Sound wave velocities in dry and lubricated granular packings: numerical simulations and experiments

I. Agnolin, J.-N. Roux
Laboratoire des Matériaux et des Structures du Génie Civil, Institut Navier, Champs-sur-Marne, France

P. Massaad, X. Jia, P. Mills
Laboratoire des Milieux Divisés et des Interfaces, Université de Marne-la-Vallée, Champs-sur-Marne, France

ABSTRACT: numerical simulations are used to investigate the origins of the different wave velocities measured in dense granular samples assembled with different methods. Glass bead packings are prepared in the lab either by pouring and vibrating the dry material in a container, or by mixing with a very small amount of a viscous lubricant. Lubricated samples, although less dense, exhibit significantly higher wave velocities for confining pressures in the 100 kPa range. Numerical predictions for elastic moduli agree much better with experimental results when the computational preparation of the samples mimics the laboratory one, albeit in a simplified manner. A plausible explanation to the laboratory observations is that the coordination number, which influences the material stiffness more than its density, is notably higher in lubricated packings.

1 INTRODUCTION

The mechanical properties of granular packings are sensitive to fine geometric details of the particle arrangement, as very small motions can modify the force-carrying contact network. In practice, direct measurements of such important internal state variables as the coordination number and the distribution of contact orientations (Radjai & Roux 2004) are usually impossible.

In this context, ultrasonic wave propagation measurements might provide useful information on the internal structure of granular samples under confining stresses. Wave propagation has been used as a probe to investigate the microstructure of granular packings by several physics groups (Jia et al. 1999; Jia & Mills 2001; Gilles & Coste 2003). At low frequencies such that the wavelengths are very long compared to the heterogeneity of the medium, the granular medium is effectively a homogeneous continuum to the propagating wave, while at high frequencies when the wavelength decreases down to the order of the grain size, scattering effects caused by the spatial fluctuations of force chains lead to diffusive transport of sound waves (Jia 2004).

Wave propagation has also become a standard method to measure elastic moduli in geotechnics laboratories (Geoffroy et al. 2003), where rheological testing devices are often equipped with specially designed transducers (Lings & Greening 2001). The recent soil mechanics literature (Thomann & Hryciw 1990; Geoffroy et al. 2003) made it clear that “dynamic” measurements of elastic moduli (wave propagation or resonance modes) agree with “static” ones (slopes of stress-strain curves), provided strain increments are small enough (below $10^{-5}$). Correctly measured elastic moduli therefore determine long wavelength sound velocities in granular materials as in ordinary solids.

Discrete particle simulations can also be used to evaluate elastic properties of model granular materials (Roux 1997; Makse et al. 2004; Roux 2004). If experimental packings are correctly simulated, such studies can clarify the relations between wave propagation measurements and sample microstructure.

We first briefly report here (Sec. 2) on experimental measurements on pressure-dependent sound velocities and attenuation in dense samples of dry glass beads (hereafter denoted as E1 samples), as well as lubricated ones in which the effects of intergranular friction are strongly reduced in the preparation stage. The resulting materials (denoted as E2 samples) are, remarkably, less dense, but stiffer (with notably larger elastic wave velocities).

In order to investigate the microscopic origins of these results, we use numerical simulations, as presented in Sec. 3 which is the main part of the present communication. We resort to suitable, yet simplified,
models to mimic laboratory assembling procedures (thus producing sets of samples denoted as A and B by a lubricated procedure, and a third series C by a “vibrated” procedure, see Sec. 3.1 for details). Comparisons of numerical results to experimental ones lead to an interpretation of the observed differences between dry and lubricated samples in terms of coordination number.

