MECHANIC WAVES IN SAND: EFFECT OF POLYDISPERSITY

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ABSTRACT

The sound propagation mechanisms inside dense granular matter are challenging the attempts to describe it because of the discrete nature of the material. Phenomena like dissipation, scattering, and dispersion are hard to predict based on the material state and/or properties and vice-versa. We propose here a simulation method using dynamic discrete elements in order to get more insight in this problem. The idea is to examine a small perturbation created on one side of a dense, static packing of grains of tiny size variations as small as typical contact deformations, during its propagation and when it arrives at the opposite side. Simulations with ordered, monodisperse and polydisperse, packings, reveal a strong impact of the system on the wave properties.

1 INTRODUCTION

A continuum description of granular materials is generally needed in field application (like oil recovery) because of the size of the system considered. Hence starting from simulations at the micro level, which are necessary to get some insight into the role of micro-parameter, one has to consider a ``micro-macro'' transition for the applications. This holds in particular for information propagation in granular materials. Regular structured packings with some weak polydispersity are used to test wave propagation. In section 2, a description of the discrete MD (Molecular Dynamics) model used and the granular packings is given. In section 3, the wave speeds (for the different packings) obtained from simulation and theory are compared and the frequency content of the waves is studied.

2 SIMULATION SETUP

2.1 DEM Model

The elementary units of granular materials are mesoscopic grains, which deform under the stress developing at their contacts. Since realistic modeling of the internal deformation of the particles is much too complicated, we relate the normal interaction force to the overlap δ of two spherical particles. If the sum of all forces, $\boldsymbol{f}_i$, acting on particle i, either from other particles, from boundaries or from external forces, is known, the problem is reduced to the integration of Newton's equations of motion for the translational and rotational degrees of freedom:

$$m_i \frac{d^2}{dt^2} r_i = f_i, \quad and \quad I_i \frac{d^2}{dt^2} \varphi_i = t_i,$$

with the mass $\boldsymbol{m}_i$ of particle i, its position $\boldsymbol{r}_i$, its moment of inertia $\boldsymbol{I}_i$, its angular velocity $\boldsymbol{\omega}_i = \mathrm{d}\boldsymbol{\varphi}_i/\mathrm{d}t$ and the total torque $\boldsymbol{t}_i$. Note that the above equation is only valid for isotropic bodies, like spheres as used in this study. The force acting on particle i from particle j can be decomposed into a normal and a tangential part. A detailed description of the model is given in [5]. For the results presented in this article we used a simple linear spring model: $|f| = k\delta$, with k (=10^5 N/m) the contact stiffness.

2.2 Particle Packing

The configuration considered here is a dense, static packing of grains, with radii a_0 (=0.001m), arranged in a Face Centered Cubic (FCC) structure (density ≈ 0.74), where square layers in the x-y plane (4x4 particles) are stacked in the z-direction (200 layers). The obtained system is thus thin and elongated in the z-direction where each particle has four contacts inside each square-layer, and eight with particles in both neighbouring layers, corresponding to a coordination number C=12.

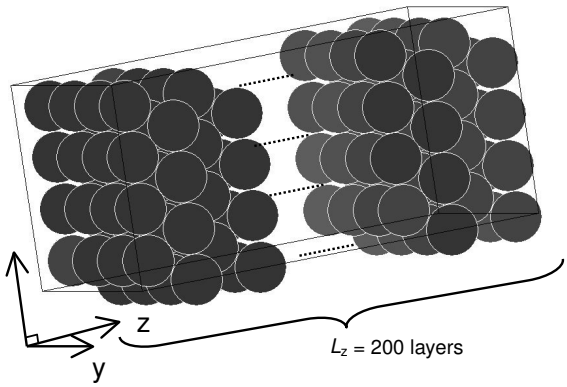

Figure 1: FCC structured packing, thin (periodic) in the x-y directions, elongated (non-periodic) in the z-direction.

