Particles, contacts and cooperative structures

(Deeltjes, contacten en coöperatieve structuren)

Rede uitgesproken bij
het aanvaarden van het ambt
van hoogleraar

Multi Scale Mechanics

aan de faculteit Construerende Technische Wetenschappen
van de Universiteit Twente,
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door

Prof. Dr. rer. nat. Stefan Luding

Prof. Dr. rer.-nat. S. Luding

Multi Scale Mechanics (MSM),
Technische Stromingsleer (TS),
Engineering Technology (CTW),
University of Twente
P.O. Box 217, 7500 AE Enschede, NL

Tel.: +31 53 489 -4212
Secretary: -4428

e-mail: s.luding@utwente.nl
http://www.msm.ctw.utwente.nl
http://www2.msm.ctw.utwente.nl/sluding

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Acknowledgements/Dankwoord

Mijnheer de Rector Magnificus
Dames en heren

Introduction

I give this presentation in English, so that our non-Dutch speaking colleagues can enjoy as well.

In October 2007 I was appointed to the chair Multi Scale Mechanics, attached to the group Engineering Fluid Dynamics in the faculty Engineering Technology (CTW), as member of IMPACT (Institute of Mechanics, Processes, and Control).

This is now already more than 7 months ago and the challenge to build up a new group is still my major activity, involving new research, appointing new colleagues, teaching and getting to know all members of the faculty and their research better.

Multi Scale Mechanics is one of the 3TU chairs, in the framework of the Center of Excellence “Fluid and Solid Mechanics”. Several examples from Fluid Dynamics and Solid Mechanics will be presented – especially, the meaning of the term Multi Scale Mechanics will be made clear. After the introduction to this fascinating new field of research, I also will present my view on teaching and other aspects of life at the University of Twente.

What is Mechanics?

To answer this question, I first looked up in Google the word “mechanics” – and find directly:

“**Mechanics** (Greek *Μηχανική*) is the branch of physics concerned with the behaviour of physical bodies when subjected to forces or displacements, and the subsequent effect of the bodies on their environment.” [Wikipedia]

Physical bodies, like you and me, are influenced by their environment via forces and displacements. But, in turn, we also have an effect on our environment, due to the fact that every action leads to a reaction – in this case our reaction. This reaction can lead to a change of our environment, which will lead to new forces, affecting us in a different way so that we behave differently. This (philosophical) loop can be repeated indefinitely; however, I will not continue in this direction, only stating that Mechanics is already a complex subject.

Physical bodies in contact and in static equilibrium

According to Wikipedia, the discipline “Mechanics” has its roots in several ancient civilizations. Think of Archimedes, who already long ago realized that a body floating in a liquid is pushed upwards by a force that is equal to the gravitational force acting on the same volume of displaced liquid: Action and Reaction again – everyone can prove this at home in the bath-tub. During the past centuries, scientists such as Galileo, Kepler, and especially Newton, laid the foundation for what is now known as Classical Mechanics.

$\vec{F} = \frac{\mathrm{d}}{\mathrm{d}t}(m\vec{v})$ is the equation referred to as Newton's second law. A force, *F*, will lead to a change of momentum, *mv*. Jump in the air and the gravity force will change your momentum – and bring you back on earth.

It is nice to know that we continue the work of such bright minds, using new tools (like computers) and defining new sub-disciplines (like Multi Scale Mechanics).

Further on, one can read: “Mechanics also constitutes a central part of technology, the application of physical knowledge for humanly defined purposes. In this connection, the discipline is often known as engineering or applied mechanics. In this sense, mechanics is used to design and analyze the behavior of structures, mechanisms, and machines. Important aspects of the fields of mechanical engineering, aerospace engineering, civil engineering, structural engineering, materials engineering, biomedical engineering and biomechanics were spawned from the study of mechanics.”

This reads – not only by coincidence – like a brief portfolio of part of our faculty CTW. A major division in the mechanics discipline separates classical mechanics from quantum mechanics. The latter is not what we are concerned about today since, historically, classical mechanics came first, while quantum mechanics is a comparatively recent invention. The laws of classical mechanics are older than written history – the apple was always falling from the tree – already before Newton told him to do so. Quantum mechanics, in some sense, provides the more general framework, encompassing classical mechanics, as a sub-discipline that applies under certain restricted circumstances. For practical problems, i.e., the circumstances of our daily life, classical mechanics allows us to solve problems – build bridges, buildings and dams – which are unmanageably difficult in quantum mechanics.

In some other applications, e.g., for very small objects, quantum mechanics is needed to understand what is going on.

Classical mechanics can be viewed as model and playground for other so-called exact sciences. Essential in this respect is the relentless use of mathematics in theories, as well as the decisive role played by experiment in generating and testing them. We will come back later to these.

Analogous to the quantum vs. classical picture, Einstein's theory of relativity has expanded the scope of classical mechanics beyond the mechanics of Newton and Galileo. In our daily life, relativistic corrections are so small that, almost always, we can neglect them. Wait: almost always? Relativistic corrections have to be applied for high-precision GPS (Global positioning system) – for more details see http://www.phys.lsu.edu/mog/mog9/node9.html.
Relativistic corrections are also needed for quantum mechanics, although relativity is categorized as a classical theory. And I would not give this presentation without modern semi-conductor based computer-industry. Computers definitely do rely on quantum effects, but relativity also limits computing power via the speed-of-light.

One could characterize classical mechanics as dealing with "large" bodies (such as engine parts, buildings, soil, sand, and powder), while quantum mechanics deals with "small" bodies (such as atoms, molecules or nano-particles). Similarly, relativistic mechanics deals with "fast" bodies, while non-relativistic mechanics with "slow" ones, where "fast" and "slow" are subjective.

Citing Wikipedia again: "… the often-used term body needs to stand for a wide assortment of objects, including *particles*, projectiles, spacecraft, stars, parts of machinery, parts of solids, parts of fluids (gases and liquids), etc."

I did not insert the word "particle" in these sentences, someone else did! Particles occur in all disciplines of

Mechanics: Sometimes hidden, sometimes obvious, sometimes during manufacturing and production, sometimes also in the end-product, like e.g., coffee-powder or muesli.

Particles are bodies with little known internal structure. They are treated as mathematical points in classical mechanics. Rigid bodies have size and shape, but retain a simplicity close to that of the particle, adding just a few so-called degrees of freedom, such as orientation in space. Otherwise, bodies may be semi-rigid, i.e. elastic, or non-rigid, i.e., fluid. The group MSM works on these disciplines (as listed in Wikipedia):

- Fluid mechanics, the motion of fluids
- Solid mechanics, elasticity, properties of rigid bodies
- Continuum mechanics, both solid and fluid
- Acoustics, sound in solids, fluids, etc.
- Statics, semi-rigid bodies in mechanical equilibrium
- Soil mechanics, mechanical behavior of soils
- Celestial mechanics, motion of planets, dust, etc.
- Applied / Engineering mechanics
- Statistical mechanics, large assemblies of particles

What is Multi Scale Mechanics?

Then, when searching for the words “Multi Scale Mechanics” (in Google), I find – to my great pleasure – the very young homepage of our group on top of the list!

There, one reads: “The group multi scale mechanics deals with fluids and solids, particles and their contacts, granular materials and powders, microfluid systems and self-healing materials, as well as a variety of multi-scale theories and modeling approaches as:

- *Microscopic/discrete models for fluids and solids*
- *Micro-macro transitions for constitutive relations.*
- *Continuum models based on micro-properties.*

Collaborations with industry involve: modern/complex material testing and optimization, sound- and wave-propagation for oil exploration, powder flow behavior, mixing and segregation, sintering, self-healing, etc.”

Multi Scale Mechanics deals with fluids and solids, where various physical phenomena take place at different length-scales. Coffee-powder in the kitchen is a good example: Vacuum packed coffee feels like a solid brick - about ten centi-meters in size. But as soon as the package is unsealed, the coffee-particles flow out easily, each particle of a size of less than a millimeter.

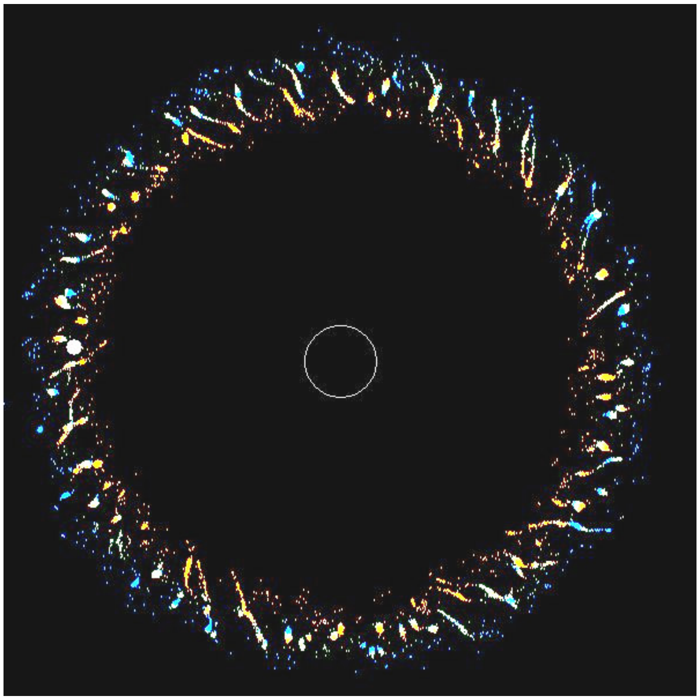
However, the contacts (on the scale of nano- to micro-meters) determine the flow behavior, e.g., due to solid-friction and contact-adhesion as described below in more detail.

In general, Multi Scale Mechanics can involve very small and very large objects. Even though numberless (small) atoms interact statistically and randomly, only a few thermodynamic parameters are needed to describe the macroscopic, large-scale behavior of a gas like air, or a solid like steel. In this sense, gases, liquids and solids are well understood.

For powders, composites, ceramics and concrete, this is much less straightforward: one has to deal with very small microscopic objects, mesoscopic domains, and very large,

macroscopic structures – all at the same time. For concrete, as an example, the cement constitution and the chemistry are as important as the filler particles (sand and stones), the steel reinforcement, and the building-structure itself.
Thus, Multi Scale Mechanics is needed to understand modern, advanced materials. Involving theory, numerical simulation and experiments for validation, these research results can then be used to optimize the design and the efficiency of buildings, machines, and materials.

In the following, some research examples of Multi Scale Mechanics will be given, involving particles, their contacts and cooperative structures like agglomerates and clusters – even examples from astrophysics show similar structures.



