma_{\text{third}}$: +25kPa</td>
<td>1792</td>
<td>6496</td>
<td>1789</td>
<td>6261</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: 0kPa, $\Delta \sigma_{\text{osc}}$: -50kPa, $\Delta \sigma_{\text{third}}$: +50kPa</td>
<td>3110</td>
<td>5998</td>
<td>1778</td>
<td>5666</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: 0kPa, $\Delta \sigma_{\text{osc}}$: 0kPa, $\Delta \sigma_{\text{third}}$: 0kPa</td>
<td>N/A</td>
<td>N/A</td>
<td>1800</td>
<td>6187</td>
<td>2460</td>
<td>6261</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: -25kPa, $\Delta \sigma_{\text{osc}}$: +25kPa, $\Delta \sigma_{\text{third}}$: 0kPa</td>
<td>N/A</td>
<td>N/A</td>
<td>1680</td>
<td>6272</td>
<td>2348</td>
<td>6149</td>
</tr>
<tr>
<td>$\Delta \sigma_{\text{prop}}$: -50kPa, $\Delta \sigma_{\text{osc}}$: +50kPa, $\Delta \sigma_{\text{third}}$: 0kPa</td>
<td>N/A</td>
<td>N/A</td>
<td>1666</td>
<td>6220</td>
<td>2778</td>
<td>6333</td>
</tr>
</tbody>
</table>
8 Conclusions

8.1 Summary

The aim of this research was to gain a better understanding of the use of bender element testing to determine the small-strain stiffness of granular materials using the numerical discrete element method (DEM). Comparisons were made between the numerical research carried out here and the experimental research carried out simultaneously at the University of Bristol on the same types of samples and same sample sizes. An important aim was to examine the mechanism by which stress waves propagate through granular material at the micro-scale and the relationship to sample scale stiffness. The particle-scale response as a stress wave propagated through the material was identified as a key research area and was explored in detail. The influence of micro-scale parameters, such as the interparticle contact model, on the wave propagation mechanism and speed were considered important.

A literature review to contextualise the research was presented in Chapter 2. Chapter 3 discussed the implementation of contact models in the PFC3D discrete element method code. The remainder of the thesis focused on three sets of DEM simulations. In each simulation the bender element was modelled as a point source. The simulations presented here grew increasingly complex and disordered as the research progressed. Chapter 4 focused on two-dimensional hexagonally packed samples of circular disks. The two-dimensional simulations were quicker to run and template algorithms for wave propagation tests and small amplitude stress probes were created that were easily adjusted for later three-dimensional simulations. Chapter 5 introduced three-dimensional regularly packed samples. Here, the complexity and computational cost has increased as there were additional degrees of freedom in a three-dimensional sample. Visualisation of the particle-scale response also became more challenging. Chapter 6 focused on three-dimensional randomly packed samples which have a cross-anisotropic fabric. The complexity and computational cost of this sample was higher than the previous regularly packed simulations; however it more closely resembled the laboratory sample at the University of Bristol. The increasing disorder in the randomly packed samples led to interesting comparisons with the more ordered simulations carried out previously. Chapter 7 focused on the effects of induced anisotropy on both the regularly packed and randomly packed three-dimensional samples in the form of anisotropic confining stresses. The randomly packed sample was subject to the effects of both induced and
inherent anisotropy leading to increased computational cost and complicated results. However, as the interpretation techniques and understanding of the system had been developed by gradually incorporating increased levels of disorder it was possible to accurately interpret the waves and achieve meaningful understanding of the system response.

For each of the samples outlined above, novel particle scale methods were used to visualise the wave propagation mechanism. Different particle scale measurements were compared including particle velocities, particle stresses, particle rotations and particle kinetic energies. Chapter 4 outlines the use of these methods on the two-dimensional sample where particle velocities and stresses were used to interpret the wave propagation. Chapter 5 presents the results for the three-dimensional regularly packed sample where particle velocities, stresses and rotations were used to visualise the wave propagation. Chapter 6 outlines the use of these techniques on the three-dimensional randomly packed sample where particle velocities, particle stresses and particle kinetic energies were considered. These visualisation methods revealed a large amount of qualitative data on the wave propagation. The wave lobes that were produced by the movement of a transmitting point source were investigated. The propagation of the wave through time and position was examined using these methods. Changes in the wave propagation mechanism incurred during parametric studies were examined as was the effect of varying the colour resolution used in these plots.