Polydisperse packings are obtained by introducing a tiny size distribution to the system. This distribution is homogeneous, centered at the original monodisperse value of the radius and width 2(Δa) of the order of the overlap δ (δ/a=10^{-3}). More precisely we studied three different cases with (Δa)=δ/2, δ and 2δ. As consequence of this small polydispersity the structured system become unstable, therefore a relaxation-simulation is needed to equilibrate the system. The polydisperse system obtained after relaxation conserves its original FCC structure at the grain scale, since the radius variation is much smaller than the value of the radius (~3 orders of magnitude), however some differences are observed at the contact level. Indeed, a radius variation of (Δa)=2δ represent a small change of 0.2% at the grain level but a large change of 200% at the contact level. Therefore polydispersity has to be related to the overlap rather than to the particle size, as it is discussed in [9]. This has a direct influence on the coordination numbers which drop down from C=12 to C=11.99, 11.22 and 9.97 for the three cases (Δa)=δ/2, δ and 2δ respectively. For the last case (**Δ**a)=2**δ** this means a non-negligible reduction of about 17% of the total amount of contacts of the monodisperse system.

3 RESULTS

An initial velocity in the z-direction $v_z=v_0$ is given to all the particles contained in the first x-y-layer ($z=z_0$ smallest) of the packing, for the other particles in the system the initial velocity is zero ($v_z=0$ if $z\neq z_0$), see Fig. 2. This excitation creates a plane compressive (P) wave that propagates through the system along the z-direction. In the following, the 'stress *versus* time' signals recorded at each layer are analyzed for each of the four systems described in section 2.1. Note that the boundary condition and the excitation method, both have an influence on the stress-time signal shape.

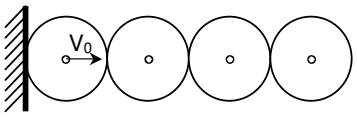

Figure 2: One-dimensional equivalent schema of the initial excitation method, where the z-direction is horizontal.

3.1 Wave velocities

One way to define the wave speed is to measure the time it takes the peak of the first pulse to travel a certain distance. Fig. 3 shows two stress-time signals for the monodisperse and a polydisperse, (Δa)=2δ, packing, both recorded at the same distance, 10 layers, from the source. From all these stress-time signals recorded at each layer in the system, plotting the z-position of the first peak against the time t when it reaches that position (not shown here) gives an almost straight line. Just assuming a constant speed, thus disregarding the acceleration of the pulse at the very beginning of the system, see [5], the slope of this line then gives the speed v_p during propagation, see Table 1 in the row labeled 'simulation'. Note that other points could have been chosen as reference, like at 10% of the first pulse for example. Due to dispersion it gives different values for v_p, still very close to those calculated here as it is observed in [1].

(Δa)	0	**δ**/2	**δ**	2**δ**
v_{pz} (Theory)	218.4	218.4	211.6	199.7
v_{pz}(Simulation)	211.4	211.2	205.5	183.8

Table 1: Comparison of the wave velocities (v_{pz} given in m/s) obtained by theoretical prediction with those obtained from simulations.

The simulation results are now compared with the wave speed obtained from the static material stiffness if the system is considered as a continuous medium. The stiffness tensor *C* of the material can be derived from the potential energy density via virtual displacement, see [3], and can be written in the following form:

$$C_{\alpha\beta\gamma\phi} = \frac{1}{V}\sum_{p\in V}\left(k\sum_{c=1}^{C}\left(l^2/2\right)n_\alpha^c n_\beta^c n_\gamma^c n_\phi^c\right)$$

with a representative volume *V*, the contact stiffness *k*, the branch vector *l* and the normal vector at the contact ***n*** . For the monodisperse packing this can be calculated analytically while for the polydisperse packings the normal vectors components are extracted from the simulation when the system is at equilibrium.
From continuum theory, the (square of the) P wave speed in z-direction is:

$$v_{pz}^2 = C_{zzzz}/\rho$$

with ρ the material mass-density (here ρ=2000kg/m^3). The results are given in the row labeled 'theory' of table 1.
This approach implies however the assumption of a **constant, time-invariant** material tensor, which can hold only for **small** deformations, and does not allow for opening or closing of contacts or even large scale rearrangements. This is all verified for the mono-disperse packing, and explains the quite good agreement between theory and simulations, where the discrepancy is 3.2% (see table 1, column '0'). As soon as polydispersity is introduced, and already for small deformations, the material tensor is no longer time-invariant and opening and closing of contacts is observed. Indeed in the case (**Δ**a)=2**δ,** the discrepancy between theory and simulation rise up to 8.5% (see table 1, column '2δ'). Although a linear contact law drives the interaction between the particles, the opening and closing of contacts introduces a non-linear interaction, and thus makes

the linear theoretical approach inappropriate. A more suitable theory should not only rely on the static initial configuration of the system but should take into account the dynamic nature of the phenomenon as well, in order to determine a realistic effective stiffness for the material. For a different approach on the moduli, that considers random arrays, see [4].