Snapshot from a clustering ring-structure around a central planet (white circle). Colors indicate the Keplerian velocity of the particles and clusters.

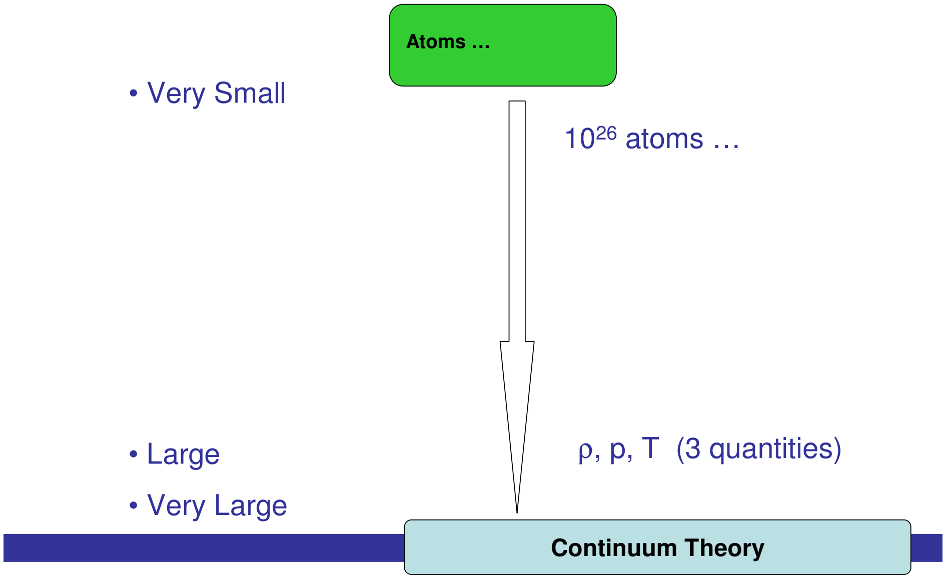
The research goals of MSM will be discussed/defined and, thereafter, a view on teaching will be given.

Examples of Multi Scale Mechanics

Multi Scale Mechanics can be seen as dealing with very small and very large objects at the same time.

The first example is a gas like the air around us. It consists of very many and very small atoms, but we typically are interested in only three quantities, namely the density, ρ, the pressure, p, and the temperature T. If the pressure is too low, as on high mountains, the density is also small and we have problems with breathing. The temperature, on the other hand, determines how comfortable we feel, but it also affects the pressure and the density. This relation is called the *equation of state* and (for gases) it can look as simple as: $p \approx \rho T$, the pressure is proportional to the product of density and temperature.

Three quantities are thus sufficient to describe the state of the gas around us. Classical thermodynamics and statistical physics, with the kinetic theory of gases, allow us to understand a gas and how it behaves, knowing only relatively little about it. Surely we do not have to know the positions and velocities of all the atoms.



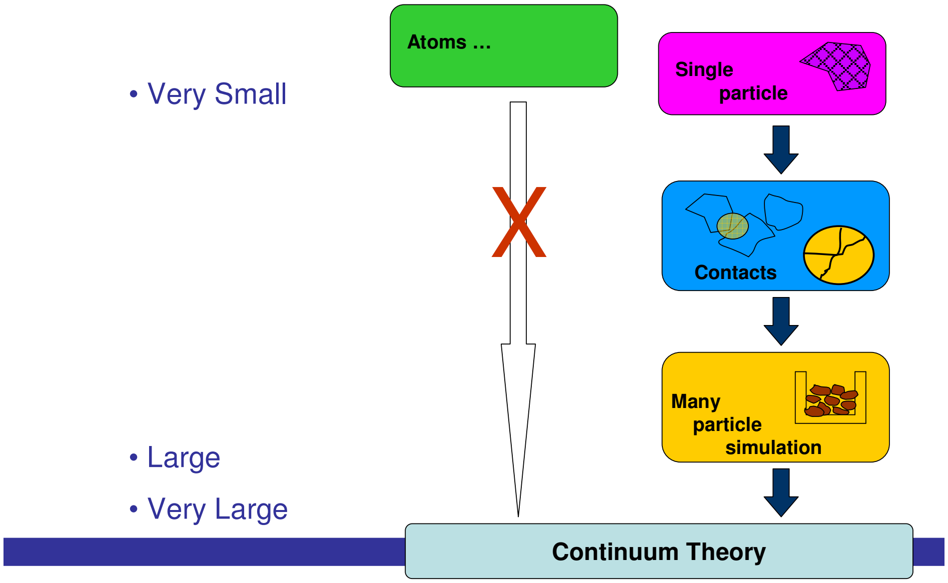
As compared to the atoms, our direct environment is large; this lecture-room is already large, our planet, i.e., its

atmospheric shell is even larger. However, the same basic rules apply even on such very large length-scales.
In this first example of a gas, it is possible to bridge the gap between the atomistic level and our macroscopic world in one step. This is called a *micro-macro transition*. The microscopic view is here on the level of single atoms or “particles” while the macroscopic view is “continuous”, since the particular nature of the atoms is not visible anymore, and it is not relevant most of the time anyway.

But is such a micro-macro transition always possible?

The answer is often: NO!

In the case of particles and multi-particle systems like sand or powder, it is not possible to jump from atoms directly to a continuum, large scale description.



Particles

Particles consist of atoms – yes – but the atoms alone do not determine what a particle looks like or how it behaves. Already one species of atoms can make very different particles, with different appearance and properties, due to the conditions at creation or production. Carbon can appear in the form of valuable diamonds or as soot. Particles can appear as ordered crystals, as amorphous glass, or as disordered, inhomogeneous combinations of various domains or sub-structures.

Thus, already the step from atoms to (rather small) particles is non-trivial and requires physics, chemistry, and other disciplines to be understood. Making particles with well-controlled properties and defined size and shape is still a challenge for the process-industry and subject to actual research at many universities.

Contacts

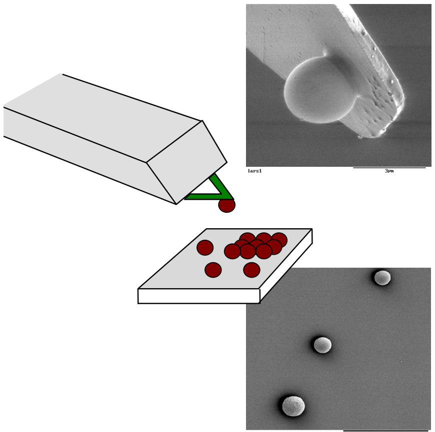
Now, consider two particles, they can look very similar, but they can behave completely differently. When the two particles are far apart, they mostly do not interact and do not feel each other. If the particles get closer, they will interact, i.e., they will exert forces on each other. (At least in the case of an isolated pair, these forces are equal, pointing in opposite direction due to the action-reaction principle.) Particles can be in mechanical contact, or they interact via short- or long-range interactions like van der Waals or Coulomb forces due to charges. Most of the time, a "contact" refers to a mechanical interaction, but in the abstract sense, contact can also mean all interactions, including longer ranged ones.

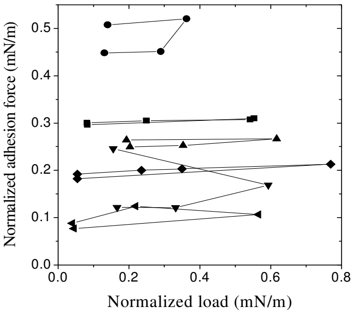
What are the forces between two particles in contact?
And how can they be measured?

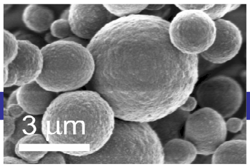
For larger particles in the millimeter range, the contact forces can be determined by mechanical force-measurement or using the help of high-speed video-recording in order to measure accelerations and thus forces directly.

For fine powder of the size of a few micro-meters, this is not possible and one can employ the AFM (atomic force microscope) technique. One can stick particles on the cantilever and measure the interaction force with another particle directly, when knowing the features of the cantilever. For even smaller particles or macro-molecules, this becomes increasingly difficult and there is only little detailed information available about the interaction of very small objects.

Contact force measurement (AFM)







Thus the understanding of particle interactions is the next step in the example of Multi Scale Mechanics. There are theories available that predict the interaction of perfect, spherical particles. However, in real life, particles are never perfect and mostly non-spherical. A perfect particle would still have its fine-structure at the atomic level, but a realistic particle has surface structures of around one to 100 micro-meters. Having atoms, surface-structures, and particles with their shape and material thus makes the “simple” interaction of two particles already a multi scale mechanics problem.

At contact, there are elastic, repulsive forces, which try to avoid that two particles occupy the same space. There are also viscous, velocity-dependent forces that disappear when the same interaction is performed slower and slower. These forces dissipate energy as well as other forces like, e.g., friction. Energy-dissipation is the main ingredient distinguishing particle or granular systems from classical gases or fluids. At each contact, energy is irreversibly transferred into sound or heat via mechanisms like viscous or plastic deformations and friction. Thus, dissipation is probably the most essential feature of particles in contact.

Multi-particle systems

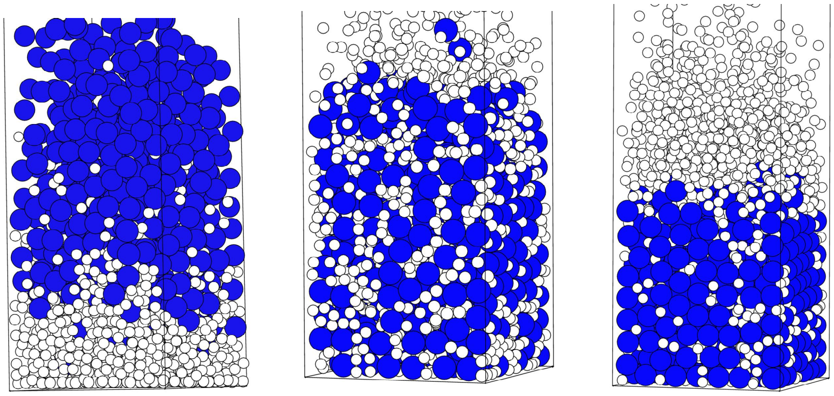
Particles in practice do not appear in pairs, they come in bigger numbers of thousands, millions, or even more.

Can we describe and predict the behavior of multi-particle systems, knowing only the particles and their pair-interaction forces?

The step from particles and their contacts to multi-particle systems can also be referred to as micro-macro transition and this is one of our groups' central research goals.

