Numerical model for granular compaction under vertical tapping

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A simple numerical model is used to simulate the effect of vertical taps on a packing of monodisperse hard spheres. Our results are in good agreement with an experimental work done in Chicago and with other previous models, especially concerning the dynamics of the compaction, the influence of the excitation strength on the compaction efficiency, and some ageing effects. The principal asset of the model is that it allows a local analysis of the packings. Vertical and transverse density profiles are used as well as size and volume distributions of the pores. An interesting result concerns the appearance of a vertical gradient in the density profiles during compaction. Furthermore, the volume distribution of the pores suggests that the smallest pores, ranging in size between a tetrahedral and an octahedral site, are not strongly affected by the tapping process, in contrast to the largest pores which are more sensitive to the compaction of the packing.

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1. INTRODUCTION

Granular materials constitute the raw materials in a huge number of human activities as in agriculture, the mining industry, pharmaceutics and are at the heart of the matter in several ecological concerns as desertification by eolian erosion or avalanches. Therefore, explaining a few current granular processes, such as storage, transport, or collapse, is a real economical challenge. Furthermore, packings of spheres which is the simplest model for granular medium, have a great fundamental interest for physicists: hard sphere systems are indeed a common description of simple liquids; moreover grains can behave, according to the external conditions, more or less like a solid, a liquid or a gas. This great variety of behaviors for a banal heap of grains makes granular mechanics a rich area of investigation only partially clarified at the moment. It is now a well-known result (although there is no theoretical explanation for it) that a disordered static packing of equal hard spheres can cover a large range of volume fraction, approximately from 56%, the random loose packing (R.L.P.), to 64%, the random close packing (R.C.P.). For a regular arrangement, the packing fraction can reach up to 74% which corresponds to the densest structures, namely the hexagonal compact (H.C.) and the face-centered cubic (F.C.C.) crystals.

As thermal energy ($k_B T$) plays no role, because it is insignificant compared to the gravitational energy of a macroscopic grain, each packing of spheres is a metastable configuration which can persist as long as there is no external excitation. In this frame, the issues of compaction of grains under vertical taps are a practical way to study the succession of jumps from a metastable equilibrium to another one. The initial packing is quite loose and can progressively reach a nearly stationary configuration (steady state) evaluated through its average volume fraction. Some experiments done in Chicago have studied the influence of the tapping intensity on the steady-state value and the dynamics of the compaction, which is approximately inverse of the logarithm of the number of taps. The experimental setup is a thin tube of diameter $D=1.88$ cm filled to about an 80 cm height with monodisperse, spherical soda-lime glass beads (of diameter $d=1$, 2 or 3 mm). The tube is shaken by an electromagnetic exciter delivering vertical taps, each of them consisting of an entire cycle of a sine-wave of frequency $f = 30$ Hz. The excitation strength is parameterized by $\Gamma$, the ratio between the measured acceleration peak and the gravitational acceleration $g$. Moreover, several numerical and theoretical works, most of them dealing with the notions of free volume and geometric constraint, found the same kind of behavior as obtained experimentally and some of them have pointed out structural ageing effects, as typically observed in glassy systems. So a parallel might exist between this granular compaction and the dynamics of out-of-equilibrium systems as glasses.

In this work, we used a simple model to simulate the compaction of a packing of monosize spheres submitted to vertical taps. We did not try to make a realistic description of the quite complex succession of collisions in a shaken packing: we have kept as the only ingredient of the model the geometric constraint between hard spheres, which is believed to be the principal origin of the compaction. Despite the fact that we deliberately forgot the mechanical dimension of the problem, the model is able to reproduce qualitatively the experimental results of the Chicago group and some further results in agreement with different numerical and theoretical studies. As the model seems to capture the physics of the problem, it is then possible to go beyond a global analysis. Indeed, as a three-dimensional packing of hard spheres, our description has the quite interesting asset that it is very close to a real granular medium. So, contrary to almost all the previous works which deal only with a macroscopic probe
(i.e. the average density in all or part of the packing), our model can provide us with realistic information on the local structure of a packing and its evolution under compaction by taps.

The paper is organized as follows. A detailed description of the model is presented in section II. Section III is devoted to the global analysis of compaction (logarithmic dynamics, hysteresis effect, and ageing behaviors). In section IV, the local analysis of the packings is described with the use of density profiles and size and volume distributions of the pores. Our conclusions and perspectives end the paper in section V.

II. THE MODEL

The model proposed here is purely geometric and deals only with the steric constraint, neither friction nor contact law between the spheres or with the walls is introduced.

The different sequences of tapping were initialized from a relatively loose packing obtained by a steepest-descent algorithm simulating a sequential gravitational deposition \[10\]. We worked with packings of 4096 spheres of radius \( R \) piled up in a square-box of dimension \( L = 32R \). Concerning the vertical walls, we used both periodic boundary conditions (P.B.C.) and fixed boundary conditions (F.B.C.) i.e. impassable vertical planes. The top of the box is open whereas the bottom is a fixed impassable plane.