After observing the propagation of the waves through the system, and observing a rough estimate for the true arrival of the shear wave, the results were examined in detail using signal analysis to determine the wave speed and ultimately the stiffness of the sample. In Chapter 4 a number of time domain techniques from the literature were used to measure wave speed. A novel method involving decomposition of the signal in the frequency domain into its constituent waves showed promise as it produced results that agreed well with the biaxial strain probe results. The resulting stiffness were compared with the stiffness of the sample measured using a small amplitude strain probe. Chapter 5 implements a number of the existing travel time determination techniques in the literature and illustrates the application of the two-dimensional fast Fourier transform method to a bender element test for the first time. The methods were tested for reliability using varying inputted frequencies and inputted waveshapes. The results were compared with the results from analytical methods and small amplitude stress probes. Chapter 6 applied the travel time techniques used in Chapter 5 on received signals produced in the randomly packed sample. The methods were tested for reliability by varying the input frequencies. The results were compared with the results form
analytical methods and small amplitude stress probes. Both time and frequency domain techniques were considered in this study.

The additional information on wave characterisation found in a frequency domain analysis was explored in this study at a level of detail that has not been applied to bender element tests before. The propagation of the wave through time at a particular point in space was transformed to the frequency domain using a fast Fourier transform function. The resulting plot was amplitude versus frequency or angular velocity. The propagation of the wave through space at a particular point in time was transformed to the frequency domain using a fast Fourier transform function. The resulting plot was amplitude versus wavenumber. These two plots were combined to form a two-dimensional fast Fourier transform plot that had the axes: angular velocity versus wavenumber. Several amplitude versus frequency plots were combined to illustrate the frequency content of oscillations at different positions through the sample. Frequency domain analysis was used to gain further insight into all samples including the two-dimensional sample in Chapter 4, the three-dimensional regularly packed sample in Chapter 5 and the three-dimensional randomly packed sample in Chapter 6. It was also used on the anisotropically stressed samples in Chapter 7.

The results of numerical simulations were compared with analytical approaches to quantify stiffness. There are many analytical methods to predict the in-situ stiffness of granular packings using particle scale data. These methods calculate a macro-scale parameter usually using a volume averaging technique and the assumption that non-affine strains do not occur. The applicability of these analytical methods was critically assessed for numerical discrete element samples with different packings. The assumptions used in analytical methods represented significant idealisations for some of the samples, particularly regularly packed samples subject to anisotropic confining stresses and randomly packed samples that were inherently anisotropic. The most ubiquitous analytical method was effective medium theory and this was implemented. The principle of virtual displacement, dispersion relation theory and the Sanchez-Salinero solution for the near-field effect were all examined. The effect of isotropic confining pressure on the results of these methods was examined. In general analytical methods are used to predict the stiffness of three-dimensional packings and the implementation of these methods is outlined in Chapters 5 and 6.

All the analytical methods that were used to give expressions material stiffness that depend on the interparticle contact stiffness. Therefore, assessing the influence of interparticle
contact models on the sample stiffness at small-strain levels was important to this study. As discussed in Chapter 3, the interparticle contact models considered in this research were the simplified Hertz-Mindlin contact model that has been used in many DEM simulations, the Cavarretta-Mindlin contact model which is a rough surface contact model and the Hertz-Mindlin-Deresiewicz contact model which is a strain energy dissipation contact model where the energy is dissipated by micro-slip of the contact. The theory or experimental evidence behind these models is outlined in Chapter 3 as is the implementation and verification exercises that were carried out. The verification exercises used for these models provided a template for how other models might be verified. The verification exercises involved single contact simulations so a simple multi-particle simulation was conducted in Chapter 3 to check if the varying interparticle contact models produced a variation in results. In Chapter 5 the effect of the contact model on the stiffness of the regularly packed sample confined at different isotropic confining pressure was examined using wave propagation tests and small amplitude stress probes.

In addition to the variation of particle packing and interparticle contact model, a number of parametric studies were carried out on the samples that varied both micromechanical parameters and macro-scale parameters. Chapter 4 considers the effects of variation in interparticle contact stiffness, particle density, frequency of the transmitted wave and viscous damping ratio. A linear contact model was used in Chapter 4 so the variation in contact stiffness was easy to control and both normal and tangential directions were varied independently of each other. Chapter 5 presents the effects of varying boundary conditions and the boundary conditions examined were flexible boundaries, rigid wall boundaries and periodic cell boundaries. Variation in frequency of the sine wave and transmitter waveshape is discussed in this Chapter. The frequencies used ranged from 7kHz to 30kHz and were representative of the frequencies used in the laboratory experiments. The waveshapes used were a single sine pulse, a single triangular pulse, a single sine pulse with a 270° phase angle and a square pulse. These waveshapes were identical to those used in the laboratory tests. The difference between plane waves and point source waves was explored. The effect of the isotropic confining pressure on sample stiffness was quantified. Chapter 6 outlines the differences due to transmitter and receiver particle connectivity and the effect that they have on the received signals. Due to the inherent anisotropy the effect of propagating waves in different planes was explored as was the effect of different isotropic confining pressures on wave speed. The variation in transmitted frequency followed a similar range of frequencies
to those examined in Chapter 5. Flexible boundary conditions and rigid wall boundary conditions were applied to samples to investigate if they affected sample stiffness. The differences between a force-driven and displacement-driven transmitter particle were explored with this sample. Chapter 7 outlined the different anisotropic stress cases that were examined and the effect on sample stiffness.