3.2 Wave frequency contents

As one can see from Fig. 3, the signal is strongly affected for (Δa)=2δ as compared to the monodisperse case, (Δa)=0. Qualitatively the first peak is shifted to the right, which is explained by a lower propagation speed (see section 3.1). Also the signal amplitude is smaller which indicates that some energy has been transferred in other type of motion (waves of different nature, shear wave for example, and/or with different propagation direction). Finally the signal looks somewhat more irregular.

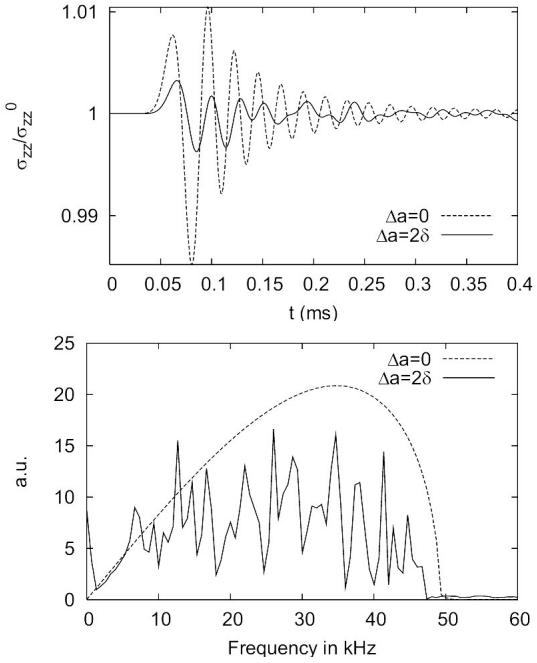

Figure 3: *Above:* Normal stress (σ_{zz}) scaled by the equilibrium stress (σ_{zz}^0) as function of time at a distance of 10 layers from the source for the monodisperse (Δa=0) and a polydisperse (Δa=2δ) system. *Below:* Fourier power spectrum of the two stress-time signals.

In order to quantify this observation we looked at the frequency content of these signals by first calculating the one-dimensional Fourier transforms in time, see Fig. 3. Due to the irregularities present at the contact level, some frequencies seem to be filtered. Fig. 4, where the frequency-space diagrams for the three different polydisperse packings are plotted, shows the evolution of the frequency content of the stress-time signals when the wave propagates away from the source. For the first case (Fig. 4, top, (Δa)=δ/2) the power spectrum does not change much, the bending observed starting at about 50 layers from the source is

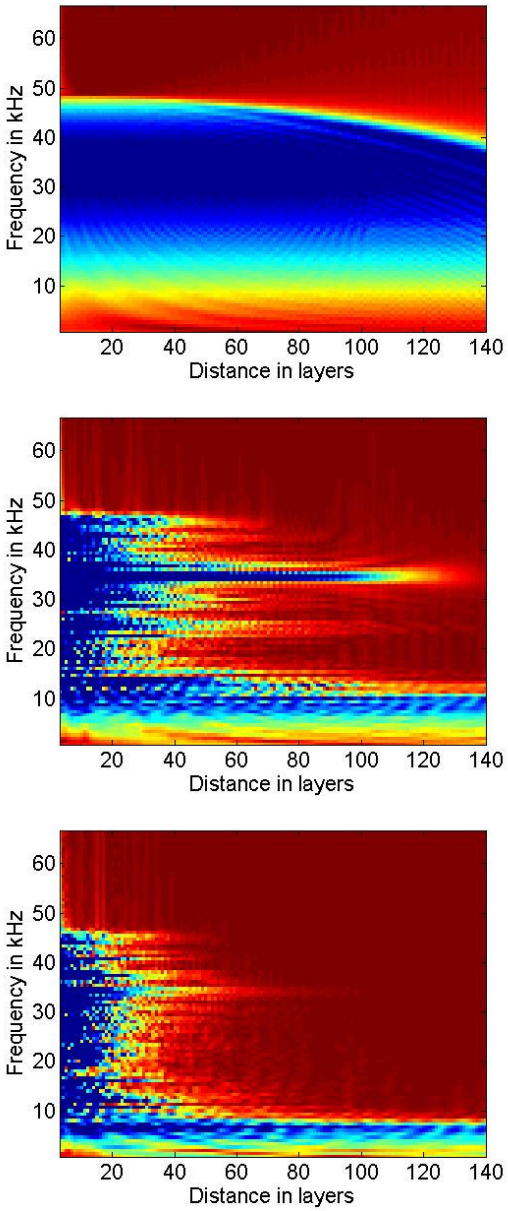

Figure 4: Frequency-space diagram (color scale correspond to the amplitude, absolute value, of the Fourier coefficients, blue is high and red is low) for the P-wave propagating in the z-direction for the three different polydisperse packings (from top to bottom: cases (Δa)=δ/2 , (Δa)=δ and (Δa)=2δ, respectively).