A tap is decomposed in two stages: first a vertical dilation and then a gravitational redeposition.

The first stage corresponds to the external excitation which will enable the packing to move from a metastable equilibrium to another one. We used the simplest way to simulate the tap by applying an uniform dilation \( \varepsilon \) to the whole packing \((z \rightarrow z(1+\varepsilon))\). This reduction is certainly far from a real tap but we assume that the way of dilating the packing is less important than the result of the dilation: a significant increase of the average free-volume of the spheres which will allow collective rearrangements during the second stage, the redeposition of the packing. This redeposition procedure must be non-sequential in order to permit such collective behaviors: so we use a monte-carlo algorithm to discretise the motion of the spheres: a great number of small displacements are computed. An individual movement procedure is structured as follows: a sphere, randomly chosen, is submitted to a small random displacement; if this displacement creates no interpenetration with another sphere or with the walls (according to the boundary conditions), it is accepted otherwise it is rejected. Because of this binary schema, two neighboring spheres can not be exactly in contact but, after a sufficient time, they get very close to contact. Figure 2 shows a typical displacement: the values of the polar angle \( \phi \) and of the displacement \( d \) are strictly randomly chosen respectively between 0 and \( 2\pi \) and between 0 and \( d_{\text{max}} \), whereas the choice of the angle \( \theta \) follows a random distribution centered on zero to mimic the effect of gravity. We used the following Gaussian distribution of width \( \theta_0 \) truncated beyond \( \pi/2 \) in order to orientate all the displacements down to the bottom of the box.

\[
P(\theta) = A \exp(- (\theta/\theta_0)^2)
\]

The choice of the distribution does not seem to be restrictive: some attempts with a Poissonian and a linear distribution give qualitatively the same phenomenology; the pertinent parameter is the width \( \theta_0 \).

With such an algorithm, agitation will persist indefinitely. So we regularly test the packing during the redeposition process. The variable checked is \( \langle Z \rangle \), the average altitude of the packing that is the average potential energy of the spheres. The redeposition is stopped when the relative variation of \( \langle Z \rangle \) becomes smaller than a threshold \( \eta \). The choice of \( \langle Z \rangle \) is motivated by its easy evaluation during the process and by its possible link with a statistical mechanics approach.

This simulation is rather close to the one proposed by Barker and Mehta \[17,18\] but with some differences especially concerning the way of introducing gravity and the end of the redeposition stage.

The model uses four parameters: \( d_{\text{max}}, \eta, \theta_0 \) and \( \varepsilon \).

The two first ones have a direct effect on the simulation time. The smaller \( \eta \), the longer the simulation time; still, \( \eta \) must be small enough if we want the redeposition to be nearly completed. The parameter \( d_{\text{max}} \) has to be optimised. A very small value of \( d_{\text{max}} \) allows almost all of the displacements to be accepted but the effect on the redeposition is very slight and the packing is therefore nearly frozen. On the contrary, for a large value of \( d_{\text{max}} \), almost of all the displacements are refused and, once again, the packing evolves very slowly. In this study, we used the intermediate value \( d_{\text{max}} = R/5 \).

\( \theta_0 \) has a significant effect on the packing behavior: a very small \( \theta_0 \) induces a decompaction whereas a large value decreases the efficiency of the compaction. We found \( \theta_0 = \pi/4 \) as the optimised value giving rise to the maximal compaction rate.

The last parameter, \( \varepsilon \), corresponds to the external excitation induced in the packing. This is our control parameter. The value of \( \varepsilon \) can be estimated from experimental results concerning the dilatation of a vertically shaken sand heap \[19\]: \( \varepsilon = \delta h/ h \approx 5/500 \approx 10^{-2} \). We can also try to link roughly \( \varepsilon \) to the experimental control parameter, the dimensionless acceleration \( \Gamma = A\omega^2/g \) where \( A \) and \( \omega \) are, respectively, the amplitude and the frequency imposed to the bottom of the heap. In first approximation, if we neglect the loss of energy in the packing, a particle at the top of the heap \((z(0) = h)\) acquires an initial speed \( \omega A \) and achieves a ballistic flight. Its maximal altitude is \( z(0^+) = h + \frac{A^2}{2\omega^2} \) and then it comes:
\[ \Gamma = \omega \left( \frac{2h}{g} \right)^{1/2} \varepsilon^{1/2} \Rightarrow \Gamma \propto \varepsilon^{1/2} \quad (2) \]

As \( \varepsilon^{1/2} \) is linked to \( \Gamma \), we will use it as our control parameter to quantify the strength of the tapping process. With this, it is possible to compare the results of our model with the experimental work of the Chicago group and with other numerical and theoretical models, almost all of them dealing only with a global description of the granular system.

