STATIC AND DYNAMIC STRUCTURE OF GRANULAR MATERIALS

(Final Report of the OTKA Project T049403, PI: János Kertész)

Granular systems are of extraordinary importance as most of the solid materials are stored ands transported in this form. Correspondingly, we meet such systems everywhere, from households to the industry, from agriculture to geology or even astronomy. In spite of their omnipresence and importance, granular systems have remained a challenge to both engineering and fundamental research due to the many open questions characteristic for them.

Granular systems are conglomerates of macroscopic solid particles characterized by friction and inelastic collisions. In the non-cohesive case the contact forces are only repulsive. In the cohesive case, adhesion forces come also into play. Because of the typical grain sizes, thermal fluctuations and Brownian motion are irrelevant; however, external driving forces can induce complex collective behavior and transition between solid, fluid, and gas-like states. The grains can be activated with shear, vibration, external volume forces (gravity, electric and magnetic fields), and flow of the interstitial fluid or gas (such as water and air). In most of the cases, the grains are in metastable states far from equilibrium. The dissipative interactions and the negligible thermodynamic effects are the main factors which determine their behavior. In fact, these are the properties which form the main source of differences between granular and ordinary condensed matter.

In recent year considerable progress has been made in the understanding of some aspects of granular materials. Static packings have been studied extensively and – among other results – a thermodynamic formalism has been developed. The characterization of the different regimes in the dynamics has been very helpful. Intensive investigations of the avalanche dynamics have revealed the nature of the intermediate regime. The analogue between thermodynamic phase transitions and the jamming transition has turned out to be a particularly fruitful idea.

Our group has worked on problems related to granular materials for more than a decade, The results immediately preceding the present project include:

- Numerical modeling of avalanches including related segregation phenomena
- Uncovering the optimal interaction cutoff for efficient simulation of magnetic grains
- Development of a theory for the geometry of shear bands
- Discovery of non-monotonic dependence of the force fluctuations on the friction in static packings of rigid discs

Based on these we formulated the following questions in the proposal of the present project:

- What is the dynamics of avalanches in a system of magnetic grains?
- How do truly three-dimensional shear bands form and what are their characteristics?
- How to generalize the theory of shear bands to include the broadening effect?
- What are the consequences of the non-monotonic force-fluctuations onto the dynamics?

The present report summarizes the progress we have made in answering these questions. The report is organized according to the above questions. At the end we give a short discussion and an outlook.

1. Avalanches in a System of Magnetic Grains

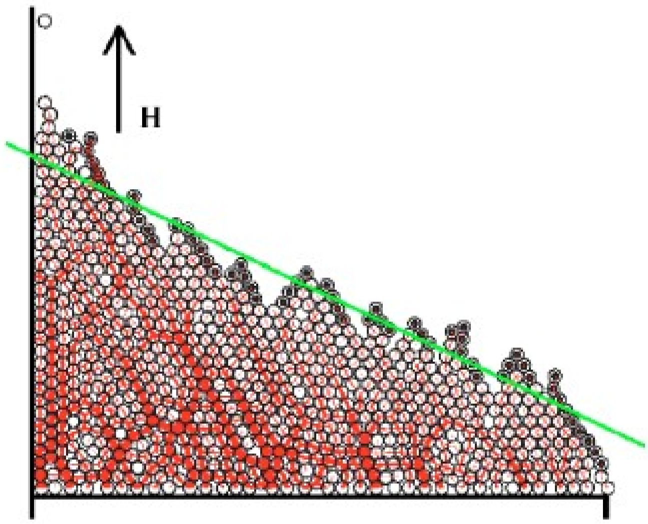
Cohesive grains behave very differently from non-cohesive ones. Some time ago Hornbaker et al. [1] addressed the question how sand castles stand. They stated that already small quantities of wetting liquid can dramatically change the properties of granular media, leading to large increase in the angle of repose and correlation in grain motion. Experimental studies of Tegzes et al. on angle of repose using the draining crater method and on avalanches using a rotating drum apparatus identify three distinct regimes as the liquid content is increased: a granular regime in which the grains move individually, a correlated regime in which the grains move in correlated clusters, and a plastic regime in which the grains flow coherently.

To study the transition from non-cohesive to cohesive behavior, Forsyth et al., adopting idea that competition between the inter-particle forces and the inertial forces determines the behavior of cohesive granular materials, suggested a method based on magnetized particles. The particles placed in an external magnetic field become magnetized, all having the same magnetic orientation parallel to the field. Varying the strength of the field allows to continuously varying the resulting inter-particle magnetic force.