Sometimes, like from atoms to a gas, this micro-macro transition can be performed for particle systems. Generalization of the classical kinetic theory for gases is one approach. While the atoms in a gas are assumed to be point-particles and their interaction conserves energy, for particle systems the finite particle volume has to be taken into account as well as the dissipative nature of their contacts.

Segregation – Mixing – Reverse segregation



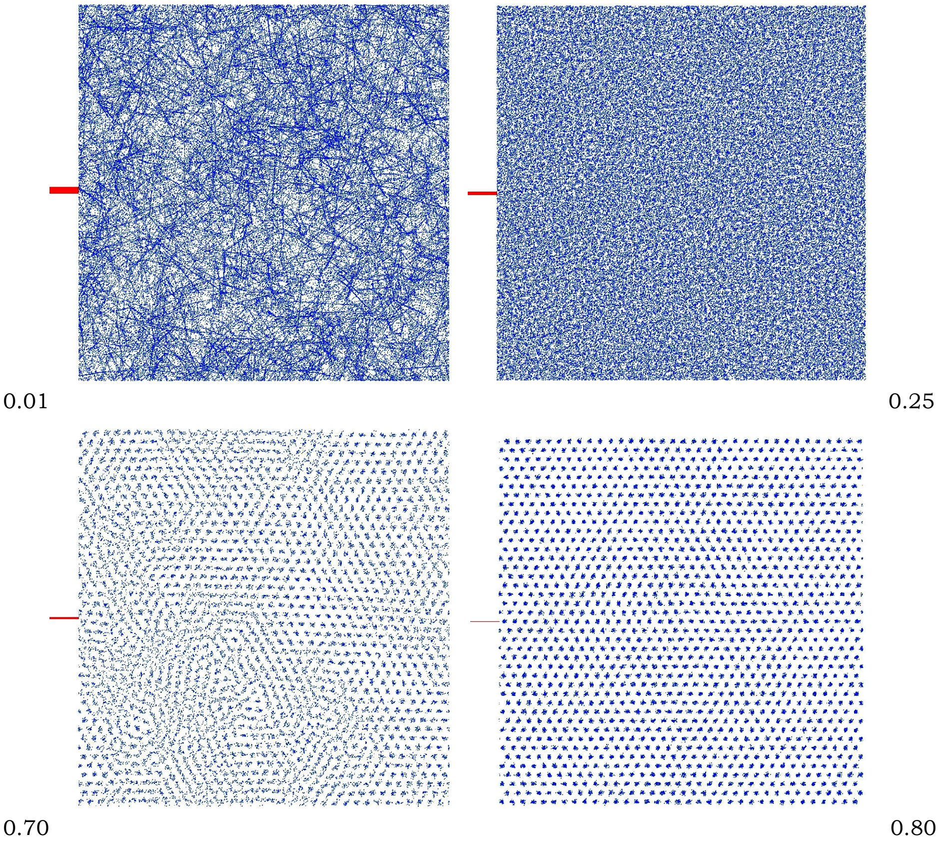
PV Quinn, D Hong, SL, PRL 2001

When putting two different species of particles into a container and shaking, one can observe segregation, mixing, or reverse segregation, dependent on the particles size- or mass-ratios, and also dependent on their shapes and other surface/contact properties. The standard, every-day example is the muesli-box, where we find the big “Brazil” nuts segregated on top. This type of segregation is, however, unacceptable for pharmaceutical products. There, the ingredients of a pill have to be mixed in certain reproducible ratios. Thus, segregation is undesired in some processes, but very well used and wanted for others, like for recycling, where different materials have to be separated.

Note that segregation or phase-separation also occurs in some gas, fluid, and solid systems, where different phases co-exist and their domains can dynamically shrink or grow. Thus separation or segregation can have many different reasons, some of them are understood, others are not. Especially the interplay of mechanisms like dissipation with the classical, geometrical or chemical sources of segregation opens a wide field for research and many open questions in industrial application.

Elastic hard sphere gas

Starting from a classical gas, the finite volume of particles (disks or spheres) already changes the behavior. The larger the particles, the more often they will interact at a given (number) density. Neglecting dissipation for the moment, classical gas theory can be generalized to higher densities. However, there is a natural limit to this expansion in small densities as proposed by Chapman, Enskog, and others. The larger the particles are – relative to the free path (related to the free volume) available – the more important their interactions and collisions become. If the free path is considerably smaller than the particle size, one observes that the particles order: instead of occupying random positions, they crystallize and organize themselves in order to maximize the free volume, since an ordered crystal occupies less volume than a disordered structure. By “saving” volume, the particles also reduce their frequency of interaction and thus the pressure. Order in the system can be visualized, e.g., by plotting the path-lines at different densities.



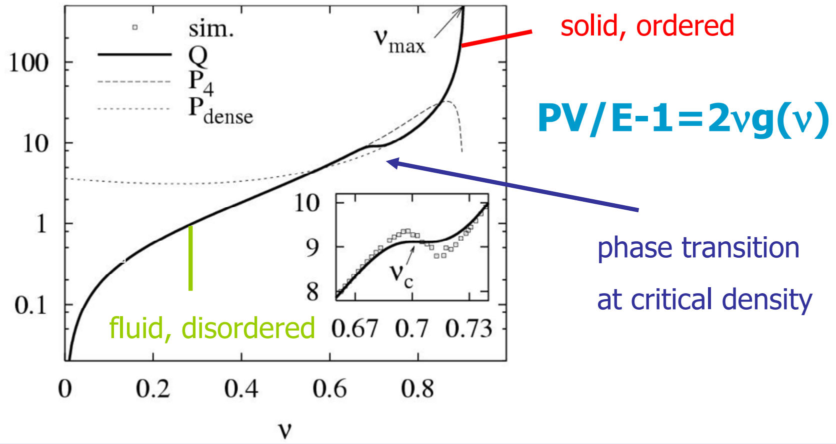
Path-lines (accumulated trace of the center of mass positions plotted as points) for a particle system with fixed number N and volume V. The density is quantified by the volume- or area-fraction, i.e., the fraction of volume/area occupied by the particles are given besides the panels.

At low density, particles have a long free path and lines become visible while, at higher density, the lines disappear and a random set of points occupies the system. At even higher density, the crystallization manifests as small, isolated “clouds” of points, when particles are caged by their neighbors and can not diffuse freely through the system anymore. For low and moderate densities, the system is in a gas- or fluid-like state, and the kinetic theory describes the behavior of the system, i.e., its equation of state, perfectly well. Around and above the crystallization density, this approach fails.

Can we generalize the classical kinetic theory to include both the low-density fluid-like and the high density solid-like ordered state?

The answer is clearly “maybe”. Even though a rigorous theory for the transition to the ordered state is not yet developed, an empirical “global equation of state” has already proven valuable to describe systems where low and high densities coexist (see the example of cooperative clustering below).

Pressure (Equation of State – 2D)



solid, ordered

$PV/E-1=2\nu g(\nu)$

fluid, disordered

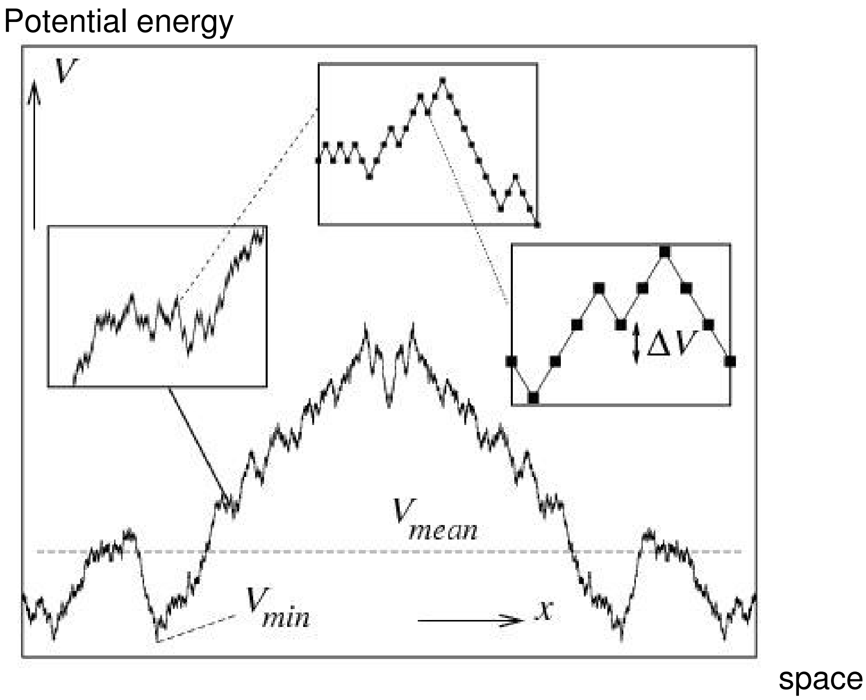
phase transition

at critical density

The global equation of state predicts the pressure for all densities. It contains the gas pressure as well as the collisional pressure, where the latter is directly affected by the crystallization. Around the crystallization density, the increased free path leads to a decreased collision frequency and thus to a reduced pressure. At even higher densities, the finite volume and shape of the particles cause an excluded volume effect that leads to a divergence of collision frequency at a special, maximal density. Even though there is free space available, this is so small, that no particle can occupy it in order to save space for others.

Cooperative Phenomena

At high densities, only *cooperative phenomena*, involving many particles at the same time, can lead to further re-organization or compaction. In general, such collective phenomena take longer and longer the more particles are involved.
This allows for another definition of multi scale mechanics that does not rely on small and large sizes: In particle systems, various times are involved: short times like the contact duration that is controlled by the contact properties and long times where the collective motion of many particles takes place. Since the latter involves many particles, it is clear that it also involves length scales possibly much larger than the particle scale.



Fractal potential energy "landscape" in a (virtual) space of configurations. The potential energy is inversely proportional to density.

Each particle is surrounded by others, which define its "configuration". One can view each particle sitting at a certain configuration that is described by a certain potential energy. Low density configurations correspond to high potential energy, whereas high density is consistent with low potential energy. Potential energy can be seen here as the potential energy in the gravitational field so that it is inversely proportional to density. The densest packing has the minimal potential energy, and some more dilute packing has a higher potential energy. The former will be stable, while the latter can be unstable.

This concept allows distributing all particles in a system on a virtual energy landscape in configuration space. When the system is unperturbed, the particles do not "move", i.e., the configuration does not change.

However, when the system is vibrated or tapped, a perturbation allows particles to "travel" in configuration space. The stronger the "temperature" of the perturbation, the higher the probability for re-organization or re-structuring will be.