### III. GLOBAL ANALYSIS

This global analysis is achieved with different average values. We did not use a direct evaluation of the packing fraction from the number of spheres in a reference volume because whether boundary effects are significant or, for a smaller volume, the statistics become too poor. Moreover, the choice of the reference volume is not unique: it can be, for example, the space that contains all the spheres or the smaller one that contains only the centers of the spheres. To avoid being partial, we evaluate the packing fraction by averaging the surface packing fraction, \( \Phi \), calculated on many horizontal cuts. This measure is permissible because of the following stereologic result: the average surface fraction of any cut in a packing is equal to the volume fraction of the packing \( \frac{2}{3} \); with horizontal cuts, this calculus is just a spatial integration which gives the exact volume fraction. The packing fraction is equal to the volume fraction of the packing between the heights 0 and 4R; \( \langle \Phi \rangle \) comes from a similar calculation on approximately 90 % of the packing and is corrected near the bottom wall by a perturbated zone model \( \frac{2}{3} \). This model uses a corrective factor for the average density of a packing near a wall (between 0 and R) with regard of a packing not perturbed by any wall. For the case of spheres near a plane, this factor is estimated to 16/11. It is also interesting to study \( \langle Z \rangle \), the average potential energy of the whole system, which is quite pertinent in a statistical mechanics description.

#### A. The dynamics of compaction

The densification of the packing is observed through the temporal evolution of the preceding mean values; here the time is the number of taps and what we call dynamics of the compaction is, in fact, the succession of metastable equilibria, each jump from one to another being induced by the taps. Figure 2 shows compaction laws obtained with fixed boundaries (F.B.C.) and three different excitation rates. This excitation intensity \( \varepsilon^{1/2} \) has a decided effect on the compaction dynamics (see section III B). The simulation curves are in good agreement with the experimental data and compatible with the following fit previously proposed \( \frac{2}{3} \):

\[ X(t) = X_\infty - \frac{\Delta X_\infty}{1 + B X \ln(1 + t/\tau_X)} \quad (3) \]

with \( X = \Phi_b \) or \( \langle \Phi^e \rangle \). For \( \langle Z \rangle \), a nearly similar fit can be proposed:

\[ \langle Z \rangle(t) = \langle Z \rangle_\infty \left( \frac{1 + B Z \ln(1 + t/\tau_Z)}{\langle Z \rangle_0 + B Z \ln(1 + t/\tau_Z)} \right) \quad (4) \]

We have noticed that a sum of two exponentials can also fit \( \langle Z \rangle(t) \) reasonably well. The dependance of these parameters on \( \varepsilon \) is difficult to characterize. We simply note that the parameter B is consistent with an exponential dependance on \( \varepsilon^{1/2} \) (i.e. \( \Gamma \)).

This compaction dynamics is quite particular: as the packing progressively densifies, the compaction efficiency decreases. So the dynamics reduces speed and the system evolves to a steady-state without never really reaching it. This slowing down is particularly remarkable for the smallest values of \( \varepsilon^{1/2} \). This specific dynamics requires the study of the densification on a logarithmic time scale. It is also interesting to analyse the fluctuations of the curves, especially when the packing becomes close to its asymptotic or steady-state (SS) limit. The power spectrum of the fluctuations X-XSS as a function of the frequency, i.e. the inverse of the taps number, shows more or less a simple power-law in a log-log diagram (with a slope in the range 1 to 1.5). The effect of \( \varepsilon \) is noticeable only for the high frequencies. Moreover, the simple standard deviation of the fluctuations, \( \sigma_X = \sqrt{X - X_{SS}} \), seems to be directly proportional to \( \varepsilon^{1/2} \) or \( \Gamma \). These results, calculated for \( X = \langle Z \rangle \), are presented in figure 3. Furthermore, we have noticed that the periodic boundary conditions do not qualitatively affect these observations; the same remark can be made concerning the results of the following section.

#### B. Hysteresis on the steady-state values

The next stage consists on studying the influence of the excitation parameter \( \varepsilon^{1/2} \) on the maximal value of the packing fraction. For this purpose, we carried out a succession of simulations with a sequence of 4000 taps. The steady-state value is estimated by averaging the packing fraction on the 1000 last taps or directly through the last \( \varepsilon \) is noticable value and an uncertain asymptotic limit has also been strong on the range of taps over which the data fitting is performed. This deviation between the steady-state value and an uncertain asymptotic limit has also been

\[ \tau_X = \frac{\ln(1 + t/\tau_X)}{1 + B X \ln(1 + t/\tau_X)} \]

\[ \langle Z \rangle(t) = \langle Z \rangle_\infty \left( \frac{1 + B Z \ln(1 + t/\tau_Z)}{\langle Z \rangle_0 + B Z \ln(1 + t/\tau_Z)} \right) \]
noticed in the experimental work of the Chicago group \cite{8} and in some theoretical studies \cite{13,15}. The dependence of $\langle \Phi^c \rangle$ on $\varepsilon^{1/2}$ is shown in figure \ref{fig:fig3} (solid black squares). The different packings are obtained after 4000 taps of strength $\varepsilon$, starting from the same initial packing. The curve has a bell shape with a maximum between 0.1 and 0.2.