We carried out computer simulations on a system corresponding to the experiments of Forsyth et al. and studied the angle of repose, the surface roughness, and the effect of magnetization on avalanching in two-dimensional particle piles. We used an own developed distinct element code and in the magnetic interaction we made use of our earlier result about the cutoff. The system is characterized by the inter-particle force ratio *f*:

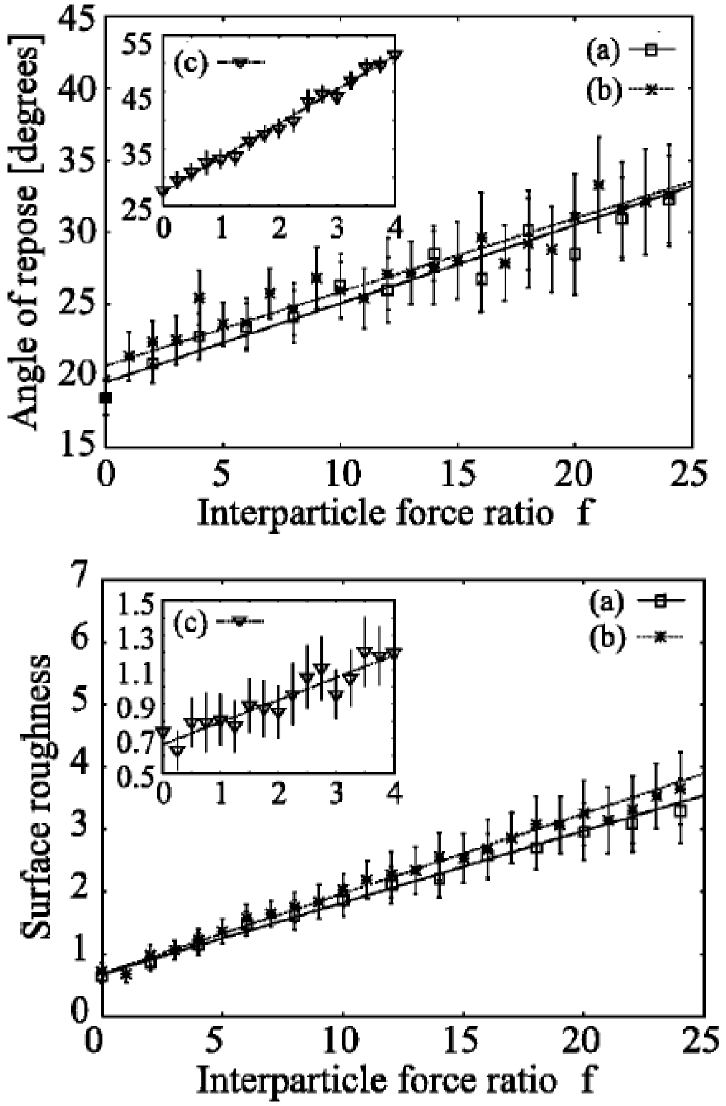
$$f = \frac{F_m}{F_g} = \frac{\mu_0}{4\pi}\ \frac{6S^2}{mgD^4} = \frac{\mu_0}{4\pi}\ \frac{\pi M^2}{\rho g D}$$

where M is the magnetization, ρ the mass density and D the particle diameter. The diameters of the particles had a Gaussian distribution around 0.8 mm. The parameters were chosen such that $f < 25$. Dissipation and friction were taken into account in the usual manner. The simulation setup is shown below.



The particles are come with constant rate one by one at small random distances from the left wall. The external magnetic field is vertical. The particles can leave the system on the right side. The angle of repose is measured by fitting a straight line over the positions of the surface particles (marked with black). The figure also shows the normal contact forces. The thickness of the lines connecting the centers of the particles in contact is proportional to the normal contact force.

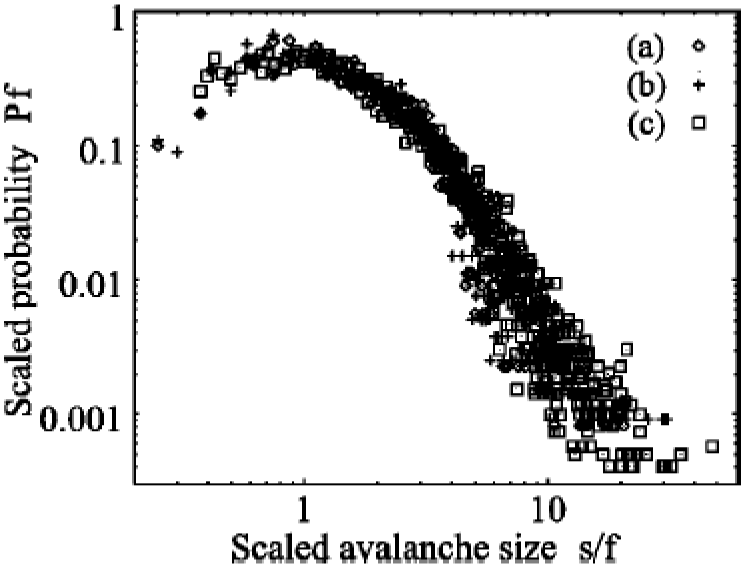
We have measured the angle of repose and the surface roughness as a function of *f*. The results are shown in the next Figure.



