Simulation Study of Granular Compaction

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Abstract. We study by numerical simulation the compaction dynamics of frictional hard disks in two dimensions, subjected to vertical shaking. Shaking is modeled by a series of vertical expansion of the disk packing, followed by dynamical recompression of the assembly under the action of gravity. The second phase of the shake cycle is based on an efficient event-driven molecular-dynamics algorithm. We analyze the compaction dynamics for various values of friction coefficient and coefficient of normal restitution.

INTRODUCTION

The phenomenon of granular compaction involves the increase of the density of granular material subjected to shaking, tapping or, more generally, to some kind of external excitation. The underlying dynamic and structural properties of compaction process are a subject of great interest for physicists in recent years [1-5].

The modeling of tapping and free evolution until the powder is settled is a rather difficult task, although some procedures have been proposed. Our numerical simulation is based on the ideas of Barker and Mehta [6, 7] and Bideau and coworkers [8], with modifications aiming at more realistic treatment of gravitational redeposition of granular particles.

Our simulations have been performed for a two-dimensional system of frictional monosized hard disks in the rectangular geometry. During the redeposition of the packing, the disks undergo instantaneous, inelastic binary collisions and propagate under gravity in between collision events. The algorithm employed in the present paper describes relatively accurately the quite complex succession of collisions in a shaken packing and provides realistic information about its microstructural transformations during compaction.

In the simulation, the compaction of \( N = 1000 \) monosize disks of diameter \( d \) and mass \( m \) under consecutive taps is studied in a rectangular container of width \( L = 1 \), with a flat bottom at \( y = 0 \) and opened top. A gravitational field \( g \) acts downwards, i.e., along the negative \( y \) direction. One shake cycle of the granular assembly (corresponding to one time step of our simulation) is decomposed in two stages: 1) vertical dilatation of the disk packing, in proportion to the shaking acceleration \( \Gamma \) and
2) formation of static granular pack in the presence of gravity. Repeated application of the shaking algorithm builds a sequence of static packings where each new packing is built from its predecessor. In the second phase of the shake cycle, the packing is compressed under gravity, using an efficient event-driven molecular-dynamics algorithm [9]. The disks are assumed to be inelastic with rough surfaces subject to Coulomb friction. Particle collisions are modeled using the Walton model [10, 11].

RESULTS AND DISCUSSION

In order to examine the effects of inelastic and friction properties of grains on compaction dynamics we used two sets of material parameters. More dissipative and rough disks (disks (A)) are characterized by coefficients of inelasticity \( \epsilon_0=0.6 \) and friction coefficient \( \mu=0.4 \), whereas with parameters \( \epsilon_0=0.9 \) and \( \mu=0.2 \) we characterize less dissipative disks (disks (B)). We used the same inelasticity and friction coefficients for grain–grain and grain–wall collisions including the horizontal base.

The variation of the packing fraction \( \rho(t) \) with the number of shakes \( t \) for several tapping intensities \( \xi \) is presented in Fig. 1, where more dissipative grains (disks (A)) have been used. The inset of Fig 1 compares the evolution of normalized packing fraction \( \rho(t) = (\rho(t) - \rho(0))/\rho(\infty) - \rho(0) \) for two kinds of grains (A) and (B), for \( \xi=3\% \). The simulation curves are in good qualitative agreement with the experimental data obtained in experiments with a reduced lateral confinement [2, 3]. We have observed that compaction dynamics gets slower when tapping intensity \( \xi \) decreases. Actually, when a small tapping intensity is applied the evolution of the density toward steady-state value \( \rho_\infty \) takes place on much wider time scale and finally a larger value of the asymptotic packing fraction is achieved.