If we now compute a unique tapping sequence with a progressive increase of the excitation $\varepsilon^{1/2}$ after every 4000 taps (constant excitation increment: $\Delta \varepsilon^{1/2} = +0.025$), we obtain nearly the same curve for $\langle \Phi^c \rangle$, as can be seen in figure \ref{fig:fig4} (open circles). When carrying out the same process in the opposite way i.e. with a progressive decrease of $\varepsilon^{1/2}$ ($\Delta \varepsilon^{1/2} = -0.025$), two things can happen: If, while increasing, $\varepsilon^{1/2}$ went beyond a critical value of $(\varepsilon^{1/2})^* \approx 0.15$, the final packing fraction $\langle \Phi^c \rangle$ does not decrease but increases a bit more to a maximum value. If we compute another increase process ($\Delta \varepsilon^{1/2} = +0.025$), we cover approximately the same values. This last upper branch, including the part above $(\varepsilon^{1/2})^*$, is represented on figure \ref{fig:fig4} (up and down open triangles). As it is relatively well reproducible, it is called “reversible”. We can also notice on this reversible branch that $\langle \Phi^c \rangle$ decreases with $\varepsilon^{1/2}$.

On the contrary, if $\varepsilon^{1/2}$ stayed below $(\varepsilon^{1/2})^*$ during the increase stage, the steady-state values do not evolve significantly; they are nearly frozen, and it is hard to estimate whether there is a compaction or a decompaction process, because the dynamics is very slow. This last branch is called “irreversible” and reflects the great metastability of the corresponding packings.

To summarize, there is a strong hysteresis effect which allows the maximum compaction rate to be reached by an $\varepsilon^{1/2}$ increase-decrease sequence. These observations are in very good agreement with the results of Nowak & al \cite{7}. In particular, Figure \ref{fig:fig4} is to be compared to the experimental data obtained with 1mm diameter beads, corresponding to an aspect-ratio of nearly 19, close to that used in our simulation ($L/2R = 16$). Surprisingly, for an aspect-ratio of 9, the experimental results show a much larger increase of the packing fraction on the reversible branch, up to nearly 66 % (i.e. more than the R.C.P. limit which may indicate a commensurability between the cylinder and the beads \cite{5}). However, for a still smaller aspect-ratio of 6, the reversible branch is more similar to the first case, with a moderate increase to a maximal value below the 64 % limit.

C. Ageing

In these kind of systems in slow evolution to a final equilibrium, it is possible to demonstrate ageing effects by comparing the system at different ages. This comparison can be made by use of temporal correlation functions of global values ($\rho, \langle Z \rangle, \ldots$) between the initial packing and the same packing after an evolution time $t_W$ (waiting time). In this study we work with the following function:

$$A(t, t_W) = \langle (\Phi^c(t) - \Phi^c(t + t_W))^2 \rangle$$

(5)

Here, $\Phi^c$ indicates the statistical average of $x$; that is, the mean value calculated for a certain number of realizations of the same experiment. The results have been averaged on only 10 realizations because of the limitation due to the calculation time. The statistics are, therefore, rather poor, that is why we use solely $\langle Z \rangle$, which fluctuates quite less than the other global values. In figure \ref{fig:fig5} are drawn the curves of $A(t, t_W)$ obtained for different values of $t_W$. There is obviously a scaling law; a similar fit as in section II.A, with the three parameters $A_\infty$ (the asymptotic limit), $B_A$ and $\tau_A$, is quite compatible with the data:

$$A(t, t_W) = A_\infty \left(1 - \frac{1}{1 + B_A \ln(1 + t/\tau_A)}\right)$$

(6)

The same kind of ageing effects have already been pointed out in previous numerical studies \cite{10,11}. These effects confirm the great similarity between granular compaction or more generally slow granular rheology and glassy systems submitted to time-dependent driving forces (see for instance \cite{22,24}).

To conclude with the global analysis of the compaction, it is satisfying to note that our simulation reproduces qualitatively well the previous results obtained both experimentally and theoretically. This model seems to capture most of the physics of the problem. Because it gives a very realistic description of a granular system as a three-dimensional packing of hard spheres, it can be a quite useful and interesting tool to go beyond a global description to a local analysis of the packings’ structure during the compaction process.

IV. LOCAL ANALYSIS

To study locally the packings of spheres more or less compacted, we use two kind of descriptions: packing fraction (or density) profiles are calculated vertically and transversely to the box, and size and volume distributions of the pores in a packing are evaluated and then analysed.

A. Density profiles

Using the surface packing fraction calculated by stereological cuts (as in the evaluation of $\Phi_\rho$ and $\langle \Phi^c \rangle$), we can have access to vertical (horizontal cuts) and transverse (vertical cuts) density profiles. Some examples of vertical profiles are shown in figure \ref{fig:fig6}. These have been obtained with fixed boundary conditions (F.B.C.), but the use of periodic boundaries (P.B.C.) induces no significant differences. The profiles are characterised in particular by a negative vertical gradient $\alpha$. 