Angle of repose (upper panel) and surface roughness (lower panel) at different magnetic inter-particle force ratios. The angle of repose is measured in degrees. The surface roughness is measured in (average) particle diameters. We carried out three sets of simulations: In (a) and (c) the particles were fired into the pile, while in (b) the particles were placed gently on the pile. In (c) an artificial side wall effect was switched on.

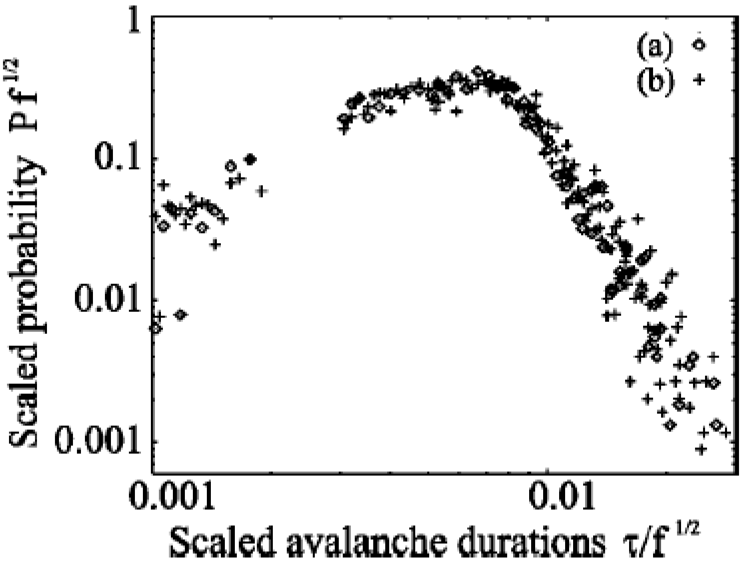
At zero magnetization the average surface roughness is about 0.7 particle diameters, and in all cases increases by approximately 0.12 particle diameters per unit change of inter-particle force ratio. This is in agreement with the observations by Hutton and on the same experiments as described by Forsyth *et al.*. As a consequence of our side wall model, the angle of repose is about 8 degrees higher at zero magnetization, in agreement with experimentally observed effects of front and back walls in Hele-Shaw cells. However, the way we model the side walls leads to a stronger increase of the angle of repose with *f* than in the experiments of Forsyth and co-workers.

We analyzed the effect of magnetization on particle avalanching and found that there is a difference in avalanche formation at small and at large interparticle force ratios: We identified a *granular* and a *correlated regime*. The transition between the two regimes is not sharp. The difference between these regimes is apparent in movies, which can be downloaded from http://maxwell.phy.bme.hu/~fazekas/magaval/ .



Scaled avalanche size distribution in granular regime. A characteristic size can be observed. We examined three different simulation setups. The avalanche size distribution at inter-particle force ratios $1 < 7$ are scaled together using the ansatz $P(s,f)=f^{-1}Q(s/f)$ where s denotes avalanche sizes. We conclude that the characteristic avalanche sizes increase linearly with f.

The difference can be made quantitative too. The statistics of the avalanches follow different rules in the two regimes as indicated in the figures.



Scaled avalanche duration distribution in correlated regime. A characteristic duration can be observed. We examined two simulation setups. The avalanche duration distribution at inter-particle force ratios $7 < f < 24$ are scaled together using the ansatz $P(\tau,f) = f^{1/2}Q(\tau/f^{1/2})$, where τ denotes avalanche durations. This justifies that the square of avalanche durations increase linearly with f.

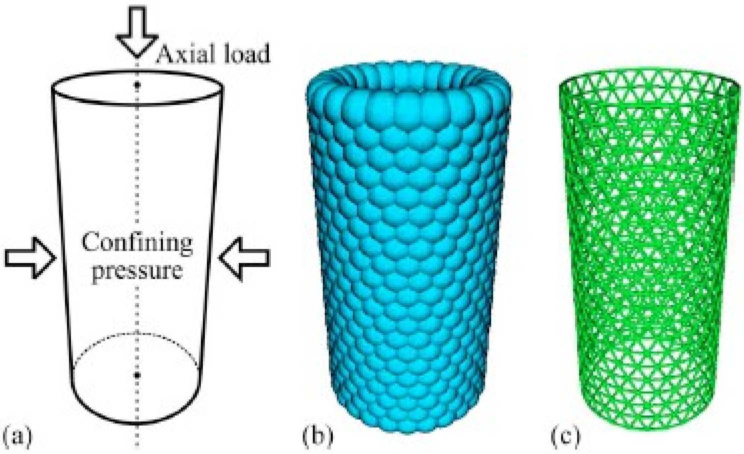
Based on our investigations we concluded that i) the simulations reproduce well the experiments on magnetic grains ii) there are strong similarities between the cohesive and the magnetic systems as reflected in the two well distinguishable regimes, although the anisotropic and long range nature of the magnetic interaction lead to some significant differences too.

