Frictional powders: Ratcheting under periodic strain in 3D

S. Luding[1], C. T. David[2], R. Garcia-Rojo[2], H. J. Herrmann[2,3]

[1] Nanostructured Materials, DelftChemTech. Julianalaan 136, 2628 BL Delft, Netherlands
[2] ICP, University of Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany
[3] Computational Physics of Materials, ETH Zürich, Switzerland

ABSTRACT

The mechanical response of grains under quasi-static cyclic loading is studied by means of a three-dimensional Molecular Dynamics scheme. The response of the system is characterized by an accumulation of plastic deformation with increasing number of cycles. From the (deviatoric) stress-strain relation a ratchet-like behavior is observed: Increasing the coefficient of friction leads to a transition from ratcheting to shake-down, i.e., the accumulation of strain stops. The strain rate shows a sharp transition when friction is increases above a certain value, whereas the fraction of sliding contacts shows a smooth, continuous transition, indicating that both effects are decoupled.

INTRODUCTION

Plastic deformation of particle systems depends on the history of the material (Vanel et. al., 2004). Hysteretic behavior under repeated, cyclic loading is in fact a very relevant characteristic of many soils and powders. The frequent use of non-cohesive, dry granular materials in foun-dations of buildings and as roadbeds makes the development of more efficient models necessary, with the goal to understand the effects caused by cyclic loading.

Element tests on small representative samples are a standard way to determine empirical laws related to the deformation behavior of powders and grains. They also permit the calculation of relevant parameters in constitutive laws. One possibility to perform these experiments is the triaxial setup, where the system is subjected to cyclic loading. Such tests are carried out in order to investigate the elasto-plastic response of granular materials. An alternative to experiments is the simulation of the system using discrete elements methods (DEM). In DEM the evolution of individual grains is obtained by the calculation of the interaction forces between particles and the integration of the equations of motion (Allen and Tildesley 1987). Contact forces include, e.g., plastic deformations, cohesion and Coulomb friction. In the simplest case visco-elastic rules can be imposed at each contact, different for the normal and the tangential direction (Luding, 2004b, David, 2005).

All natural materials, when subject to increasing load, produce relatively high stress, and exhibit corresponding deformations, hysteresis and creep. Given a cyclic perturbation of a granular material, the main question is whether the material accumulates plastic deformation in each cycle (ratcheting) or whether it adapts to the excitation (shakedown). Materials in which the excitations “shake down”, i.e., do not accumulate, should best be considered for constructions. Goal of this study is to better understand the transition between the two regimes.

The concept of ratcheting was introduced in soil mechanics in order to describe the gradual accumulation of a small permanent deformation (Lekarp et al., 2004). Ratcheting is however a much more general concept that has also been observed for steel (Colak, 2003), biophysical systems, and others. In a 2D granular packing of discs, subjected to stress controlled cyclic loading, strain accumulations could be classified as shakedown, or ratcheting, depending on the amplitude of the stress variations and the strength of friction (Alonso-Marroquin et al., 2004; Garcia-Rojo et al., 2004); first 3D results on cyclic loading (David 2005) are elaborated further here.

MODEL

The particles that make up a powder, deform locally under stress at the contact point. A realistic modeling of this would be computationally too expensive to allow for the simulation of many particle systems. Thus the interaction force is only expressed as function of the overlap of two particles – if they are in contact (short range forces). The force between them is usually decomposed into a normal and a tangential part.

The *normal force* is, in the simplest case, a linear spring that takes care of repulsion, and a linear dashpot that accounts for dissipation during contact.

The *tangential force* involves dissipation due to Coulomb friction, but also some tangential elasticity that allows for stick-slip behavior on the contact level. A literature overview and more details on the model used can be found in (Luding, 2004, Luding, 2006, Luding 2007).

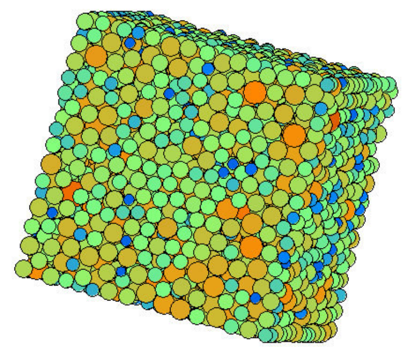
In our DEM simulations, a three-dimensional triaxial box is used. The walls are either fixed or stress controlled. Typical values of the test include a confining stress p_0=1 kN/m^2, a wall-mass m_w=2 kg, and a viscosity of the wall, γ_w=200 kg/s, which corresponds to a viscous relaxation time t_w=0.01 s.