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and by large peaks near the bottom of the box. These peaks reflect a partially ordered packing due to the wall and are very close to previous experimental observations. The gradient can be roughly estimated in an intermediate zone \(5 \leq z/R \leq 22\) for F.B.C. and \(5 \leq z/R \leq 26\) for P.B.C. after smoothing the profile. This gradient, directly linked to \(\varepsilon\), is qualitatively different from previous numerical results, where a local densification is obtained at the interface. It could be objected that this gradient comes directly from the modeling of the tap through an uniform dilation. Nevertheless, despite this gradient comes directly from the modeling of the previous numerical results [11], where a local densification \(\varepsilon_{\text{26}}\) for P.B.C.) after smoothing the profile. This gradient, being inspired by a Fermi level profile [26], we can propose the following average fit for a typical vertical profile:

\[
\Phi(\tau) = \frac{\Phi_0 - \alpha \tau}{1 + \exp(\beta(\tau - \tau_0))} \quad \text{where} \quad \tau = z/R \quad (7)
\]

Figure 7 presents a few transverse profiles in fixed boundary conditions; they are qualitatively close to experimental profiles [25]. Here again, some peaks indicate a local organisation in layers due to the walls; this effect has approximately a three layers range. The average lateral density increase (at a distance less than 7R from the walls corresponding roughly to this wall effects range) is noted \(\delta \Phi_{\text{lateral}}\) as is the central increase \(\delta \Phi_{\text{central}}\). The last one is systematically smaller than the other. Both of them are calculated in comparison with the initial profiles and reflect the spatial repartition of the bulk compaction. These profiles with periodic boundaries reveal no peak, due to the absence of walls. The central zone is a bit larger but keeps the same qualitative shape and densities as well during a tapping sequence. This observation of an obvious compaction even in P.B.C. ensures that compaction is not, or at least not principally, due to wall effects. This was not evident considering the small aspect ratio used in the experience of the Chicago group. Quantitatively, the absolute value of the packing fraction is larger in the periodic conditions but its increase due to compaction is a bit smaller.

As global values, \(\delta \Phi_{\text{lateral}}\) and \(\delta \Phi_{\text{central}}\) have the same dependence on \(\varepsilon^{1/2}\) (bell shaped curves) than the others. It is also possible to study their evolution with the number of taps. The results, presented in figure 8, point out, once again, the nearly frozen dynamics for small values of \(\varepsilon^{1/2}\). Moreover, we can remark that the initial packing in F.B.C. presents a great metastability. This one is particularly noticeable on the transverse profile (see fig. 7) with an “under-population” of the spheres near the walls. This explains the significant compaction of \(\delta \Phi_{\text{lateral}}\) caused by the first tap (see fig. 8). This metastability is due to the construction of the initial packing: it was built by a gravitational algorithm [16] with periodic conditions, and a slight agitation was then induced in the packing to adapt it to fixed boundary conditions (F.B.C.). This last stage was not sufficiently efficient.

### B. Size and Volume Distributions of the Pores

Another way to analyse a packing of particles is to study the interstitial voids. This void-space is more difficult to apprehend because, in contrast to a particle, a cavity has no geometric limit. We then introduce the notion of pore as the “void” between four neighboring spheres. Previous studies have already been made on this issue, both theoretically and experimentally. Gotoh [28] introduced the pore size distribution \(P_0\) as the probability for a randomly positioned sphere of radius \(r^\prime\) to intercept no particle center. He proposed a theoretical expression for \(P_0\) derived from the Percus-Yevick approximation which agrees well with previous results on random close packings [29,30]:

\[
0 \leq \sigma \leq 1, \quad P_0(\sigma) = 1 - \Phi \sigma^3 \quad (8)
\]

\[
1 \leq \sigma, \quad P_0(\sigma) = (1 - \Phi) \exp\left[\frac{\Phi}{(1 - \Phi)^2}(-1 - 2\Phi)\sigma^3 + \frac{1}{2\Phi\sigma^2} + 1 - 5/(2\Phi)\right] \quad (9)
\]

where \(\sigma\) is the ratio \(r^\prime/R\) (R is the radius of the hard spheres) and \(\Phi\) is the average volume fraction. Figure 8 confronts this expression with the distribution calculated in one of the packing obtained after a compaction sequence of 4000 taps (\(\Phi = 60.6\%\)) and with periodic boundaries. The distribution calculated in the initial packing (\(\Phi = 58.4\%)\) is also represented and is quite close to the other. This slight difference means that the distribution \(P_0\) is insufficiently sensitive to small structural changes as compaction.

Hence we find that it is more efficient to work with a direct statistical analysis on the size of the pores. To do this, we use the Voronoï tesselation of a packing [31]: a Voronoï polyhedron around a sphere is the region of space in which all the points are closer to this given sphere than to any other. Two neighbors correspond to two Voronoï polyhedra that share a face. Each vertex is equidistant from the center of four neighboring spheres and therefore constitutes a pore. More precisely, we define the pore as the virtual sphere in contact with these four neighboring spheres which interpenetrates none of them. The size of the pore is then the radius of this “void-sphere”. The
volume of this sphere reflects partially the total void-volume situated inside the tetrahedron formed by the centers of the four neighboring spheres. In a packing, it is possible to calculate the size distribution of the pores \( \rho_V(\xi) \), where \( \xi = r/R \) with \( r \) the radius of a pore and \( R \) the radius of the hard spheres. The normalisation of the distribution gives \( \int \rho_V(\xi) d\xi = N_P \), the total number of pores in the measurement volume. This distribution is linked to Gotoh’s one. Thus, \( P_0(\sigma = r'/R) \) is more or less the sum of the pores of size greater than \( r' \). Therefore \( P_0 \) is a cumulative distribution in comparison with \( \rho_V \), which is expected to be more sensitive to the local structure. A rather similar analysis by use of the size distribution of the pores was previously sketched out by Barker and Mehta [17].