2. Formation and characterization of shear bands in granular materials

2.1 Three-dimensional shear bands in triaxial axisymmetric shear cells

The description of the rheological properties of dry granular media is a key question which controls the ability to handle – mixing, storing, transporting, etc. – these particulate systems. An interesting and sometimes annoying feature of such materials is strain localization, which appears almost always when a sample is subjected to deformation. In the past 20 years the formation of shear bands has gained increasing attention as experimental tools like computer tomography – CT – became available. Such experimental studies revealed complex localization patterns and shear band morphologies depending on the test conditions. Simulations of two-dimensional systems have contributed considerably to the understanding of the related phenomena, but so far realistic numerical experiments on three-dimensional systems were missing.

We applied distinct element method simulation to a triaxial axisymmetric shear cell, which is a standard testing tool of granular materials.



The triaxial axisymmetric shear cell. (a) A granular sample was subjected to axial load and confining pressure. (b) The rubber membrane surrounding the sample was simulated by overlapping spheres initially arranged in a triangular lattice. (c) The neighboring spheres were interconnected with linear springs. The confining pressure acted on the triangular facets.

First we had to identify the shear bands. The mean deformation gradient tensor can be calculated for a region Ω as:

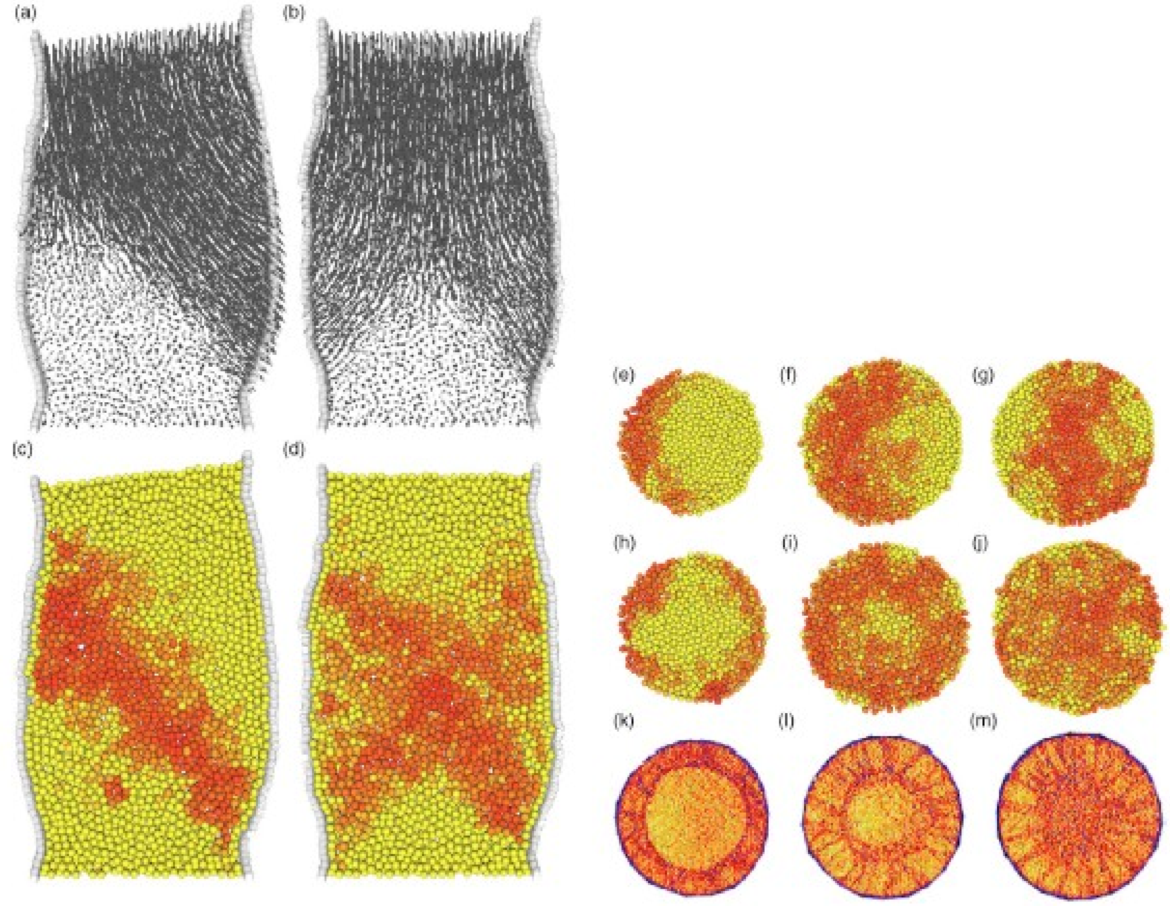
$$\langle u_{ij} \rangle = \frac{1}{V} \oint_{\partial\Omega} n_i u_j dS$$

where the integral has to be evaluated numerically over a small region. The symmetric part of this tensor is the strain tensor, the ε_k eigenvalues enable us to define the local shear intensity:

$$S = \max_k \left| \varepsilon_k - \frac{1}{3} \sum_l \varepsilon_l \right|$$

This quantitiy is well suited to characterize the position of the shear bands as the loci of the highest shear intensity. We have shown that the angular velocity and the coordination number could also be used for this purpose.