The resulting compaction dynamics is strongly consistent with the Mittag–Leffler law [12]

\[
\rho(t) = \rho_\infty - \Delta \rho \exp \{ -(t/\tau)\}^\gamma, \quad \Delta \rho = \rho_\infty - \rho_0
\]

\( \rho_0 \) is the initial packing fraction and \( \rho_\infty \) is the mean value of the packing fraction at the stationary state. \( \exp \{ \cdot \} \) denotes the Mittag–Leffler function of order \( \alpha \). Our data are reasonably well fitted by a Mittag–Leffler function (1). These fits are shown by the dashed lines in Fig. 1. As can be seen, the intermediate–long time behavior of the packing fraction can be accurately described by Eq. (1). In Fig. 2 the values of two fitting parameters \( \tau \) and \( \alpha \) versus control parameter \( \xi \) are reported for the both kinds of grains, (A) and (B). The parameter \( \tau \), for a given type of grains, seems to be a simple power law of the vibration intensity \( \xi \), i.e., \( \tau = \kappa \xi^{\gamma_1/2} \).

As one can see from Fig. 2, the slope of \( \tau \) vs \( \xi^{1/2} \) curves is almost independent on the material properties of the grains. For disks of type (A) and (B) the exponents are \( \gamma_1(A)=2.50 \) and \( \gamma_1(B)=2.85 \), respectively. However, parameter \( K \) of the power law (2) depends appreciably on the material properties of the grains. We have obtained that \( K(A)=30.3 \) and \( K(B)=13.1 \) for disks (A) and (B), respectively. One striking feature of
Fig. 2 is the fact that the fitting parameter $\alpha$ depends considerably on the tapping intensity $\xi^{1/2} \propto \Gamma$ and on the material properties of the grains. For large values of $\xi^{1/2}$, there is a rapid approach to steady-state density $\rho_\infty$, and consequently the parameter $\alpha$ reaches a value close to 1. The steady-state density $\rho_\infty$ is also sensitive to material properties of disks. The decrease of $\rho_\infty$ with $\xi^{1/2}$ is more pronounced for disks of type (A). However, for given tapping intensity, system of disks (B) achieves a larger value of the asymptotic density $\rho_\infty$ than the system of more dissipative disks (A).

Figure 1: Temporal evolution of the packing fraction $\rho(t)$ obtained for the grains of type (A) and for various tapping intensities $\xi = 0.1\%$ (red), 0.7\% (green), 2\% (blue), 3\% (violet) and 5\% (light blue). The dashed curves are the Mittag–Leffler fits of Eq. (1), with the parameters $\tau$ and $\alpha$ given in Fig. 2. Inset: evolution of the normalized packing fraction for two kinds of the grains (disks (A) – solid line and disks (B) – dashed line), at $\xi = 3\%$.

CONCLUSION

We have demonstrated that large scale simulations of granular compaction offer insight into dynamics of the compaction process and evolution of the packing structure during its progressive densification. Unlike to almost all previous models for granular compaction, whose essential ingredient is geometrical frustration, our model is based on realistic granular dynamics. One of its main features is that during the second phase of the shake cycle the whole system is reassembled by using event–driven molecular–dynamics algorithm. We employed the Walton model [10, 11] that captures the major features of granular interactions.

We have fitted the time dependences of the packing fraction with the Mittag–Leffler function (1). Our data show that the compaction dynamics strongly depends on the material properties of the grains. It was shown that the relaxation behavior is appreciably slowing down with the increase of the inelasticity of the
grains. The characteristic timescale $\tau$ is found to decay with tapping intensity $\Gamma$ according to a power law (2), $\tau \propto \Gamma^{-\gamma}$. The exponent $\gamma$ is almost independent on the material properties of the grains. The model presented here can be easily generalized to mixtures of several kinds of grains, allowing the study of segregation phenomena.

Figure 2: Fit parameters $\tau$ (empty symbols) and $\alpha$ (full symbols) of (1), as functions of vibration intensity $\xi^{5/2} \propto \Gamma$ for two kind of the grains. Squares and circles correspond to the grains of type (A) and (B), respectively.

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REFERENCES