8.2 Key observations

The key observations in this research are related to the objectives of the PhD programme given in Chapter 1.

1. Samples used
   a. As the samples became more the disordered the propagation of the waves through the medium was affected. The wave speed was slowed by disorder and this meant that the more disordered a sample, the less stiff it was.
   b. Disorder affected the applicability of analytical methods. The methods usually rely on the existence of solely affine plastic/elastic strains, homogenous interparticle contact forces and monodisperse samples. Each of these assumptions was more easily violated as the sample became increasingly disordered. It was difficult to accurately measure the degree of randomness of a granular packing and existing methods only gave a partial insight. Fabric tensors, histograms of particle connectivity, contact force rose diagrams, void ratio distribution plots and radial pair distribution plots showed that the randomly packed sample was generally truly random except for around the boundaries.
   c. In the frequency domain the location of peaks on the plots of amplitude versus frequency were a function of the disorder of the system, largely in agreement with previous studies by Lawney & Luding (2013) and Leibig (1994). Hu et al. (2008) relate these peaks to the phenomenon known as Anderson localisation that is well documented in the quantum mechanics literature but has not received much attention in condensed matter physics. The value of the threshold or maximum frequency was a function of the disorder as was how the frequency content was filtered as it travelled through the sample.

2. Micro-scale analysis
a. Using micro-scale analysis to visualise the propagation of stress waves through the sample it was possible to achieve a rough estimation for the arrival of the true shear wave.

b. It was also possible to visualise the near-field effect and reflections travelling through the sample in a level of detail that was not achieved in previous analyses. The near-field effect was observed to be associated with movements along the boundaries. The reflections were observed to initiate when the propagating wave interacted with the boundaries and reflections were produced by all the boundary conditions implemented in this research.

c. Parametric studies were carried out that varied both the micro-scale and macro-scale sample parameters. The variations in sample properties were observed to affect the propagation of the wave visualised using the particle-scale properties.

d. The effects of the direction of wave propagation and wave oscillation were observable in the visualisation plots. The connectivity of the transmitter influenced the amplitude of the waves propagating through the system with highly connected transmitter particles producing waves with higher amplitudes. Compressional waves were confirmed to travel faster than shear waves.

3. Travel time determination techniques

a. After critical assessment the two-dimensional fast Fourier transform method, which is a frequency domain method, was found to be the most reliable. It varied least with changing transmitter waveshape and changing frequency of the sine wave. It produced the expected exponent relationship between elastic moduli and confining pressure which was 1/3 due to Hertz-Mindlin contact mechanics.

b. Time domain methods were found to be unreliable as there was an infinite number of characteristic points, such as first zero-crossing or first local minimum, could be picked.

4. Frequency domain analysis

a. From enhanced frequency domain analysis a non-linear relationship between angular velocity and wavenumber was uncovered indicating that the speed of a wave through granular material was non-linear. Granular material was found to be inherently dispersive.
b. Diffusion was found to occur in the time domain as the received signal amplitude was lower than the transmitted signal amplitude. A more nuanced interpretation for the loss in amplitude was obtained from the frequency domain analysis undertaken here. Some of this loss in amplitude was found to be from standard diffusion as the wave generated by a point-source spread out in a spherical lobe and the intensity was spread over a larger area. That was not the only reason for a loss in amplitude. Frequency filtering, observed as a maximum or threshold frequency in the frequency domain plots, meant that at higher frequencies the waves produced were standing waves and their energy did not propagate. Therefore the amplitude of the received signal did not contain any amplitude from waves with high frequencies.

c. It was true that frequency filtering was observed in the time domain as the received waves were oscillating with a visibly lower frequency but the observation was qualitative. Quantitative observations were made in the frequency domain where the amplitudes associated with each frequency were readily available. The location of the maximum frequency decreased with increasing disorder as the randomly packed sample had a lower maximum frequency than the regularly packed sample. The maximum frequency was found to be proportional to $\sqrt{(k/m)}$ where $k$ is the interparticle contact stiffness and $m$ is the particle mass. It was found to be more sensitive to the normal interparticle contact stiffness and less sensitive to the shear interparticle contact stiffness.