If we now use directly the normalized volume \( v = \xi^3 = \frac{4}{3\pi r^3} \), as new variable, the corresponding statistical density is \( \rho_v(v) = \xi \rho_V(\xi) \) (here the “volume” of a pore is reduced to \( 4/3\pi r^3 \)). The distribution \( \rho_v(v) \) reflects the contribution of the pores to the total porosity according to their size; this last distribution seems to be the more pertinent in problems of free volume and compaction. We have noted that, by integrating \( \rho_v(v) \), a new global value is obtained and corresponds to the average normalized volume of a spherical pore: \( \langle v \rangle = \frac{1}{N_P} \int \rho_v(v) dv = \langle v \rangle / V \), where \( \langle v \rangle \) is the average volume of a pore, \( V \) is the volume of the hard spheres, and \( N_P \) is the number of pores. The average pore volume \( \langle v \rangle \) has the same dynamics and the same kind of reversible-irreversible behavior as described in section IIIB. Figure IIb shows the distributions \( \rho_v(v) \) for a given packing at different stages of its compaction (in F.B.C. and with an excitation strength \( \varepsilon = 2 \times 10^{-2} \)). The statistics are calculated in a smaller box of height 18R located at a distance 2R from the walls to avoid some boundary problems. In this measurement volume, \( N_P \) varies approximately from 9550 to 10250 for the different packings analysed. These different volume distributions \( \rho_v(v) \) are slightly affected by the taps in the small pore domain, whereas the variation of the packing fraction clearly appears in the progressive reduction of the tail of the distribution in the large pore zone. So, there is more or less a persistence of the distribution for the values of \( v \) approximately limited by the volume of an octohedral site (\( \xi_O = \sqrt{2} - 1 \approx 0.414 \) and \( v_O \approx 0.0711 \)). The distribution \( \rho_v(v) \) is bell-shaped with an over-population for the largest pores (the tail) and with a minimum size of the pores corresponding to a tetrahedral site (\( \xi_T = \sqrt{3/2} - 1 \approx 0.225 \) and \( v_T \approx 0.0114 \)). With respect to the small pores, this is in contradiction with a Poisson distribution proposed in a previous theoretical model for logarithmic dynamics [22]. But, in figure IIb, we note that, in the range of volume corresponding to the tail of the distribution, \( \rho_v(v) \) is compatible with a Poisson law: \( \rho_v(v) \propto e^{(-v/v_0)} \), where \( v_0 \) is directly linked to \( \nu \), the average normalized volume already defined, or to \( \langle \Phi^0 \rangle \), the average packing fraction.

These results must be compared with previous work on the issue. First, Bernal [1] analyzed the arrangements of spheres by characterizing the cavities between the spheres. To do this, he studied the different polyhedra formed by the sphere centers as corner. He found five canonical holes. Table I [33] presents his results obtained on a mechanical model of hard spheres and concerning the statistical weight (in number and in volume) and the \( \xi \)-value corresponding to each hole. In fact, these canonical holes are more or less distorted (otherwise \( \rho_V(\xi) \) would be an addition of Dirac peaks) and the \( \xi \)-value corresponding to the regular hole is therefore a lower limit. So we can note that the tetrahedron and the tetragonal dodecahedron correspond to the smallest values of \( \xi \) for which we have shown that the volume distribution \( \rho_v(v) \) is not greatly affected by the tapping process. In contrast, the octahedron, the trigonal prism and the archimedian antiprism (the two last in very low proportions) appear in the large pores range and are consequently more sensitive to the compaction state of the packing. So, according to this Bernal’s classification on the structure of the pores, we can suggest that compaction is principally due to rearrangements of the three largest canonical pores.

V. CONCLUSIONS AND PERSPECTIVES

A simple model of hard spheres under vertical taps based solely on geometric constraint is sufficient to qualitatively describe previous experimental and numerical results: the same kind of compaction dynamics, hysteresis effect on the steady-state values, and ageing behaviors. The originality of this model, i.e. a realistic description of a granular system as a three-dimensional packing of hard spheres, permits a structural analysis of the packings. A semi-local study on density profiles suggests the existence of a negative vertical gradient in the packings but with no clear hysteresis effect. It also confirms a compaction in the bulk which can not be caused only by wall effects, which are particularly noticeable with fixed boundaries (F.B.C.). A more local analysis on the void space of the packings shows, in a model of spherical pores, a volume distribution sensitive to the packing fraction for the large pores and nearly stationary for the small ones. Compaction could then be principally explained by collective rearrangements of the largest pores.