In this picture, the particles are an ensemble of points traveling on the landscape: at high temperature they will travel faster. The term "traveling" corresponds to a re-organization or re-structuring in the environment of a particle. Short-distance travel means local reorganization and long-distance travel corresponds to cooperative re-organization.

The various types of "travel" in this space are:

Short distance "travel":

1 "Falling" into a valley means compaction, i.e., a locally increased density.

2 Moving "up-hill" one step means a less stable/favorable situation with lower density.

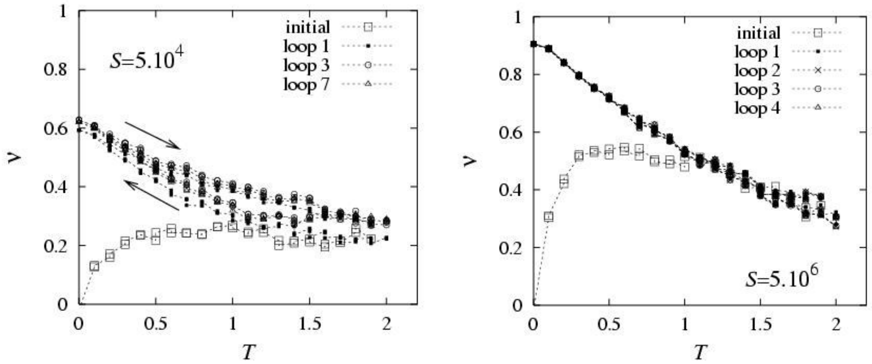
Long-distance travel:

3 Travelling to the top of a mountain corresponds to de-compaction of large parts of the system.

4 Travelling from one valley to a distant valley corresponds to a large scale re-organisation.

A particle (configuration) sitting on a "mountain" is unstable, whereas a particle (configuration) in a "valley" is stable. Usually, the former has a low density and the latter has a high density. However, there are plenty of possible configurations in between, including also meta-stable ones.

If the energy landscape is rough – or even fractal – this model picture explains qualitatively why local re-organization is relatively fast, whereas cooperative re-organization is slow and becomes extremely slow when larger parts of the system are involved. Travel to a distant valley takes a long time.



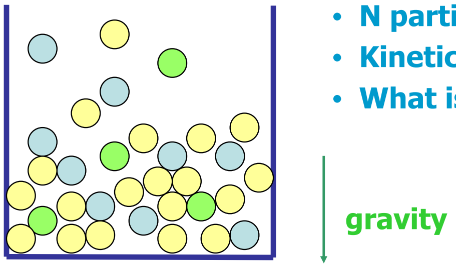
Density plotted against shaking strength (T), starting from the initial loose packing density, ν=0, and during several loops approaching ν=1, the densest packing possible. S indicates the time between changes of T.

Translating inverse potential energy to density, ν, and shaking strength to temperature, T, allows now to model loops of increasing shaking and subsequent relaxation. Starting from a loose packing, the shaking intensity is increased slowly, where S is inversely proportional to the rate of change. The first branch (starting from a loose, unconsolidated packing) always displays increasing density and – if shaking becomes too strong – the density decreases again. At high intensity, slowly reducing T allows the packing to compact even further (because now collective re-organization is possible). Repeating the loop several times leads to further compaction as also observed in experiments. The slower the loops are performed, the stronger the cooperative compaction.

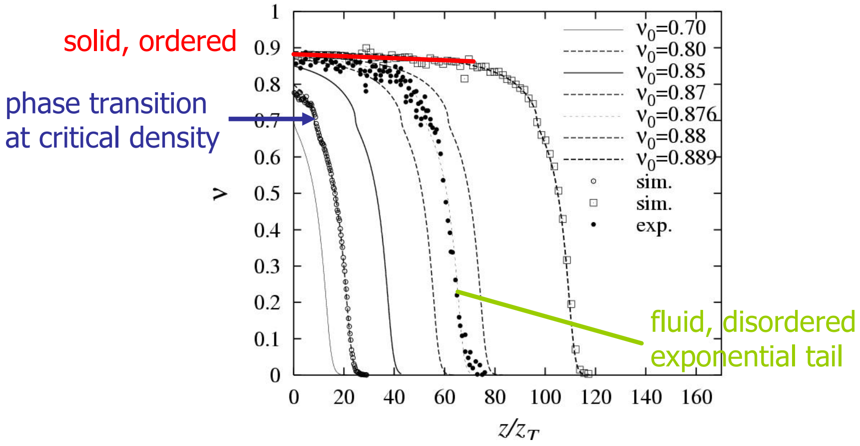
In summary, the multi-time- and multi-length-scales are clearly related to each other. The phenomenology and the understanding of this relation in the framework of “energy-landscape” models, so far, is only qualitative and subject to further research.

Solid-liquid-gas co-existence

The global equation of state (GEQS) allows the (fluid-like) description of a system where gas, fluid, and solid phases co-exist. Theory, based on the GEQS, predicts the density profile of corresponding simulations, but also of experiments [SL, Phys. Rev. E, 63, 042201, 2001].



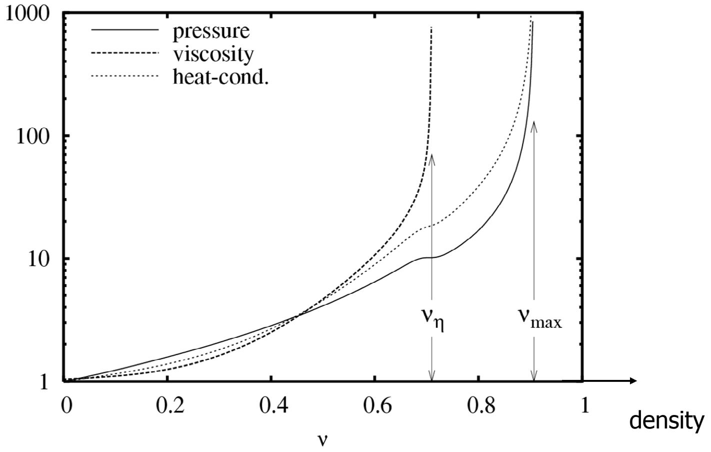
- **N particles**
- **Kinetic Energy**
- **What is the *density profile* ?**



However, life is not that simple!
The global equation of state for pressure has, in general, to be accompanied by the corresponding equations for heat conductivity, viscosity and possibly many others. All those are summarized as transport coefficients. Again, like for pressure, the kinetic theory predicts the transport coefficients well for low and moderate density.

But this is not true for all of them. The coefficient of diffusion is already badly predicted for rather low density, and viscosity brings a surprise: At moderate density, the kinetic theory prediction becomes unreliable and, close to the crystallization density, the viscosity (=shear stress divided by shear rate) diverges. This is not foreseen by the kinetic theory since the beginning order close to the crystallization density is not accounted for – perfect disorder (non-correlation) is assumed in this theory.

Are there global equations of state? (2D)



RG Rojo, SL, JJ Brey, PRE 2006 and E Khain, PRE 2007

Thus, multi scale mechanics brings a new challenge: Starting from low density systems (with small particles), fluid- and even solid-like regimes can show up and do co-exist. New theories and multi scale mechanics methods are necessary to understand and describe such challenging fluid, solid, and particulate systems.

Cooperative structures due to dissipation

When a number of particles is left alone, as for example interstellar dust floating in space, they will move and, from time to time, collide. At collisions they will dissipate energy.

What is the effect of dissipation?

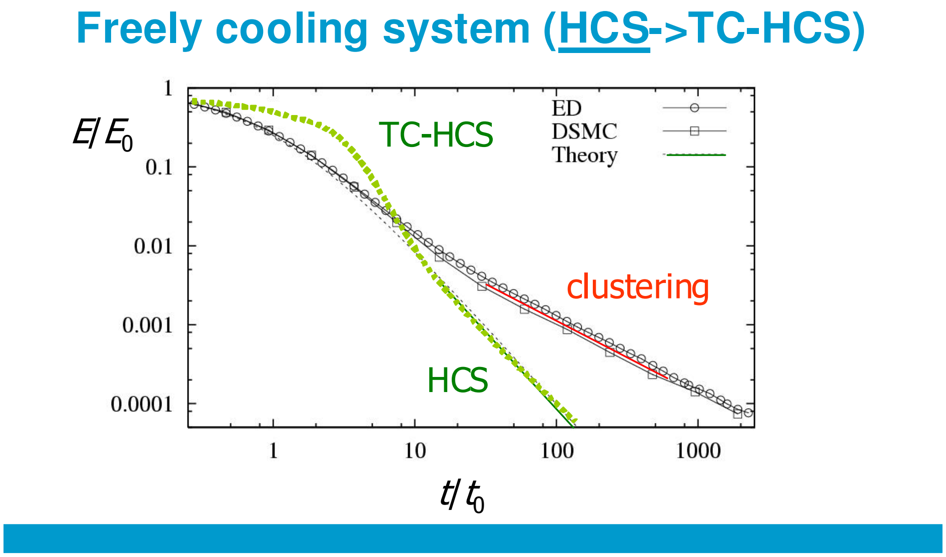
A granular gas can be idealized as an ensemble of hard spheres in which the energy loss that accompanies the collisions of the particles is quantified by a single number, the coefficient of restitution r. In the simplest case the particles are identical in size and mass and for $r=1$, one has the elastic gas as above.

The simulation volume consists of a square with periodic boundary conditions in 2D. An initial state with random particle positions and velocities is prepared in the following way: The particles first sit on a regular lattice and get random velocities with a total momentum of zero. Then the simulation is started without dissipation ($r=1$) and run for 100-1000 collisions per particle so that the system becomes a homogeneous elastic gas and the velocity distribution approaches a Maxwellian. This state is now used as initial configuration for the dissipative simulations.

The dissipative collisions lead to a decay of the kinetic energy, the collision frequency and the pressure. Besides that, one observes three different regimes:

1. The *homogenous cooling state* (HCS), when no clusters have formed yet at short times, can be described by mean-field kinetic theory. The decay of the kinetic energy E is governed by the dissipation at collisions and is proportional to the squared inverse time, $E \approx 1/t^2$.
2. In the *cluster growth regime*, the decay of energy and collision rate deviate from the laws that describe the HCS. The decay of kinetic energy slows down proportional to the inverse time, $E \approx 1/t$, the collision frequency strongly fluctuates, and the average collision frequency may even increase during cluster-cluster interactions.
3 Finally, in the *saturation regime*, when the largest cluster in the population approaches system size, the

cooling resembles to the homogeneous cooling state in so far that the proportionality with time is similar. The quantities energy and collision frequency show large fluctuations due to the enormous changes of both during cluster-cluster interactions and collisions – again largely cooperative phenomena.