2 EXPERIMENTS

The glass beads used in our experiments are of diameter $d = 0.3-0.4$ mm, randomly deposited by pouring and vibrating in a duralumin cylinder of diameter $W = 30$ mm and varying height from 10 mm to 30 mm. The container is closed with two fitting pistons and a normal load is applied to the granular sample across the top piston. Before the ultrasonic measurements, one cycle of loading-unloading is performed in the granular packing in order to consolidate the sample and minimize its hysteretic behavior. A plane-wave generating transducer of diameter 30 mm (top piston) and a detecting transducer of diameter 30 mm are placed on the axis at the top and bottom of the cylindrical container in direct contact with the glass beads. Once the cell is filled, a normal load corresponding to apparent pressures $P$ ranging from 30 kPa to 1000 kPa is applied to the upper piston using a jackscrew arrangement, while the lower piston is held fixed, as in oedometric loading. (The preloading pressure cycle reached up to 400 kPa). Broadband short pulse excitations of $2\mu s$ duration centered at a frequency of 500 kHz are applied to the source transducer. The time of flight of the transmitted ultrasonic signal is used to measure the sound speeds, which are shown on figure 1, and to which results of numerical simulations will be compared in Sec. 3.2 (Figure 3).

Measurements are first performed on assemblies of dry beads, initially prepared in a dense state by layerwise deposition and tapping (samples E1). Then, to study the influence of intergranular friction on the initial structure and elastic properties of the medium, we mix a small amount of liquid lubricant (trioleine, volume fraction 0.5%) with the granular sample for tens of minutes to distribute the oil uniformly among the grains. We observe (figure 1), that the solid fraction in the obtained lubricated samples (denoted as E2) is about 0.62, lower than in the dense dry ones E1 ($\sim 0.64$), while sound wave speeds are significantly higher for E2 specimens (by 10 to 20%) than in the E1 case. It is also apparent on Figure 1 (a logarithmic plot), that the increase of sound velocities with pressure is slightly faster in E1 samples.

3 NUMERICAL SIMULATIONS

We now turn to numerical simulations to explore the origins, at the scale of the contact network, of the differences between the dry (E1) and the lubricated (E2) samples. Our numerical simulations, like others (Makse et al. 2004) (but, admittedly, unlike the experiments of Sec. II) focus on homogeneous, isotropic states, under varying pressure $P$. The samples – the same as those studied by Agnolin & Roux (2005)– comprise 4000 identical beads of diameter $a$ in a periodic cell which changes size as stresses are applied. Averages and standard deviations are evaluated on 5 such samples. Spherical grains are attributed the elastic properties of glass beads (Young modulus $E = 70$ GPa, Poisson coefficient $\nu = 0.3$), and assembled by a standard molecular dynamics method. The contact laws involve Coulomb friction and a suitably simplified form of (Hertz-Mindlin) contact elasticity (see (Agnolin & Roux 2005) and references therein).

The most frequently used numerical procedure (Makse et al. 2004) to obtain dense configurations is to suppress friction altogether while compressing a granular gas to mechanical equilibrium under a given isotropic pressure, thus simulating perfect lubrication. This results in typical isotropic random close packing structures (O’Hern et al. 2003), the properties of which are not sensitive to the details of the procedure, provided it is fast enough to bypass crystal nucleation entirely. On applying this method with prescribed pressure $P = 10$ kPa, we ob-
tained samples we denote as A. Their coordination number \( z^* \), evaluated on eliminating inactive grains ("rattlers") from the count, is close to 6, the value it should approach (Roux 2000; Makse et al. 2004) in the rigid limit, as the average contact deflection \( h \) becomes negligible, \( h/a \propto (P/E)^{2/3} \to 0 \). On imposing larger pressure levels (up to quite high values in simulations) a friction coefficient \( \mu = 0.3 \) is introduced. This implicitly assumes that the perfect lubrication of the assembling stage (in which intergranular forces are transmitted through a very thin layer of lubricant) disappears as large static pressures bring solid surfaces into contact. Another series of numerical samples, type B ones, are also made assuming only a very low friction in the initial stage (\( \mu_0 = 0.02 \)), as a first model of imperfect lubrication. Finally, in order to imitate the preparation of dense dry samples of type E1 in the laboratory, a third series C of initial states under 10 kPa is prepared as follows. First, A configurations are slightly dilated, scaling coordinates by a common factor \( \lambda = 1.005 \); then grains are mixed at constant volume, as by thermal agitation: the system is thus strongly shaken in a dense state; the final step is a compression, with friction (\( \mu = 0.3 \)) and some viscous dissipation to mechanical equilibrium at \( P = 10 \) kPa.