Further to this numerical work, an experimental study of the compaction induced by vertical taps is being carried out. The packing fraction is deduced from a measure of absorption of a horizontal gamma-rays beam. In addition to the average volume fraction in the bulk, our set-up permits the evaluation of the vertical density profile in the packing; these measurements would be crucial in order to test the results of our numerical model, especially concerning the existence of a negative vertical gradient. Furthermore, compaction is studied in quite different ex-
peripheral conditions than in the previous work of the Chicago group. In this later one, the set-up is a tube of height 80 cm and with an approximate diameter of 2 cm filled with 1 mm diameter soda lime glass beads. So, transverse wall effects are very significant and the vertical pressure on the packing is saturated for almost all of the height of the heap, the overload being completely held up by the walls. Inversely, the cylinder used in our set-up has a diameter of 10 cm and a height of 15 cm; about 80 percent of it is filed with 1 mm diameter glass beads. Here, the wall effects become negligible and the vertical pressure is definitely not saturated in the packing. It will be interesting to see to which extent these differences can qualitatively and quantitatively affect the compaction under vertical tapping.

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[1] J.D. Bernal, Proc. Roy. Soc. London A, 280, 299 (1964).
[2] H.M. Jaeger, S.R. Nagel and R.P. Behringer, Rev. Modern Phys., 68(4), 1259 (1996).
[3] G.Y. Onoda and E.G. Liniger, Phys. Rev. Lett., 64(22), 2727 (1990).
[4] J.G. Berryman, Phys. Rev. A, 27(2), 1053 (1983).
[5] G.D. Scott and D.M. Kilgour, J. Phys. D: Applied Phys., 2, 863 (1969).
[6] J.B. Knight, C.G. Fandrich, C.N. Lau, H.M. Jaeger and S.R. Nagel, Phys. Rev. E,51(5), 3957 (1995).
[7] E.R. Nowak, J.B. Knight, M.L. Povinelli, H.M. Jaeger and S.R. Nagel, Powder Tech., 94, 79, (1997).
[8] E.R. Nowak, J.B. Knight, E. Ben-Naim, H.M. Jaeger and S.R. Nagel, Phys. Rev. E, 57(2), 1971 (1998).
[9] E. Caglioti, V. Loreto, H.J. Herrmann and M. Nicodemi, Phys. Rev. Lett., 79(4), 1575 (1997).
[10] M. Nicodemi and A. Coniglio, Phys. Rev. Lett., 82(5), 916 (1999).
[11] A. Barrat and V. Loreto, J. Phys. A, 33, 4401 (2000).
[12] P.L. Krapivsky and E. Ben-Naim, J. Chem. Phys., 100(9), 6778 (1994).
[13] J. Talbot, G. Tarjus and P. Viot, Phys. Rev. E, 61(5), 5429 (2000).
[14] S.F. Edwards and D.V. Grinev, Phys. Rev. E, 58(4), 4758 (1998).
[15] D.A. Head, Phys. Rev. E, 62(2), 2439 (2000).
[16] R. Jullien and P. Meakin, Europhys. Lett., 4(12), 1385 (1987).
[17] G.C. Barker and A. Mehta, Phys. Rev. A, 45, 3435 (1992).
[18] G.C. Barker and A. Mehta, Phys. Rev. E, 47, 184 (1993).
[19] E. Van Doorn and R.P. Behringer, Europhys. Lett., 40(4), 387 (1997).
[20] L. Oger and J.P. Jernot, in Disorder and Granular Media, edited by D. Bideau and A. Hansen (North-Holland, 1993).
[21] R. Ben Aim, Ph.D. thesis, Faculté des Sciences de l’Université de Nancy, 1970 (unpublished).
[22] L. Berthier, L.F. Cugliandolo and J.L. Iguain, cond-mat/0010266, (2000).
[23] M. Sellitto and J.J. Arenzon, cond-mat/0006146, (2000).
[24] A. Barrat, J. Kurchan, V. Loreto and M. Sellitto, cond-mat/0011492, (2000).
[25] R.F. Benenati and C.B. Brosilow, A.I.Ch.E. Journal, 8(3) 359 (1962).
[26] H. Hayakawa and D. Hong, Phys. Rev. Lett., 78(14), 2764 (1997).
[27] L. Vanel, Ph.D. thesis, Faculté des Sciences de l’Université de Paris VI, 1999 (unpublished).
[28] K. Gotoh, M. Nakagawa, M. Furuchi and A. Yoshigi, J. Chem. Phys., 85(5), 3078 (1986).
[29] J.L. Finney, Proc. Roy. Soc. London A, 319, 479 (1970).
[30] E.M. Tory, B.H. Church, M.K. Tam and M. Ratner, Can. J. Chem. Er., 51, 484 (1973).
[31] P. Richard, Ph.D. thesis, Faculté des Sciences de l’Université de Rennes I, 2000 (unpublished).
[32] T. Boutreux and P.G. de Gennes, Physica A, 244, 59 (1997).
[33] H.J. Frost, Acta Metall., 30, 889 (1982).