Freely cooling system (HCS->TC-HCS)

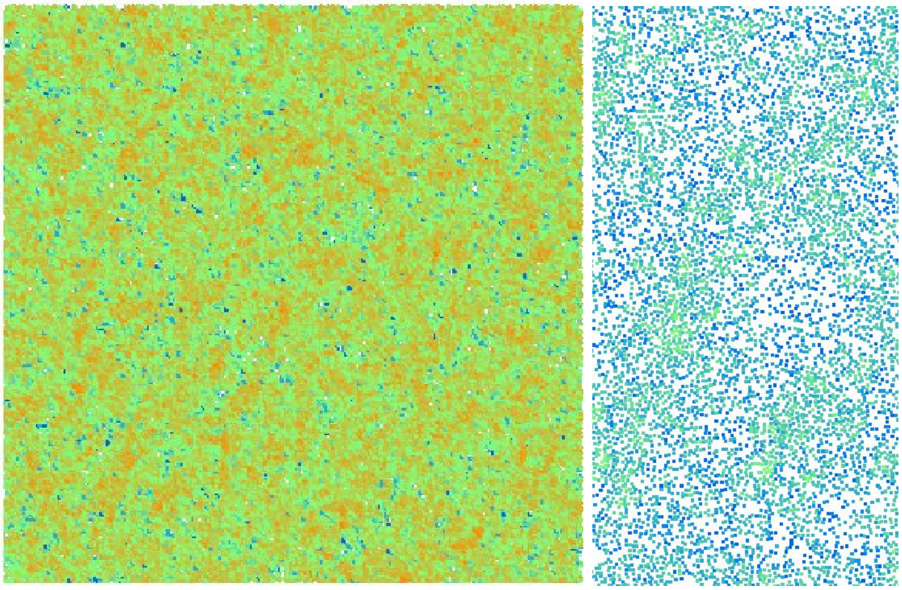
Energy plotted against time from different simulations (symbols). The HCS is indicated by the thin black dotted line, while the cluster growth regime is indicated by the red line. The most realistic TC-HCS model that takes into account the softness of the particles is plotted as green line.

On the following pages, snapshots from the different regimes of evolution are given together with zooms into some clusters where, again, the gas-liquid-solid/crystal coexistence is evident.

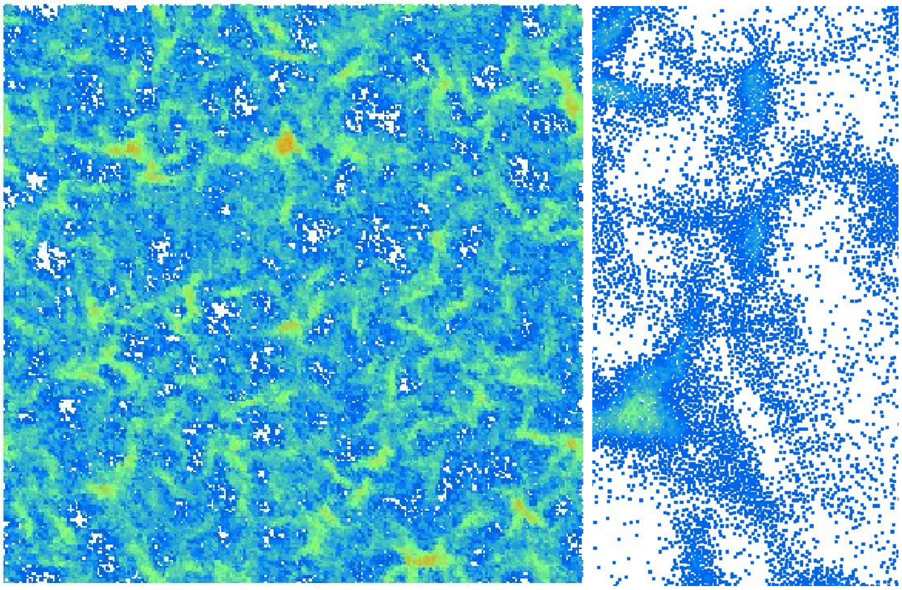
But before, we note that there is a material property missing in both simulations and theory as presented so far, namely the stiffness of the particles and the contact duration TC related to it. The fact that particles are soft makes their interactions take a finite time and, therefore, also the rate of dissipation is limited. Especially at large dissipation rate (early times), this leads to a delay of dissipation. This is included in the TC-HCS model [SL and A. Goldshtein, Granular Matter 5(3), 159-163, 2003] but will not be discussed here in more detail.

From HCS to cluster growth

$t/t_0=16$

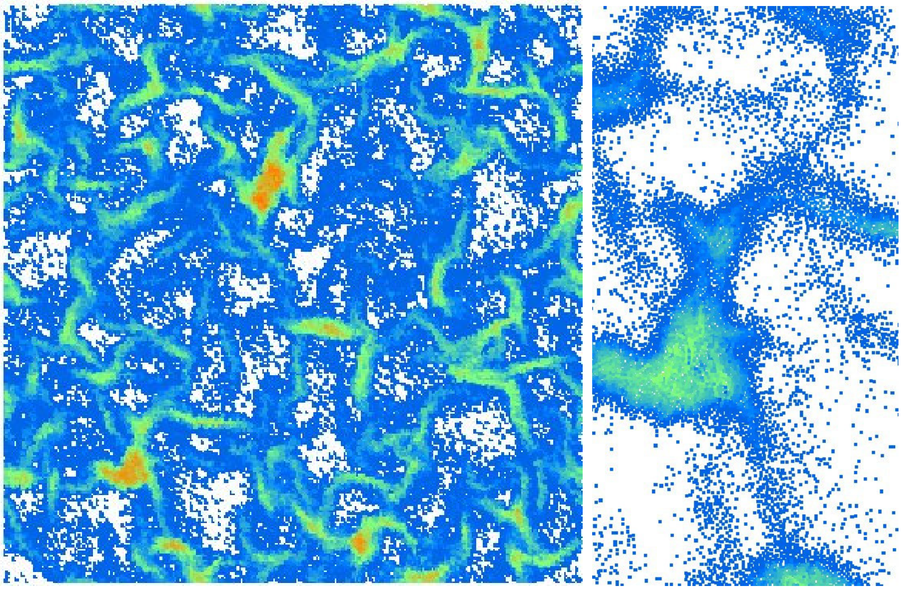


$t/t_0=125$

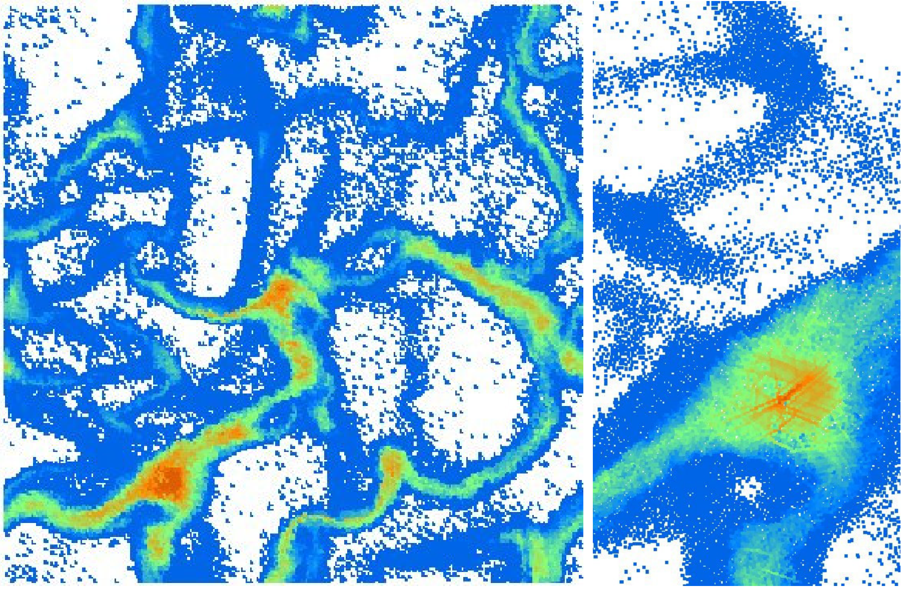


Cluster growth regime and saturation regime

$t/t_0=500$



$t/t_0=8000$



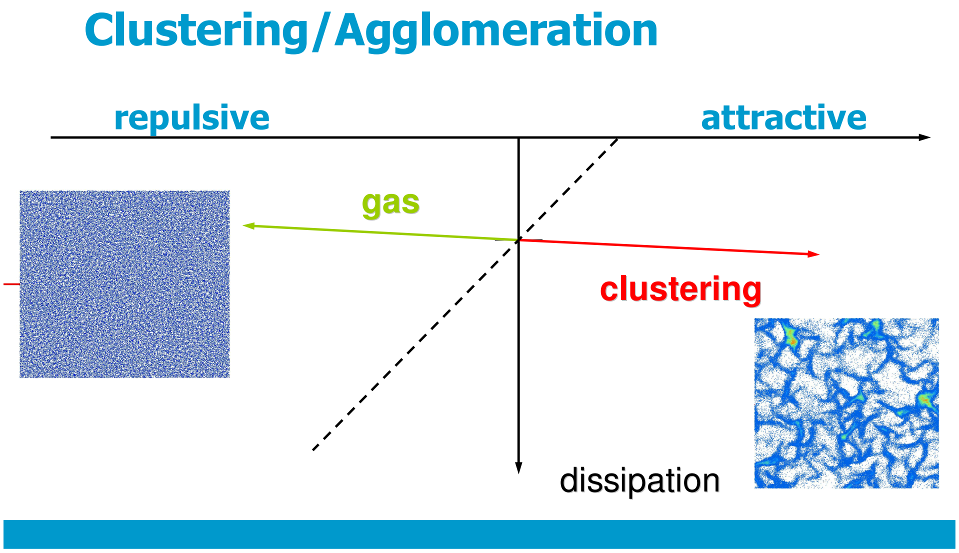
The above example of cooperative phenomena has shown that particles prefer to come and stay together – only due to dissipation. Collisions dissipate energy, and dissipation will be strongest in those parts of the system where – due to statistical fluctuations – a few more particles collide. Strong dissipation reduces energy, temperature and thus pressure. A reduced pressure allows more particles to come along, thus increasing dissipation, so that the collective phenomenon is self-enhanced. More and more particles will merge to the clusters, and also existing clusters will interact, collide and merge. This leads to the cluster-growth described before.