For the initial preparation of the sample, the spheres (with radii randomly drawn from a Gaussian distribution centered at 5 mm, a minimum of 3 mm and a standard deviation of 0.7 mm) were placed on a square lattice (big enough for them not to overlap). Then the box is compressed by imposing a confining pressure, p_0, in order to achieve a homogeneous, isotropic initial condition. The preparation stage is finished when the kinetic energy becomes much smaller than the potential energy stored in the contacts. A periodic loading with period t_0 is applied next through one side of the box, while keeping the other stresses constant. The fact that all walls are stress controlled can lead to a moving center of mass of the system; however, we checked various combinations of stress-controlled and also fixed wall boundary conditions and coule not see much systematic difference bettween the different boundary conditions.

RESULTS

Different friction coefficients and numbers of particles have been investigated (David, 2005): The particles studied have a density ρ=2000 kg/m^3, which leads to a mass m=1 g for a sphere with the mean radius a=5 mm. The normal and tangential spring constants used are k_n=5000 N/m, and k_t=1000 N/m, respectively. For viscous damping (normal, tangential, and beackground) the following values were applied: γ_0=0.05 kg/s, γ_t=0.01 kg/s, γ_b=0.2 kg/s, and γ_{br}=0.05 kg/s; the latter two correspond to backround translational and rotational damping, respectively. These material parameters leads to a typical contact duration, t_c=10^{-3} s, restitution coefficient, r=0.95, and background damping relaxation time, t_b=0.005 s. The DEM step used is Δt_{MD}=2.10^{-5} s, such that we can be sure that $\Delta t_{MD} << t_c < t_b < t_0$. If not explicitly mentioned, the friction coefficient is μ=0.1. See Fig. 1 for a snapshot of a typical system before the cyclic loading starts.

Figure 1: Snapshot of a model system with N=3375



particles. The color code indicates the size of the particles (large=red, medium=green, small=blue).

In the following, the stress is modified with the amplitude $\Delta\sigma = 0.2 p_0$, where p_0 is the static pressure, the sample was prepared with. The horizontal stress is the average of the stress on the left and the right wall: $2\sigma_{xx} := \sigma_{xx}^{left} + \sigma_{xx}^{right}$, and $2\sigma_{xx} = 2p_0 + \Delta\sigma[1-\cos(2\pi t/t_0)]$ is the functional variation of stress with time t, and t_0 =10 s is the period of one cycle. Simulations with different periods t_0 =20 s and 40 s, did not lead to significant differences. Different amplitudes, however, change the behavior strongly.

When deviator stress $\sigma_D = 2(\sigma_{xx} - \sigma_{yy})/3$ is plotted against strain $\varepsilon_D = 2\left(\varepsilon_{xx} - \varepsilon_{yy}\right)/3$ (also deviator), with the active strain in horizontal direction $\varepsilon_{xx} = 1 - L_x / L_x^0$ and the inactive strain, perpendicular, $\varepsilon_{yy} = 1 - L_y / L_y^0$, the stress-strain relation consists of open hysteresis loops with slow accumulation of deviator strain.

The accumulated strain, ε_N, becomes smaller after each cycle until a roughly constant rate of increase is reached. The system size has a strong influence on strain accumulation (David, 2005). Here, N=1728 is used, as a compromise between large (size-independent) and small (faster) simulations. For very small samples, the strain accumulation is constant after a few cycles, while for larger samples, ratcheting remains over hundreds of cycles, see Fig. 2 for a typical deviator stress strain plot. During each cycle, the number of sliding contacts increases during the first half-period, then rapidly drops and increases again until the end of the period, before it drops again, see Fig. 3. The variation of the fraction of sliding contacts is of order 0.10 for a friction coefficient of μ=0.1 and can be as large as 0.6 for a small friction coefficient of μ=0.05. Note, however, that some later shakedown after thousands or more cycles cannot be excluded from our finite size and finite time simulations.