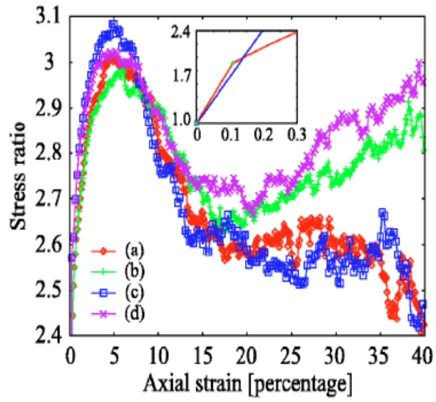
The main results of our investigation are summarized in the next figure.



Cross sections (a), (c), (e), (f), (g) of sample C and (b), (d), (h), (i), (j) of sample D shown at 10% axial strain. (k), (l), (m) present CT scans [3] (Experiment No. F2075). The vertical cross sections (a)–(d) were taken at the middle of the sample. The horizontal cross sections were taken at different heights: close to the top (e), (h), (k), at the middle (g), (j), (m), and in between (f), (i), (l). The gray (red) color encodes the local shear intensity (c)–(j) and the local void ratio on (k)–(m). (a), (b) show the velocity field.

Here sample C means freely tilting upper platen, while on sample D the axisymmetry is enforced. We have found that in the former case spontaneous symmetry braking takes place in the shape of the shear bands. Our findings are in excellent agreement with the experiments carried out in space experiments under microgravity conditions (k,l,m figures above).

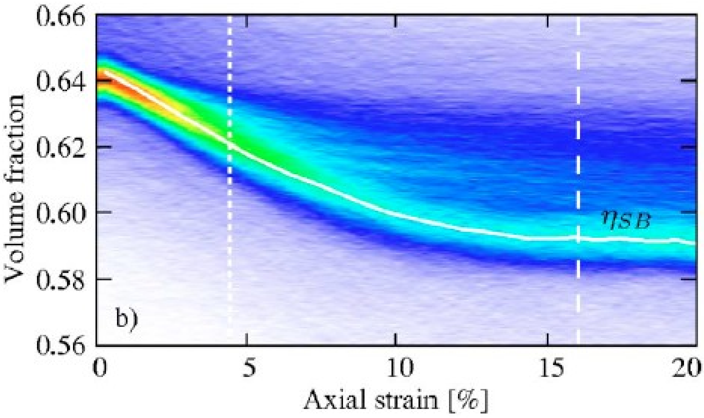
A further interesting related phenomenon is strain hardening. The figure below shows, in good agreement with the experiments, that in the case of forced symmetry the stress rate increases after a minimum as a function of the strain (green and magenta), while no such effect is observed for the symmetry breaking case (red and blue).



2.2 Critical density in shear bands

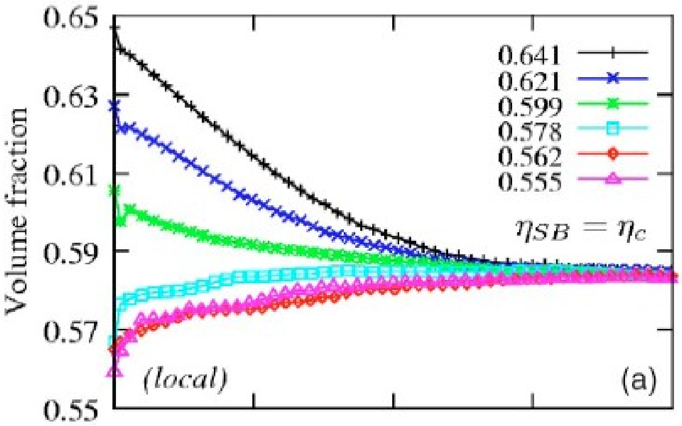
One of the most important characteristics of granular systems is the packing density. It has been a long standing problem how this quantity behaves, when the material is imposed to shear such that shear bands form. It has been suggested that system organizes itself to a critical density: For large initial density dilatation takes place, while starting from a loose ensemble of grains the system becomes denser. This picture could only be verified for relatively small systems.

We proposed that the concept of critical density can be applied within the shear band only. In order to prove out hypothesis we carried out computer simulations and measured carefully the local density during shear. The system had the same axisymmetric arrangement as described above. The results are shown in the following figure.



Development of the critical density as a function of the strain. The curve in white shows the value as measure in the shear band.

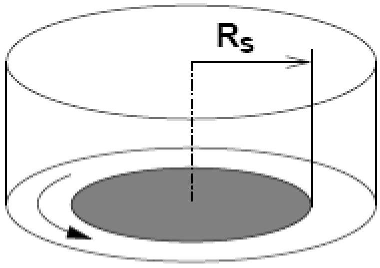
The next figure shows that the asymptotic density becomes indeed independent of the initial packing density. The latter are marked in different colors.