Figure 2 displays the values of solid volume fraction \( \Phi \) and coordination number \( z^* \) as functions of pressure \( P \) in states A, B and C. While B samples are similar to A ones, with somewhat lower values of \( \Phi \) and \( z^* \), C configurations, remarkably, although very nearly as dense as A ones (as expected given their preparation method), and actually denser than B ones, exhibit much lower coordination numbers. The difference between C and A states is gradually reduced as \( P \) grows.

3.2 Wave velocities.
Isotropic states A, B, C possess two independent elastic constants, the bulk \( (B) \) and shear \( (G) \) moduli, from which the velocities of longitudinal \( (V_P) \) and transverse \( (V_S) \) sound for large wavelengths are deduced as \( V_P = \sqrt{\frac{B + 4G/3}{\rho}} \) and \( V_S = \sqrt{\frac{G}{\rho}} \), \( \rho \) denoting the mass density in the granular material.

Once mechanical equilibrium states are obtained with sufficient accuracy, the stiffness matrix of the contact network is built, and both elastic moduli are obtained on solving a linear system of equations, in which particle displacements and rotations as well as strain increments are the unknown, and the imposed stress increments determine the right-hand side. Figure 3 presents the simulated values of \( V_P \) and \( V_S \) for all three sample types and compares them to experimental results. Scarcely coordinated C samples are clearly in much better agreement with experimental data on dense, dry packings than A or B ones in the \( P \sim 100 \) kPa range. The difference between B and C systems is qualitatively the same as the one between dry and lubricated laboratory packings: a lower density, but higher wave velocities that increase a little slower with pressure. Some indications about the pressure dependence of elastic moduli \( B \) and \( G \) in A and C configurations, and a discussion of their pre-

![Figure 2: Volume fractions and coordination numbers as functions of \( P \) in isotropically compressed samples of types A (square dots), B (stars), and C (open circles).](image)

![Figure 3: Comparisons between numerical and experimental values for \( V_P \) (bottom plot) and \( V_S \) (top part).](image)
numerical procedures, even for the interpretation of the observed larger wave velocity in lubricated packings is due to their larger coordination number.

We therefore conclude that C-type samples are better models for dense dry granular packings (of type E1). Such a statement apparently contradicts the good agreement reported by Makse et al. (2004) between numerical measurements of sound speeds on samples of type A and experiments on dry specimen of type E1, such as those by Domenico (1977), shown on Figure 3. However, on confronting simulation results with experimental ones, those authors focussed on a higher pressure range (above several MPa, see Figure 3), in which A and C-type systems are much less differentiated. We checked that our numerical results on A samples coincide nearly perfectly with those of Makse et al. (2004). Thanks to our experimental results for smaller confining pressures we can also distinguish between dense systems with high and low coordination numbers, the latter ones being more appropriate as models for dense, dry granular assemblies.

It might also be noted that in a different communication in the present proceedings (Roux 2005), it is argued that the mechanical properties of C-type samples in quasistatic, axisymmetric triaxial compression are closer to those observed in the laboratory with sand or glass bead samples assembled by pouring and shaking than those of A configurations.