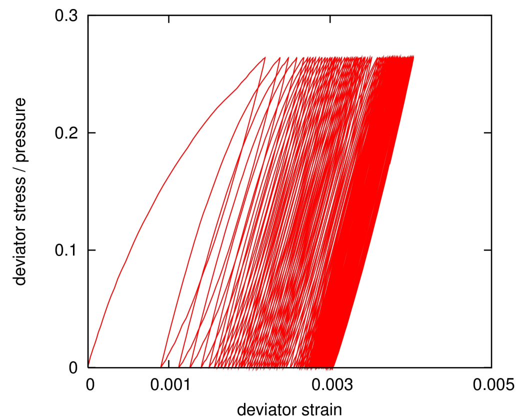


Fig. 2: Deviatoric stress versus deviatoric strain during the first 100 cycles for a sample of N=3375 spheres.

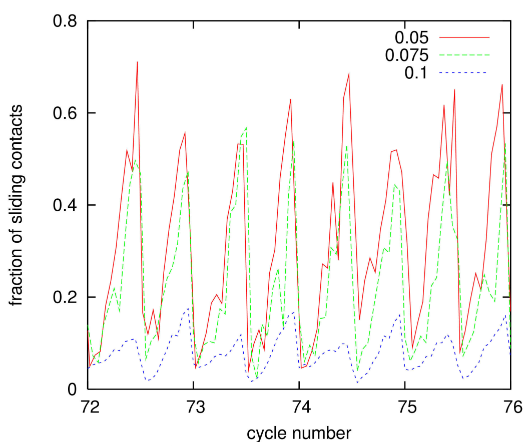


Fig. 3: Fraction of sliding contacts during 4 cycles of a sample with N=1728, for different coefficients of friction, as given in the inset.

The effect of friction in detail

We study the influence of friction, in a system with N=1728 spheres, covering various friction coefficients between $\mu = 0.01$ and 10. The area enclosed by the first cycle (which quantifies the dissipated energy in this cycle) is smaller for larger friction, see Fig.4, and also the apparent modulus (the slope of the hysteresis loop) changes with friction; a larger friction leads to a stiffer material with less plastic strain.

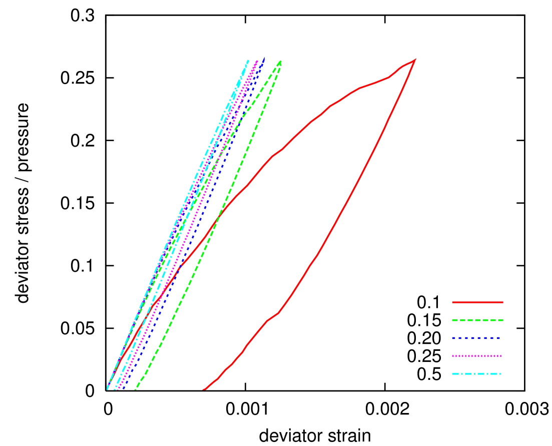


Fig. 4: Deviatoric stress-strain relation for the first cycle for different coefficients of friction as given in the inset.

The system therefore crosses the boundary between ratcheting and shakedown when friction is increased above μ=0.1-0.5, see Fig. 5. This transition is rather sharp: a drop over two orders of magnitude can be observed.

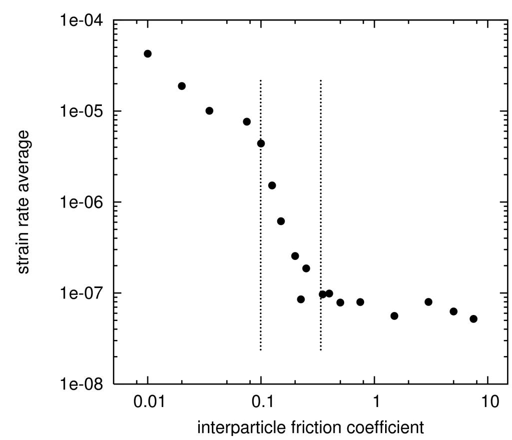


Fig. 5: Strain accumulation rate, as a function of the coefficient of friction. Each point indicates the rate of change of deviatoric strain between the first and the 100^{th} cycle.

The fraction of sliding contacts, in contrast, shows a smooth transition without the drop. This indicates that the two phenomena strain-accumulation and massive contact sliding are related to the friction coefficient, but the different transition behavior indicates different physical origins and effects responsible.