Note, however, that cluster growth is not observed in small systems and for too weak dissipation. In that situation, the statistical fluctuations become so strong as to overcome the cooperative cluster growth and rapidly destroy evolving clusters.

In realistic systems, it is not enough to consider only the particles and the dissipation at collisions. Dependent on the material, attractive or repulsive forces can be activated. For example, van der Waals forces are always active, but show a strong attractive or adhesive effect only for small particles like in fine powder. Coulomb forces due to charges on the particle surface are repulsive when the charges are equal.

What is the effect of attraction/repulsion?

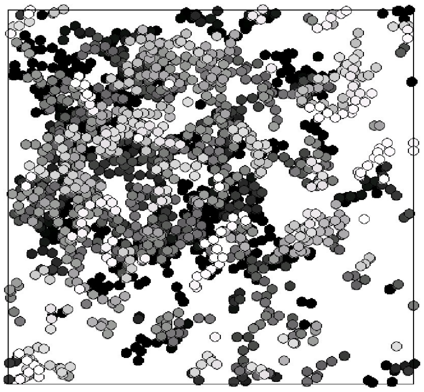
The cooperative clustering due to dissipation will be delayed or even hindered when the interaction forces are repulsive. In contrast, for attractive forces, one can expect that cluster growth will be enhanced.



Clustering/Agglomeration

Interestingly, there are two counter-intuitive regimes:
No clustering is observed for weak attractive forces and weak dissipation, but clustering is observed for weak repulsion and strong dissipation. The dashed line indicates the (unknown) phase boundary between a homogeneous regime and a clustering regime and the trianglular regions close to the dissipation axis correspond to these two regimes.

Finally, as last remark, clusters also can look very different when realistic fine powder particles with strong adhesion, friction, roughness and other surface interaction phenomena collide. Then these clusters are called agglomerates which can be very loose or even fractal in structure – in contrast to the dense, solid clusters shown above.

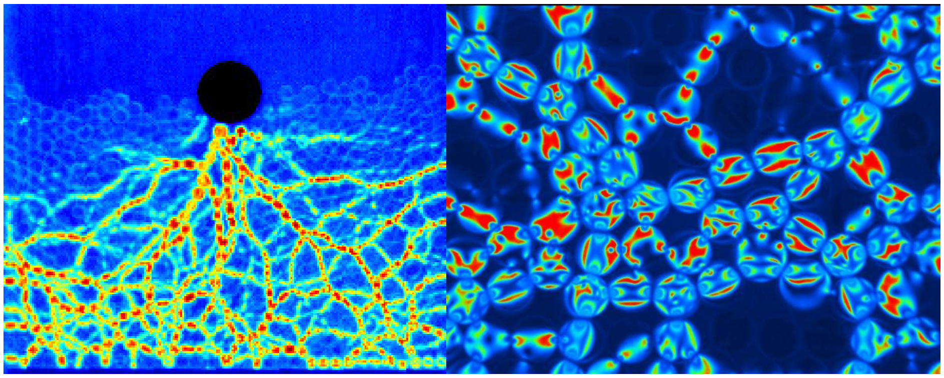


Snapshot of a fractal agglomerate, where the grey-scale indicates the distance from the viewer, light=close and dark=far.

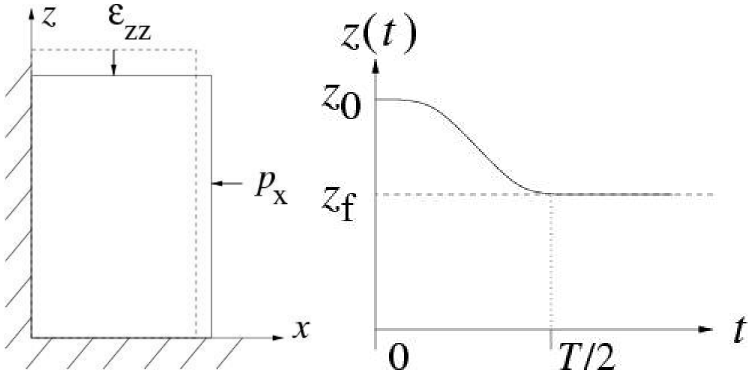
Having noted that, starting from a dilute, gas-like situation, particles tend to form dense (or loose) clusters by themselves due to dissipation, already in the absence of attractive forces, in the following, denser, solid-like systems will be examined closer: The particles are now either compacted by walls pushing them together, or by gravity pulling them downwards and thus also keeping them together.

Force chains and shear bands in dense packings

One possibility to gain insight into the material behavior of a granular packing is to perform elementary tests in the laboratory. The images below are taken from Bob Behringer's experiments on photo-elastic particles and display the peculiar force-chains. Low stresses (blue) and high stresses (red) and contact forces co-exist very close to each other. Forces are transmitted almost linearly over several particle diameters. They form a beautiful and interesting network spanning the whole system, on a scale larger than the particles and much larger than the contacts – thus a nice example for multi scale mechanics again.

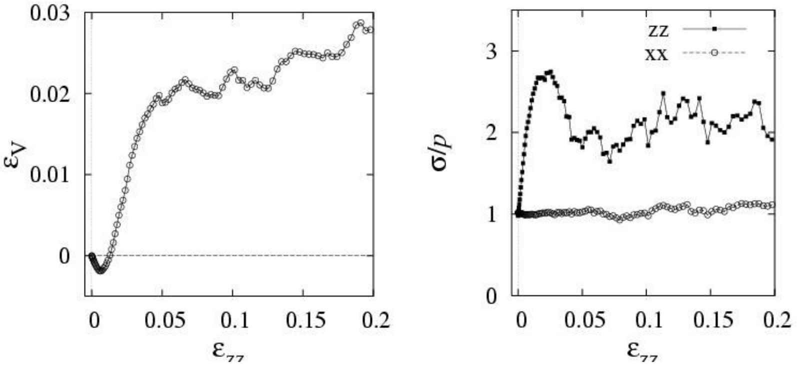


Simulations with the discrete element model (DEM) show the same features. In my favorite set-up for two-dimensional (2D) numerical "experiments", the so-called bi-axial box, the left and bottom walls are fixed. Stress- or strain-controlled deformation is applied to the side- and top-walls, respectively. In a typical simulation, the top wall is slowly shifted downwards, while the right wall moves, controlled by a constant stress p_{x}, responding on the forces exerted on it by the material in the box.



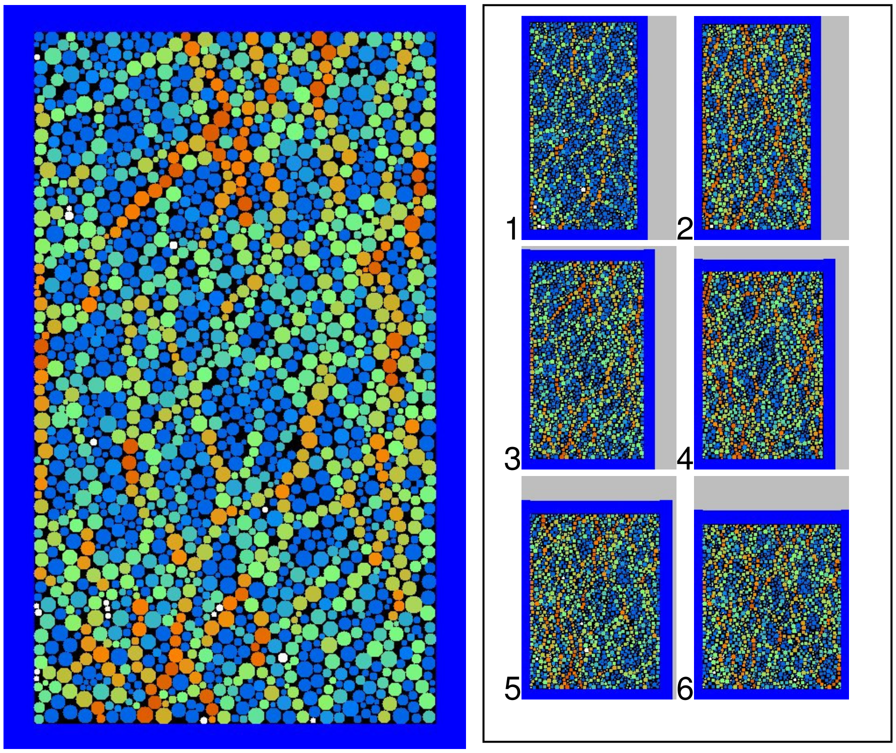
(Left) Schematic drawing of the model system. (Right) Position of the top-wall as function of time for the strain-controlled situation.

The system examined in the following contains N=1950 particles with radii randomly drawn from a homogeneous distribution with minimum 0.5 mm and maximum 1.5 mm. The friction coefficient used in the two-dimensional simulations is μ=0.5. Initially, the particles are randomly distributed in a huge box, with rather low overall density. Then the box is compressed, either by moving the walls to their desired position, or by defining an external pressure p, in order to achieve an isotropic initial condition. Starting from this relaxed, isotropic initial configuration, the vertical deformation strain ε_{zz} is applied to the top wall and the response of the system is examined. The volume change of a typical simulation shows first compression, then dilatancy, and eventually saturates with strong variations at larger deformations. At the same time, the stress response (xx and zz denote horizontal and vertical stresses, respectively) becomes more and more anisotropic, i.e., the vertical stress increases strongly until it reaches a maximum. After the peak, softening behavior is evidenced with a smaller, fluctuating stress-saturation for larger deformations.