4 CONCLUSION

Numerical simulations show that wave propagation in dense bead packings assembled with various procedures can reveal differences in their microstructure, beyond the sole density. Admittedly, more accurate comparisons with experiments are certainly necessary. This requires a more detailed knowledge of laboratory samples and their anisotropic state of stress (Khidas & Jia 2005), a possible consideration of the effects of capillary adhesion, as well as more realistic numerical models for laboratory procedures (Emam et al. 2005). However, the results presented here show that discrete numerical simulations can relate experimentally accessible data on wave speeds to internal variables such as coordination number or fabric. They clearly stress the need for a better understanding of the influence of the preparation procedure on the subsequent mechanical properties in quasistatic conditions. They suggest a plausible interpretation of the observed larger wave velocity in lubricated systems. Numerical procedures, even for isotropic samples, should not be selected as appropriate because they produce the right density. Coordination number, a largely independent state variable, strongly influences elastic properties and quasistatic stress-strain laws (Roux 2005).

REFERENCES

Agnolin, I. & Roux, J.-N. 2005. Elasticity of sphere packings: pressure and initial state dependence. These proceedings.

Domenico, S. N. 1977. Elastic properties of unconsolidated porous sand reservoirs. Geophysics 42(7): 1339–1368.

Emam, S., Canou, J., Corfdir, A., Dupla, J.-C., & Roux, J.-N. 2005. Granular packings assembled by rain deposition: an experimental and numerical study. These proceedings.

Geoffroy, H., di Benedetto, H., Duttine, A., & Sauzéat, C. 2003. Dynamic and cyclic loadings on sands: results and modelling for general stress-strain conditions. In H. di Benedetto, T. Doanh, H. Geoffroy, & C. Sauzéat (eds), Deformation characteristics of geomaterials: Lisse: 353–363. Swets & Zeitlinger.

Gilles, B. & Coste, C. 2003. Low-frequency behavior of beads constrained on a lattice. Physical Review Letters 90: 174302.

Jia, X. 2004. Coidalike multiple scattering of elastic waves in dense granular media. Physical Review Letters 93: 154303.

Jia, X., Caroli, C., & Velicky, B. 1999. Ultrasound propagation in externally stressed granular media. Phys. Rev. Lett. 82: 1863–1866.

Jia, X. & Mills, P. 2001. Sound propagation in dense granular materials. In Y. Kishino (ed.), Powders and Grains 2001: Lisse: 105–112. Swets & Zeitlinger.

Khidas, Y. & Jia, X. 2005. Acoustic measurements of anisotropic elasticity in glass bead packings under uniaxial stress. These proceedings.

Lings, M. L. & Greening, P. D. 2001. A novel bender/indicator element for soil testing. Géotechnique 51(8): 713–717.

Makse, H. A., Gland, N., Johnson, D. L., & Schwartz, L. 2004. Granular packings: Nonlinear elasticity, sound propagation, and collective relaxation dynamics. Physical Review E 70: 061302.

O’Hern, C., Silbert, L. E., Liu, A. J., & Nagel, S. R. 2003. Jamming at zero temperature and zero applied stress: The epitome of disorder. Physical Review E 68(1): 011306.

Radjai, F. & Roux, S. 2004. Contact dynamics study of 2D granular media: critical states and relevant internal variables. In H. Hinrichsen & D. E. Wolf (eds), The Physics of Granular Media: Berlin. Wiley-VCH.

Roux, J.-N. 1997. Contact disorder and non-linear elasticity of granular packings: a simple model. In R. P. Behringer & J. Jenkins (eds), Powders and Grains 97: Rotterdam: 215–218. Balkema.

Roux, J.-N. 2000. Geometric origin of mechanical properties of granular materials. Physical Review E 61: 6802–6836.

Roux, J.-N. 2004. Internal state of granular assemblies near random close packing. preprint (archive [cond-mat 0405358]).

Roux, J.-N. 2005. The nature of quasistatic deformation in granular materials. These proceedings.

Thomann, T. G. & Hryciw, R. D. 1990. Laboratory measurement of small strain shear modulus under $K_0$ conditions. ASTM Geotechnical Testing Journal 13(2): 97–105.