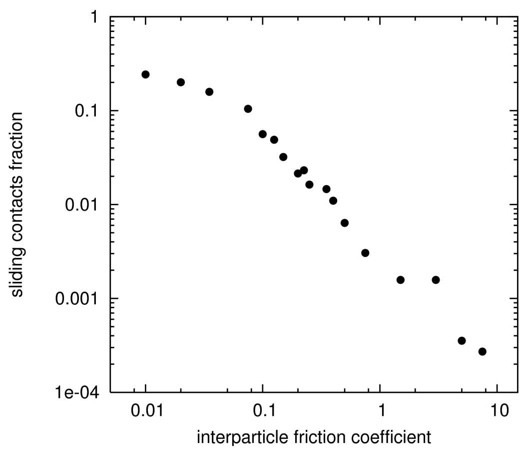


Fig. 6: Fraction of sliding contacts from the same simulatons as in Fig. 5, averaged over the first 100 cycles.

DISCUSSION AND CONCLUSIONS

In summary, ratcheting was examined in a three dimensional cuboid volume filled with poly-disperse, frictional spheres. The limit between shakedown and ratcheting depends on both system size and friction, the latter is examined more closely here. For the chosen magnitude of deviatoric stress change, clear ratcheting is only observed for rather weak friction, while stronger friction seems to work against ratcheting by stabilizing the packing due to the stronger tangential forces. Interestingly, the transition from ratcheting to shakedown is rather sharp when the deviatoric strain rate is considered, but the transition is smooth and continuous for the ratio of sliding contacts. This indicates that the sliding contacts cannot solely be responsible for ratcheting. A more detailed exploration of the influence of various other material- and system-parameters is in progress, involving variations of the stress amplitude, of the friction model parameters, boundary conditions, and others.

ACKNOWLEDGEMENTS

The authors acknowledge support from the EU project Degradation and Instabilities of Geomaterials with Application to Hazard Mitigation (DIGA) in the framework of the Human Potential Program, Research Training Networks (HPRN-CT-2002-00220), the Deutsche Forschungsgemeinschaft (DFG), and FOM (Fundamenteel Onderzoek der Materie), financially supported by the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO). Many helpful discussions with Sean McNamara, O. Mouraille, and F. Alonso-Marroquin are acknowledged.

REFERENCES

1. Allen, M., P. Tildesley (1987). *Computer Simulation of Liquids.* Oxford: Oxford University Press.
2. Alonso-Marroquin F. and H. J. Herrmann (2004). *Ratcheting of granular materials*, Phys. Rev. Lett. 92, 054301 (2004).
3. Colak, O. U. and E. Krempl (2003). Modelling of uniaxial and biaxial ratcheting behavior of 1026 Carbon steel using the simplified Viscoplasticity Theory Based on Overstress, Acta Mechanica (New York) 160, 27-44.
4. David, C. T., Garcia-Rojo, R., Hermann, H. J., and Luding, S. (2005), *Hysteresis and Creep in Powders and Grains*, in: Powders and Grains 2005, Eds. R. Garcia Rojo, S. McNamara, and H. J. Herrmann, Balkema.
5. García-Rojo, R. and H. J. Herrmann (2005). Shakedown of unbound granular material, Granular Matter 7(2), in press.
6. Lekarp, F., U. Isacsson and Dawson A (2000). *Permanent strain response of unbound aggregates,* J. Transp. Engng.-ASCE 126 (1). 66-83.
7. Luding, S. (2004), *Micro-macro transition for anisotropic, frictional granular packings*. Int. J. Sol. Struct. 41, 5821-5836.
8. Luding S. (2004b), *Molecular dynamics simulations of granular materials*. In H. Hinrichsen and D. E. Wolf (Eds.), The Physics of Granular Media, Wiley VCH, Weinheim, Germany, pp 299-324.
9. Luding, S. (2006), *About contact laws for frictional granular particles*. In: Behavior of Granular Media (research report).
10. Luding, S. (2007), *Tensile tests with a new contact laws for frictional granular particles*. submitted to Granular Matter.
11. Vanel, L., D Howell, D. Clark, R.P. Behringer and E. Clement (1999), *Effects on construction history on the stress distribution under a sand-pile*, Physical Review E 60, 5.