d. The location of peaks in the frequency domain plots was relatable to Anderson localization which was originally applied in a quantum mechanics context. Leibig (1994) and Rosenstock & McGill (1962) show how Anderson localization can be used to describe wave propagation through condensed matter.

e. Anderson localization was a function of the disorder of the system and was related to the stiffness of the sample.

f. Frequency domain analysis of the propagation of waves at a grain scale lead to the theoretical support for $\lambda_{\min}/d > 2$ where $\lambda_{\min}$ is the minimum wavelength that can propagate through the system and $d$ is the particle diameter. This was because the maximum value of $k$, the wavenumber, was $\pi/d$.

5. Analytical methods
a. The assumptions used in calculating effective moduli for granular samples were found to generally hold true for regularly packed, isotropically compressed, granular material. They led to inaccurate results for granular material subject to inherent or induced anisotropy such as the pluviated randomly packed sample and anisotropically compressed regularly packed sample.

b. When used to calculate the effective sample moduli of the regularly packed samples, the magnitudes of the moduli agreed well with the results from bender element tests and small amplitude stress probes.

c. The principle of virtual displacement predicted the cubic anisotropy of the sample stiffness that was found by the bender element tests also.

d. Dispersion relation theory predicted the cubic anisotropy of the packing and the presence of frequency filtering. Frequency filtering was confirmed by examining the results in the frequency domain as has already been outlined in the key observations. Dispersion relation theory also predicted dispersion where the phase and group velocities of the waves were different and there was a non-linear relationship between wavenumber and angular velocity.

e. The Sanchez-Salinero method was used to accurately predict the arrival of the near-field effect relative to the arrival of the true shear wave in both randomly packed and regularly packed samples. Shear wave speed was a necessary input for this method and the shear wave speed calculated using effective medium theory was used to achieve the results for the regularly packed sample. The shear wave speed was measured using the two-dimensional fast Fourier transform method for the randomly packed sample.

f. The results of the methods that predicted stiffness were examined at different isotropic confining pressures.

6. Contact models examined

a. The Hertz-Mindlin contact model produced the highest magnitudes of the sample shear modulus, $G$, with a 1/3 exponent relationship with confining pressure.

b. The Hertz-Mindlin-Deresiewicz contact model produced lower magnitudes of the sample shear modulus than the results from the Hertz-Mindlin contact model. The exponent relationship with confining pressure was 1/3.
c. The Cavarretta-Mindlin contact model produced lower magnitudes of the sample shear modulus than the results from the Hertz-Mindlin-Deresiewicz contact model. The exponent relationship with confining pressure was 1/2 at low confining pressures and 1/3 with higher confining pressures.

d. The variation in wave speed with varying interparticle contact model was observed in the particle-scale visualisations.

7. Other micro- or macro-scale parametric studies

a. The samples were examined under different isotropic and anisotropic stiffness. Non-linear contact models used in the three-dimensional samples meant that the sample stiffness was a function of the confining pressure.

b. The regularly packed sample was cubic-anisotropic based on the results of wave propagation tests in different directions and on different shear planes.

c. The fabric of the randomly packed sample was investigated by propagating waves in different directions and different planes. Wave propagation results for the compressional waves matched the measured fabric tensor showing the sample to be cross-anisotropic. Shear wave propagation results indicated the sample was anisotropic but not cross-anisotropic, however, the influence of the connectivity of the transmitter and receiver may affect the results.

d. Variation in sample boundaries did not produce a large variation in wave speed and therefore sample boundaries did not affect sample stiffness. The boundaries considered in this study were flexible boundaries, rigid wall boundaries and periodic cell boundaries.

e. There was little difference in wave speed regardless of whether the transmitter particle was displacement-driven or force-driven.

f. Plane waves were easier to interpret than point-source waves as they were subject to less diffusion. The amplitude of received plane waves was larger than the amplitude of point-source waves.

g. The particle densities and contact stiffness were varied in a parametric study in Chapter 4 and both parameters were found to influence the shear wave speed recorded. Both the normal and shear contact stiffness influenced the shear wave speed and therefore the sample stiffness.

h. The DEM results compared favourably with the results of equivalent tests carried out in the laboratory.
8.3 Recommendations for future research

It is hoped that this research creates a platform from which further novel research projects can be launched to further the understanding of granular material behaviour. Some recommendations are outlined below.