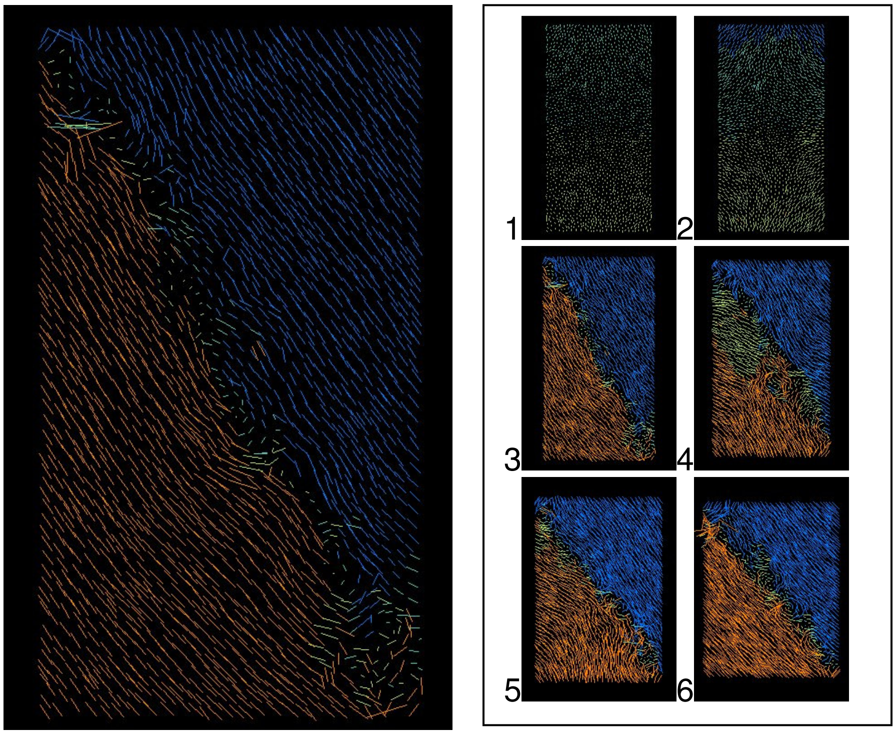
Volumetric strain (left) and stresses (right) during bi-axial deformation.

In the following pictures, snapshots from one simulation are shown and discussed with respect to different color-codes highlighting different interesting features of the granular material. As first example, the potential elastic energy of the particles is shown, indicating the inhomogeneity of the forces and stresses. From one particle to the next, the stress (the potential energy density) can change by orders of magnitude. This inhomogeneity manifests in so-called stress- or force-chains, which can be formed and destroyed during deformation. The former takes place with high probability in the (vertical) direction against the applied deformation, the latter in the perpendicular (horizontal) direction. With other words, the deformation causes an anisotropic change of the (initially isotropic) structure, acting against the direction of compression by creating new contacts. At the same time, in the perpendicular direction, contacts can open, until the structure is not stable anymore – shear-band localization is the consequence.



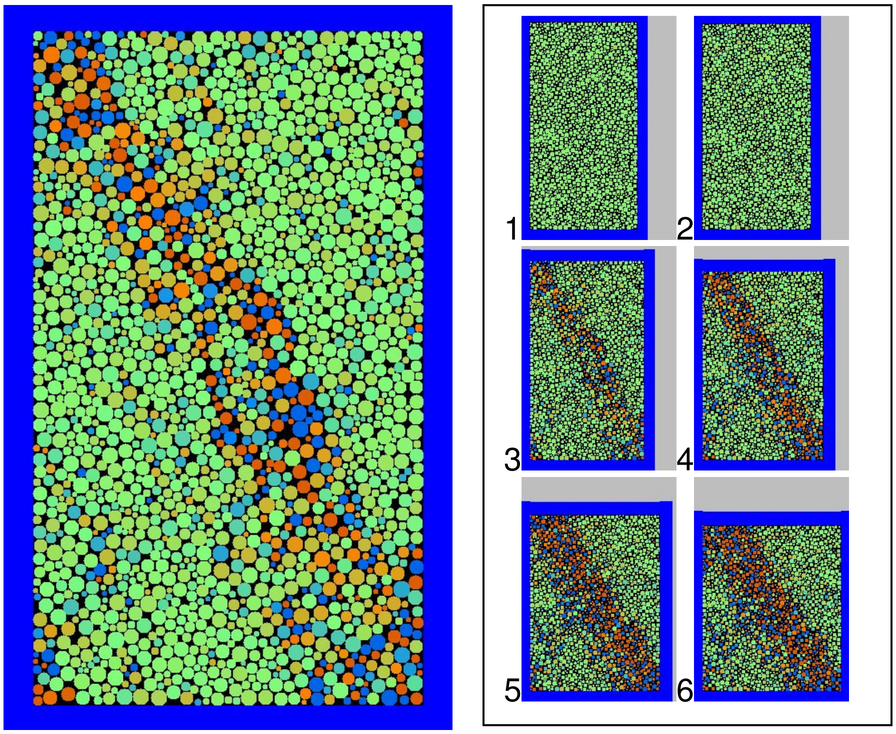
Snapshots of the simulation at different strains. The color-code corresponds to the potential contact-energy of each particle, decaying from red, green to blue. White particles are so-called "rattlers" and do not carry stress at all. The small pictures (1-6) are taken at strains ε_{zz}*=0.0027, 0.011, 0.042, 0.090, 0.151, 0.205; the magnified one is #3.*

A peculiar aspect of the system becomes evident when the displacement field in the center-of-mass reference frame is shown. First, the deformation is isotropic (1 and 2), but at a larger deformation (3-6) a shear band forms, breaking the overall symmetry of the system. The two triangle shaped parts of the system slide along each other along the shear band. When compared to these more or less static areas, the shear band is rather narrow, only a few particle diameters in width. Note that the shear band always tries to emerge from one of the corners of the system, where the shear deformation is largest and the particle structure is least stable.



Snapshots of the simulation with the displacement field in the center of mass reference frame. Blue and red correspond to opposing diagonal (top-left to bottom-right) directions of motion.

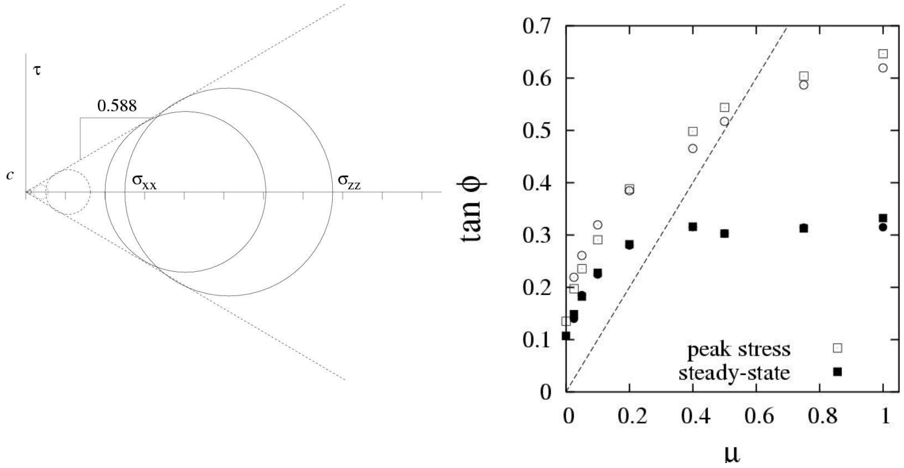
The rotation of the particles is the next quantity to examine. The particles rotate either clockwise (red) or counter-clockwise (blue) – or they remain without rotation (green). Rotation is connected to the large shear displacement in the shear band. The corresponding (clockwise) continuum-rotation is, however, not the only rotation mode. In addition, the particles have a peculiar eigen-rotation on top of the continuum rotation. Some particle rotate faster than the continuum, some slower, and some even turn “backwards”. The material outside the shear band remains practically a solid block and rotations do not occur; only inside the dilated shear band are rotations possible. Note that the integrated field of strong rotations is much wider than the local shear bands above, due to the superposition of several more narrow shear-bands, one occurring after the other.



Snapshots with the integrated particle rotations color coded. This displays shear-band positions as well as the memory of the particles concerning their total rotation during the simulation.

Now it is possible to examine the flow behavior of the system by plotting “Mohr-circles” on the horizontal stress axis, through the maximum stress (right-most point on the circle) and for different confining stresses (left-most point). The tangent to these circles can be seen as the yield-surface or -function for peak material strength. It is linear, for the parameters used, with a slope different from the microscopic friction coefficient at the contacts alone. Since we have not used cohesive forces, the macroscopic cohesion c is non-existent here, i.e., the yield-function hits the origin. Note that the peak-strength depends on the history of the sample, i.e., on its initial configuration, whereas the saturation strength does not.

Relating the macroscopic friction coefficient (as measured from this multi-particle simulation or from experiments) to the microscopic friction coefficient is one example for the micro-macro transition. For small contact friction, the sample shows considerable macroscopic friction. Increasing the contact friction leads also to increasing macro-friction that, however, saturates at a certain level. Even larger friction at the contacts does not hinder the packing from being deformed and sheared, since the particles find other ways (like rolling) to overcome the interlocking resistance from their neighbors.



(Left) Mohr circle representation of the yield-function at maximum stress and (Right) micro-macro transition for friction, i.e., the macroscopic friction coefficient (the slope of the yield-function) is plotted against the microscopic coefficient of friction at the contacts. Open symbols denote the results for different initial conditions, while solid symbols come from the steady, saturated large deformation regime.

Even though, the bi-axial box has improved our understanding of shear bands, the open question, as posed by Jim Jenkins, remains:

What is the reason for shear bands?

We are sure that shear bands are not caused by either friction, contact-adhesion, particle-shape or dimension, since they appear in frictionless, adhesionless packings of disks or spheres equally likely. Especially, it turns out that anisotropy of both structure and stress is of eminent importance.

The micro-macro transition for anisotropic particle systems and the formulation of the corresponding constitutive relations in the continuum theoretical framework is one of the major research goals of MSM.

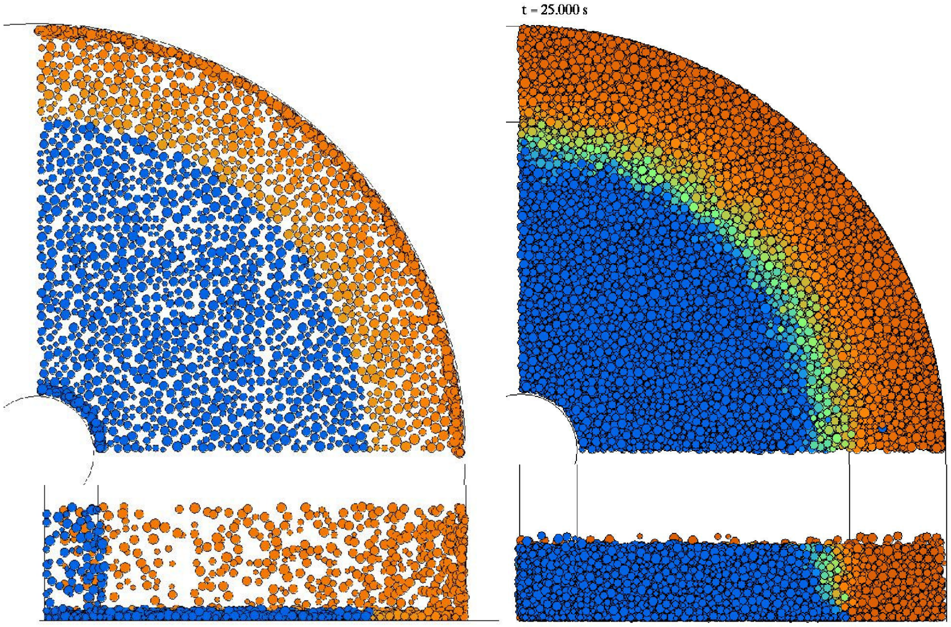
Above, the observable quantities volume, structure, stress, and their anisotropy, are obtained from the over-all system, i.e., a global averaging is performed. Thus the conclusions drawn rely on the assumption that global averaging is allowed. In experiments, it is usually impossible to perform otherwise. In simulations, local averaging is possible to test this hypothesis, see below.