However, we observed a clear dependence of the asymptotic density on the friction. In the limit of infinite friction the critical density depends only on the shape of the grains, therefore this limiting case can be considered as new, dynamic characteristic packing of granular materials.

2.3 Theory of wide shear bands

Recently, in a series of very interesting experiments, van Hecken and collaborators demonstrated that shear bands widen if they are not pinned to the walls of the apparatus. In order to avoid the latter effect, they introduced a modified Couette-cell, where, instead of two concentric cylinders rotating in opposite directions only the outer cylinder is left and a bottom split is introduced such that a disc in the middle of the cell is at rest. This way universal shape functions could be obtained for the position and the width of the bands. The next figure shows the geometry:

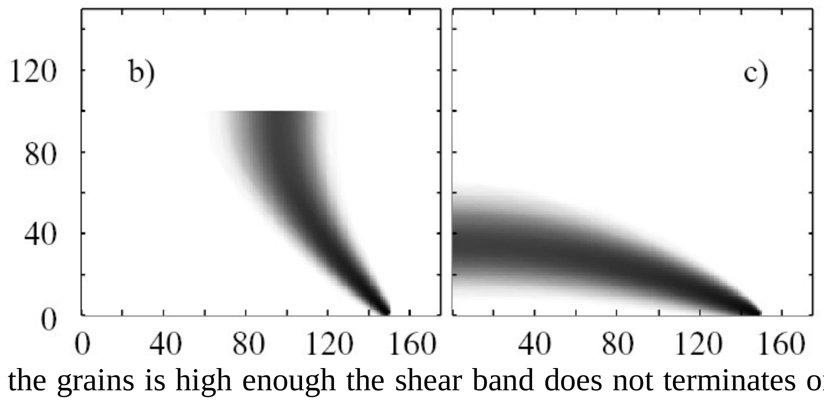


Setup geometry. The rotating (white) and the stationary (gray) parts induce shear flow in the granular material held by the container. The developing shear band is pinned to the bottom split, but its widening is not hindered by the wall.

In an earlier paper we proposed a theory based on a varational principle for the position of the shear band. Using the principle of least dissipation we suggested that the shape should minimize the following functional:

$$\int_0^H r^2 \sqrt{1 + (dr/dh)^2}\, \sigma_{tn} dh = \min.$$

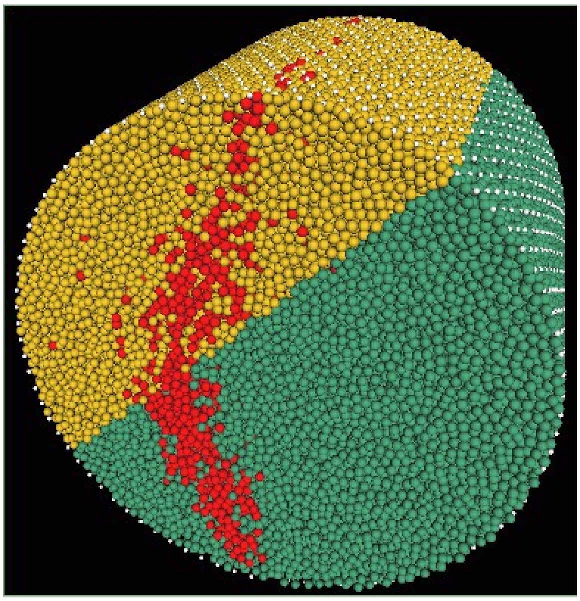
Here σ_{tn} is the shear element of the (two-dimensional) stress tensor. We solved the problem under the simplifying assumption that the tangential variation of the band is negligible (which enables to reduce the problem to two dimensions) and, more importantly, that the band is infinitely narrow. Our results were surprisingly good for the position of the band, and we could predict the existence of closed, cupola shaped bands, which were later found in experiments. However, one of the most important aspects, namely the widening of the bands escaped of that treatment. Our aim in the present project was to generalize the theory in order to account for this latter, important effect as well. The next figure illustrates the two generic cases for the shear band geometries (axial cuts).



If the packing of the grains is high enough the shear band does not terminates on the surface but closes itself underneath. These figures were obtained by using our model.

The main idea is that instead of using a simple optimization as we did for the narrow band limit, we consider the shear bands as a result of a time dependent phenomenon. There is a narrow band solution at every instant of time; however, the formation of the shear band rearranges the material. This way a new optimization problem is defined where a new band is found and so on. In other words, the shear band is formed in a self organized random potential and is measured as a wide band is a time average of this fluctuating object. This model is closely related to several problems of statistical physics including self-organized criticality and the directed polymer in a random potential. These relations already give a hint why universal behavior was seen in experiments. The grayscale in the above figure reflect the frequency of shear bands at some position, which can be transformed easily to relative velocity. This way we have a complete description of the wide shear bands and the agreement with experiment is again surprisingly good.