FIG. 1. A typical displacement during the redeposition stage of the algorithm.

FIG. 2. Bottom packing fraction $\Phi_b$ versus $t$, the number of taps, in logarithmic (up) and linear (down) time scale for three excitation rae ($\varepsilon = 5 \times 10^{-3}$, $5 \times 10^{-2}$, and $1.5 \times 10^{-1}$). The solid lines are the simulation results and the dotted lines are the inverse-logarithmic fits.

FIG. 3. The power spectrum of the fluctuations of $\langle Z \rangle$ versus frequency (the inverse of the number of taps) (up) and the simple standard deviation of $\langle Z \rangle$, $\sigma(\langle Z \rangle)$, which is nearly linear with $\varepsilon^{1/2}$ (down).
FIG. 4. Steady-state values of $\langle \Phi^c \rangle$ obtained after 4000 taps with different values of $\varepsilon^{1/2}$ (solid black squares) and hysteresis during a sequence of increase (open circles), decrease (open up-triangles) and increase again (open down-triangles) of the excitation with an increment $\Delta \varepsilon^{1/2}$ every 4000 taps.

FIG. 5. Ageing effects on the time-correlation function $A(t, t_W)$ for several waiting times $t_W$ : the different curves (up) and a collapse according to the fit in dotted line (down).

FIG. 6. Two examples of vertical density profiles with their fit : for the initial packing (dotted line) and for a packing obtained after 4000 taps with $\varepsilon = 10^{-1}$ (solid line).

FIG. 7. Two examples of transverse density profiles : for the initial packing (dotted line) and for a packing obtained after 4000 taps with $\varepsilon = 10^{-1}$ (solid line). The two vertical dotted lines indicate the frontiers in the calculus of $\delta \Phi_{\text{lateral}}$ and $\delta \Phi_{\text{central}}$.

FIG. 8. Lateral (up) and central (down) packing fraction increases (in comparison with the initial packing) versus $t$, the number of taps for 4 values of $\varepsilon$.

FIG. 9. Theoretical pore size distribution $P_0$ (thick solid line) compared with the numerical calculation for a packing with the same average volume fraction (open circles). No significant difference with the calculations for the initial packing (thin solid line) which has a quite smaller volume fraction.

FIG. 10. a) Volume distribution of the pores $v\rho_v(v)$ for a packing at different stages of its compaction (F.B.C. and $\varepsilon = 2 \times 10^{-2}$): $t+1 = 1, 100, \text{ and } 10000$. As the packing progressively densifies (i.e. as $t$ increases), the tail of the distribution corresponding to the largest pores tends to vanish (as symbolized by the arrow). Here, T and O indicate the v-values for tetrahedral and octahedral sites in a dense packing (F.C.C. or H.C.). b) Plot of $\ln(\rho_v(v))$ versus $v$ for the same packings. The different tails are compatible with a Poisson law.

|                | $\xi=r/R$ | Number (%) | Volume (%) |
|----------------|-----------|------------|------------|
| tetrahedron    | 0.225     | 73.0       | 48.4       |
| half-octahedron| 0.414     | 20.3       | 26.9       |
| trigonal prism | 0.528     | 3.2        | 7.8        |
| tetragonal dodecahedron | 0.353 | 3.1 | 14.8 |
| archimedian antiprism      | 0.645     | 0.4        | 2.1        |

TABLE I. Characteristics of the Bernal canonical holes.
$\epsilon = 5 \times 10^{-2}$
\[ \Delta \varepsilon_{1/2} = +0.025 \]
\[ \Delta \varepsilon_{1/2} = -0.025 \]
\[ \Delta \varepsilon_{1/2} = +0.025 \]
$A(t, t_W)$

$t_W = 1$

$t_W = 2$

$t_W = 3$

$t_W = 5$

$t_W = 20$

$t_W = 50$
$A(t_{W},t) / A_{\infty}$

$B. \ln(1+t/\tau)$

$t_{W} = 1, 2, 3, 5, 10, 20, 50, 100, 500$
\[ \delta \phi_{\text{lateral}} (\%) \]

\[ \varepsilon = 10^{-4} \]
\[ \varepsilon = 10^{-3} \]
\[ \varepsilon = 2 \times 10^{-2} \]
\[ \varepsilon = 0.1 \]

$t+1$
$\delta \Phi_{\text{central}}$ vs. $t+1$

- $\varepsilon = 10^{-4}$
- $\varepsilon = 10^{-3}$
- $\varepsilon = 2 \times 10^{-2}$
- $\varepsilon = 0.1$
theorical curve ($\Phi = 60.6 \%$)

4000 taps ; $\varepsilon = 5 \times 10^{-3}$ ($\Phi = 60.6 \%$)

initial packing ($\Phi = 58.4 \%$)
$t+1 = 0$
$t+1 = 100$
$t+1 = 10000$

$\ln(\rho_v(v))$