8.3.1 Numerical studies

In general, the computational cost of a discrete element method simulation is a function of the number of particles simulated. To reduce the number of particles created, relatively large glass ballotini particles were simulated in this research. The particle size of 2.54mm is much larger than the particle size of real soils. The largest number of particles simulated in this research was 81,576 particles which were used to simulate the three-dimensional regular packing simulation. In the future this will be considered a small-scale simulation due to the increasing computational power of individual computers, the development of more efficient algorithms and the proliferation of parallelised DEM codes, such as LAMMPS. The aim of future research must be to carry out larger scale simulations so that real soil particle size distributions are simulated in 1:1 scale models of experimental apparatuses. Small-scale simulations should be used in initial validation work of the algorithms employed in large-scale simulations as happened in this research.

The application of flexible, stress-controlled boundaries in DEM simulations is rare and the method used in this research could be refined further to capture more aspects of the physical flexible boundary. The membrane simulated here behaved like a two-dimensional plane membrane when in reality the physical membrane would wrap around the particles as it is three-dimensional. Capturing the true three-dimensional behaviour of flexible boundaries would be an improvement in the ability to model the important geotechnical apparatuses with flexible boundaries such as the triaxial cell and cubical cell.

Variation in particle shape was found to affect wave propagation in experimental work carried out by Cho et al. (2006). DEM has struggled to accurately model particles that are not spherical in shape. A number of researchers including Cleary & Sawley (2002) and Lu & McDowell (2007) have made attempts to model non-spherical particles in DEM. Investigation of the variation in particle shape using a DEM simulation would help explain the mechanism behind the experimental variations and improve the ability of DEM to model particles of non-spherical shape. There is a growing database of particle scale characteristics
including measurements of angularity and sphericity available in the work of Altuhafi & Coop (2011), Cavarretta et al. (2010), Cho et al. (2006) that could be used to help create numerical models.

Varying the interparticle contact model produced some of the most interesting results in this study. They were also some of the most cross-cutting results that attracted interest from the other research fields that use discrete element simulations and have investigated the influence of interparticle contact models on their results. There are many other interparticle contact models that could be investigated. Some of the most widely used ones that were not implemented in this research are the Thornton model that accounts for particle plasticity, see Thornton & Ning (1998), and the JKR model that accounts for adhesion between particles, see Thornton & Yin (1991). An investigation into the effect of these models on sample stiffness is recommended and would be complimentary to the study outlined here.

The micromechanical interaction between the bender element and the granular material warrants further investigation. The influence of the connectivity of the transmitter and receiver particles illustrates that the placement of the transmitting and receiving benders in the packing may influence the signals produced. The development of a discrete element model of the bender element using parallel or contact bonds is recommended to explore the behaviour of the cantilever transmitter in comparison with the behaviour of the single particle transmitter. Laser measurements of the movement of bender elements in air carried out in the University of Bristol during this study would provide useful insight into the modes of vibration and fundamental frequencies of bender elements that would aid the development of a discrete model of a bender element. A larger, cantilever bender element is less likely to be influence by the particle connectivity as the particle connectivity of all the particles used to create the cantilever will average out to similar values in a truly heterogeneous sample.

**8.3.2 Experimental studies**

Further investigation of the interaction between the bender element and the sample should be carried out in the laboratory. Micro-scale analysis using micro-computed tomography could illustrate how the bender displaces in the soil sample when a signal sent to it by the function generator. Any plastic deformation of the bender in the sample and the movement of the sample particles surrounding the bender could be recorded in this analysis. Particle image velocimetry could track the velocities of individual particles surrounding the bender element as it displaces and provide insight into how the stress waves are produced by the bender
element. This will complement existing finite element research in the literature on bender elements.

Frequency domain analysis of bender element signals has led to new insight regarding the characterisation of waves produced by bender elements. The lack of knowledge of the variation of the wave as a function of position in the experimental apparatus hinders the quantification of the propagating wavenumber. The use of transducers along the length of the sample to measure the wave amplitude as a function of position similar to the work of Liu & Nagel (1993) in future experimental work on bender elements would allow two-dimensional fast Fourier transform plots to be created and compared with the equivalent plots created in this research.

The location of the peaks in the frequency domain plots of amplitude versus frequency spurred much analysis towards the end of the current study. The relationship between the peaks and the phenomenon known as Anderson localization of wave energy became apparent but there was insufficient time left to fully explore this fascinating relationship. It is recommended that future researchers consider the importance of exploring the location of these peaks and what they might reveal about sample properties such as stiffness. It is possible to explore this in both a laboratory and numerical context. Investigation of Anderson localization will provide some new insights into the behaviour of physical and numerical granular material.
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