Another, very interesting outcome of the variational approach is that a new phenomenon could be predicted: The refraction of shear bands on the boundary of two granular materials with different friction. Here the analogy to the Fermat-principle of optics could be used and the result is in full analogy; even Snell's law holds. The predictions of the theory were checked in computer simulations and good agreement was found. The following figure shows the simulated refraction of a shear band.

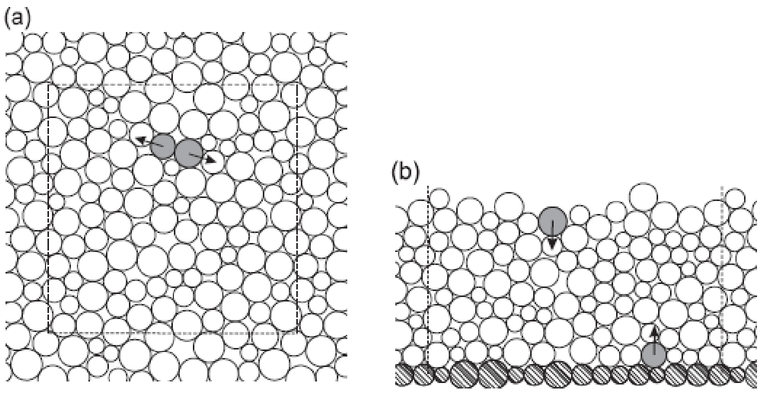


Refraction of shear bands on the boundary of two granular materials with different frictions. The two materials are shown in different colors. The system is driven by shear such that the left and the right parts move in the opposite, axial direction. There is split both on the top and at the bottom thus the band is pinned on these lines. In a homogenous material a vertical band would develop.

3. Unjamming due to local perturbations in granular packings

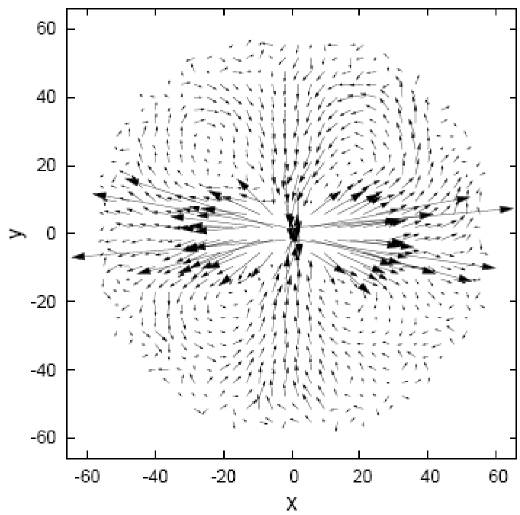
Recently much effort has been devoted to understand the jamming transition in granular systems. We asked ourselves the question: How does the already jammed state get again into motion? Our method is primarily computer simulation of two-dimensional systems.

We produced dense packings in two different ways: First, we let the particles aggregate as a consequence under gravity. The second, more demanding arrangement was to produce homogenous arrangements with periodic boundary conditions and isotropic compression. The next figure illustrates the geometries together with the perturbations applied.

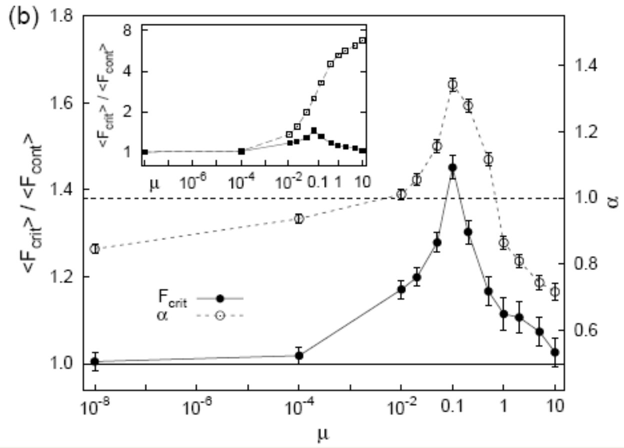


Schematic picture of the two types of granular packings confined by an external pressure bath (a) and by gravity (b). The dashed lines mark periodic boundaries. Some typical perturbations are illustrated with gray particles and arrows showing the direction of perturbation.

We study the mechanical response generated by local deformations in jammed packings of rigid disks. Based on discrete element simulations we determine the critical force of the local perturbation that is needed to break the mechanical equilibrium and examine the generated displacement field. When averaged over many perturbations in the homogenous case we observed a quadrupole-type displacement field:



Averaging over the different angles too, the displacement field decays as a power law with a friction-dependent exponent α. This dependence is non-monotonic, as shown in the next figure.



The same figure shows also the critical force F_{crit} in units of the average contact force as a function of the friction μ.. Again, a non-monotonic dependence can be observed. The maxima of both α and F_{crit} are at the same value of the friction coefficient, $\mu \approx 0.1$.