only due to a limitation of available data. The same diagram for the monodisperse case does not offer visual differences with this case and is hence not shown here. However for the two other polydisperse cases ((Δa)=δ and (Δa)=2δ) the frequency range is strongly reduced as the wave

propagates away from the source, with a clearly persistent small frequency range around 8kHz. Also

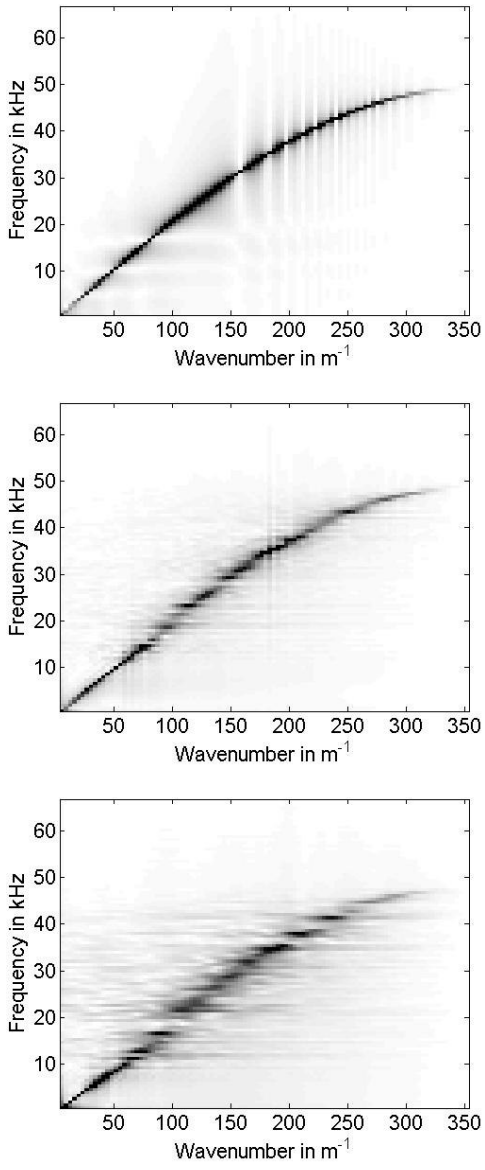

Figure 5: Dispersion relation (grayscale correspond to the amplitude, absolute value, of the Fourier coefficients) for the P-wave propagating in the z-direction in the three different polydisperse packings (cases $(\Delta a)=\delta/2$, $(\Delta a)=\delta$ and $(\Delta a)=2\delta$ respectively).

an other quite strong persistent frequency range observed around 35kHz for the case $(\Delta a)=\delta$, exists in both cases, but tends to vanish much earlier with polydispersity increasing. Also the two-dimensional Fourier transform in time and space has been calculated for the waves traveling in the whole system. The dispersion relation (Frequency *versus* Wave number) obtained for the monodisperse and the polydisperse (case $(\Delta a)=\delta/2$) packing is a sinus (see Fig.5, top, both being visually identical). This has been studied in more details in [5] for a different excitation method but showing similar behaviour.

For the two more polydisperse packings ($(\Delta a)=\delta$ and $(\Delta a)=2\delta$) the dispersion relations obtained (see Fig. 5) are much broader, more noisy, and random gaps seem to appear, although the sine shape is still visible.

4 CONCLUSION

Wave propagation was examined in three-dimensional regular (crystal) monodisperse and slightly polydisperse packings of spheres, for compressive (P) propagation modes.

For the wave speeds, quantitative agreement was obtained between simulations and theoretical predictions based on a micro-macro computation of the stiffness material tensor for the monodisperse packing. However the quality of agreement decays when the polydispersity is increasing. The opening and closing of contacts already present for small perturbation creates non-linear effects.

Finally an interesting filtering of frequencies is observed as polydispersity is increasing. Also the dispersion relation becomes noisier while maintaining its sine profile approximately.

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