In an earlier study we found that the force fluctuations in the static packings also show this non-monotonic character, with a maximum at $\mu \approx 0.1$. It is tempting to look for a relationship between these phenomena. Qualitatively, the larger fluctuations provide more freedom for the force rearrangement when perturbing the system, which naturally leads to a higher critical force. The faster decay of the displacement (larger exponent) has similar roots. This picture got a quantitative confirmation, when we showed that the breaking critical forces at single contacts indeed get the limiting values enabled by the fluctuations. As a byproduct of this investigation we could conclude that the force-ensemble, i.e., the ensemble of static configurations with the same contact geometries but different forces is able to determine the critical force at each contact. For the gravity governed case the displacement is better characterized by the penetration depth, the measure of the range affected by the perturbation. Again, we found non-monotonic behavior; however, the maximum in this case does not entirely coincide with that of the force fluctuations. It should be mentioned at this point that the perturbation is not at contacts like in the homogenous case but rather at particles, which drives the system out of the force ensemble. This seems to be a significant difference.

4. Conclusions

We have demonstrated that distinct element simulations are efficient tools to investigate relevant problems of granular systems. We have used two methods: Contact dynamics and molecular dynamics. In both cases we developed our own code.

The studies focused on three problems: Magnetic avalanches, shear bands and unjamming. We managed to show that in several respects the magnetic particles behave similarly to cohesive ones enabling fine tuning of the interactions by changing the magnetization. The two regimes as a function of the interaction parameter f could be clearly distinguished and characterized by different avalanche dynamics, which was reflected in the different statistical behavior.

Realistic three-dimensional simulations of shear band formation revealed the importance of the external constraints: If they allowed, a spontaneous symmetry breaking occurred in the geometry of the bands. The concept of critical shear density could be made more precise: We showed that it develops in a self-organizing manner inside the shear band.

We generalized our theory of wide shear bands to describe not only the position but also the width of the bands. The model is related to that of self organized criticality and of directed polymers in a random medium. We managed to give a rather accurate account of the related experiments. The theory predicted a new effect: refraction of shear bands on the boundary of granular materials with different frictions.

We studied the response of dense packings on perturbations. We have found that the the critical force needed for unjamming and decay of the displacements are non-monotonic functions of the friction and we related this dynamic phenomenon to the force fluctuations found earlier in static packings.

Many interesting, open questions remained for further investigations. These include: How to describe the velocity field within the framework of a continuum theory in the quasistatic limit? What is the mechanism of force transmission in the early stage of unjamming? What is the consequence of soft potentials for the dynamics of unjamming? We hope to be able to come back to these problems on forthcoming projects.

Within the framework of the present project the following papers were prepared:

S. Fazekas, J. Kertész, D. E. Wolf: Piling and avalanches of magnetized particles Phys. Rev. E, 71, 061303 (2005)
S. Fazekas, J. Török, J. Kertész, D. E. Wolf: Morphologies of three-dimensional shear bands in granular media, Phys. Rev. E 74, 031303 (2006)
S. Fazekas, J. Török, J. Kertész: Computer simulation of three dimensional shearing of granular materials: Formation of shear bands, Powders & Grains 05, R. Garcia-Rojo, H.J. Herrmann and S. McNamara (eds.) Proc. of the conf.2005 in Stuttgart p. 223-226 (Balcema, Leiden, 2005)
S. Fazekas, J. Török, J. Kertész: Critical packing in granular shear bands, Phys. Rev. E 75, 011302 (2007)
T. Unger, J. Török, J. Kertész, D. E. Wolf: Shear band formation as a variational problem Powders & Grains 05, R. Garcia-Rojo, H.J. Herrmann and S. McNamara (eds.) Proc. of the conf. 2005 in Stuttgart p. 227-231 (Balcema, Leiden, 2005)
T. Unger: Refraction of shear zones in granular materials, Phys. Rev. Lett. 98, 018301 (2007)
J. Török, T. Unger, J. Kertész, D. E. Wolf: Shear zones in granular materials: Optimization in a self-organized random potential, Phys. Rev. E75, 011305 (2007)
M. R. Shaebani, T. Unger and J. Kertész: Unjamming of granular packings due to local perturbations: Stability and decay of displacements , Phys. Rev. E 76, 030301(R) (2007)
M. R. Shaebani, T. Unger and J. Kertész: Unjamming due to local perturbations in granular packings with and without gravity, Phys. Rev. E 78, 011308 (2008)
M. R. Shaebani, T. Unger and J. Kertész: Generation of homogeneous granular packings: Contact dynamics method with coupling to an external pressure bath, submitted to Journal of Computational Physics
M. R. Shaebani, T. Unger and J. Kertész: Extent of force indeterminacy in packings of frictional rigid disks, submitted to Phys. Rev. E

PhD theses from the research of the present project

S. Fazekas: Disitinct Element Simulations of Granular Materials (BME, 2007)
M. R. Shaebani: Unjamming due to local perturbation (BME-Zanjan IABS, 2008)

Budapest, August 2008

János Kertész, PI