Local vs. global view (shear-cell in three dimensions)

A special three-dimensional ring shear cell is shown as the next example. The system, based on an experiment by Martin van Hecke in Leiden, is a quarter of a cylindrical ring shear-cell with fixed inner and moving outer wall with radii 0.015 m and 0.110 m, respectively. The bottom wall consists of a disk with radius 0.085 m that is attached to the inner wall (static), and an outer flat ring that rotates with the outer wall. In order to enhance the roughness of the walls, about 10 percent of the particles are glued to the walls. The system (open to the top) is then filled with particles, ranging from 0.75 mm to 1.5 mm in radius, up to a height of some ten average particle diameters.

The slit at the bottom of the shear cell induces a shear band (green transition region from red to blue in the color coded pictures) with a position moving inwards. The width of the shear band is about ten particle diameters, increasing from bottom to top. The shear band position and its width are in good quantitative agreement with the experimental results for frictionless particles already (~80%) and the agreement is even better when friction is switched on (~90%).

Like in 2D, the shear band originates from the most unstable wall position – here from the slit. In the bulk, the shear band develops where the shear stress is largest: it moves inwards and widens. In the shear band, dilatancy occurs and rotations can be observed (faster and slower) than the continuum. Thus, the phenomenology is dimension independent. In 3D, the advantage is that one can average in space over many particles – along the angular ring-direction. The continuum quantities density, stucture, stress and strain are now obtained at different radial and vertical positions in a local averaging approach.

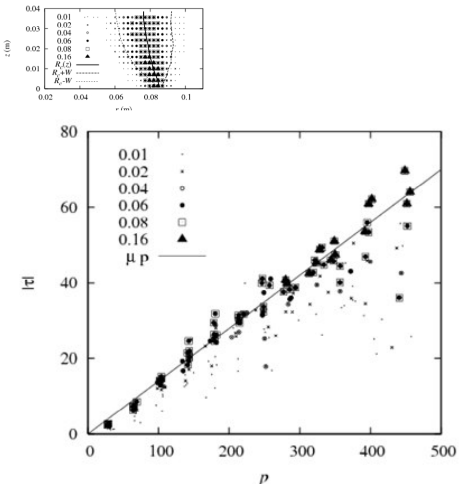


Snapshots (top-view and front-view) of a quarter of the ring shear cell, either empty (left) or filled with 22400 particles (right). About 2200 particles (left) are glued to the bottom and the cylindrical walls (indicated by the lines). The inner wall and a fraction of the bottom are at rest (blue), while the outer wall with the outer part of the bottom is rotating around the symmetry axis. Gravity acts in direction of view (top-) or vertically downward (bottom) and the color codes kinetic energy.

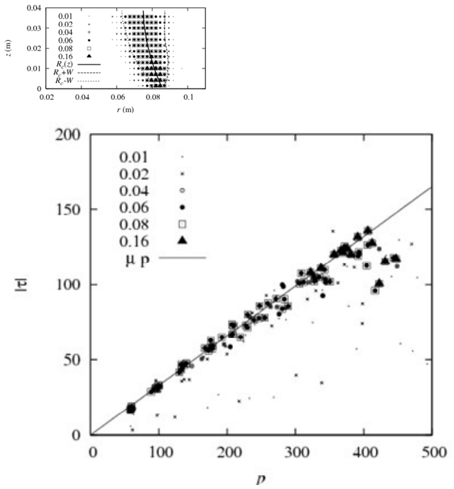
As an example, the shear stress can be plotted against the pressure for various points in the system. Different symbols indicate different shear rates, where larger symbols correspond to larger velocity-gradients and thus faster deformation. Before, by means of global averaging, several simulations had to be performed to obtain a yield-function. Now, from a single simulation by means of local averaging, the same is achieved – clearly an advantage.

The yield functions for frictionless and frictional material are close to linear and all points in the system with considerable shear rate are found with similar shear- to normal-stress ratio along the yield function – within some scatter.

Constitutive relations: Mohr-Coulomb



no friction



friction

Thus, local averaging allows obtaining similar information as global averaging, but with a much finer resolution, so that the inhomogeneity of shear vs. no-shear is avoided. Information is accumulated, disregarding the force-chain inhomogeneity, however. Results can be obtained at different positions with different values of density, stress, and shear rate. Then, ideally, constitutive relations can be deduced from a single reference simulation.

What do these constitutive relations look like?

Whether we will succeed to implement them in continuum theory models, in order to finalize the micro macro transition, the next years of fascinating research will show.

Finally, I regret that I cannot continue and also present other interesting research examples from our group, involving sound propagation, solids-fracture and self-healing, dunes, micro-flows, and many others.

Teaching/Onderwijs

In parallel to research-activities, teaching is another major task at a university. Teaching means conveying *compiled*[1], *selected*[2], *sorted*[3], and *well-prepared*[4] facts to a special audience.
Teaching involves, in general, rather short scientific talks during conferences and workshops for more specialist audiences, as well as teaching courses to students, post-graduates or amateur-audience at various levels of expertise and background, during several days, weeks or months.

Independent from the type of presentation, the first and most important thing to know is:

Who is sitting in the audience?

During the year, I give many short presentations and often I know well the audience in advance and thus know exactly what and how to present. But sometimes, I attend a conference with, or give a course for a new community, mostly unknown to me. Then I first listen as long as possible, grasp the mood, and then adapt my strategy. Often, re-sorting is necessary, sometimes a changed selection better fits to the audience and, in a few cases, a completely new talk must be prepared – those were the longest nights.
A short talk allows for rhetorical and technical tools that catch the attention of the audience and keep it. Due to the short time, usually, the talk should be perfectly adapted to the audience from the beginning. For a long lecture or lecture-series, even though one has more time and the possibility to better adapt during the event, still the audience must be the starting point and, at the end, should leave a memorable event. I want to keep my “clients” happy and satisfied while, at the same time, conveying my message.

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[1] *compiled facts:*
After years of research, ideally, it is possible to present the insight in compiled form, in simple words and pictures, such that the audience returns home with the same insight ("aha-effect"). For a researcher it might take years to obtain the insight, it will take several attempts to compile it properly, but for the audience it should take only minutes to grasp it.

[2] *selected and* [3] *sorted facts:*
No one can present all details of a certain subject due to the limited time available for the talk or the course. It requires boldness to leave out most of the details, and even some of the (supposedly important) insights – in the spirit of a selection appropriate to the audience. After such a selection, a different order or sequence of presentation often turns out to be desirable for didactical or practical reasons.

[4] *well-prepared facts:*
Without doubt, a presentation should be well-prepared in the technical sense and according to the previous points. Power Point has added value when compared to a classical lecture on black-board or transparencies, but also many dangers and pit-falls: too fast, too overloaded, too fast, too small fonts, too fast, or too many animated features, just to name a few. Whenever possible, in order to teach calculations or more complicated subjects, I prefer the old-fashioned black-board: The subject will be sequentially developed and there is a speed-limit built-in for the lecturer. The problem of unreadable or too small writing is remaining, though.
But too much preparation works against flexibility, adaptivity and improvisation. Those lectures I had prepared so well that I did not even have to look at my notes anymore are NOT my best lectures. When giving a lecture from my memory, I might do it too fast, jump ahead, get sloppy, forget something, change the sequence or nomenclature or, sometimes, start to side-step and detail

on an issue that was not planned. Much discipline is required to avoid those problems and find a healthy equilibrium between well-prepared and adaptive.
Sometimes a mistake made during a lecture triggers a lively discussion. A planned error or a left-out subject cries for a question from the audience – but sometimes the unplanned flaw appears more natural and even better initiates interaction between student and teacher, audience and lecturer. Since I tend to make mistakes, standing with the nose close to the black-board, I try to make the best out of them.

The following “stelling” is a statement about research:

> The place for curiosity-driven research is the university – where else can it be done? Even at a technical university, in an engineering faculty, there must be a healthy equilibrium between curiosity- and application driven research – and teaching.

Its implications for the curiosity-driven approach for teaching can be best clarified by referring to TV series like “Sendung mit der Maus” or “Kopfball” (Sunday morning 11:00, 1st german TV channel ARD). They proof how curiosity can be grown and harvested. Already small children can be interested in science and engineering subjects without using any complicated terms or formulas.

I believe starting already at youngest age, not only teachers but also parents and relatives can and should encourage children to ask the question “Why?”.

In this spirit, I conclude by stating that the questions “What is this good for?” or “Why do I have to learn this?” are not valid questions in a class-room or at a university. I hope not to hear these questions very often and rather prefer to answer questions like: “What is the reason?” or “How can I understand?”

Acknowledgements/Dankwoord

Mijnheer de Rector, geachte aanwezigen,

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View from our appartment in Cargese, Corse.

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All my students and colleague-researchers, I thank for their hard work and fascinating research results, as there were Master students (chronological order): Oliver Strauß, Steffen Schöllmann, Jürgen Falkner, Chiara Corticelli, Tom Winkels, and Maarten Drummen, as well as PhD students: Dr. Marc Lätzel, Dr. Stefan Miller, and Dr. Micha-Klaus Müller, and those who are not promoted (yet) Rostyslav Tykhoniuk, Ciprian David, Antina Ghosh, Robert Andersson, Orion Mouraille, and Fatih Göncü. I am also looking forward to the collaboration with the new colleagues, especially Dr. Katia Bertoldi and Dr. habil. Holger Steeb, who already helped me with proposals and plans for teaching.

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Stolwijk, and Anjenet Mettivier-Meyer for their competent support and advice whenever and wherever needed.

In memoriam:
Prof. Brian Scarlett and
Prof. Daniel Hong, both
are not among us to share
the joy of research on
particles.

In deutsch bedanke ich mich bei meinen „Mit-Wohnern“ Uli Franz (während des Studiums in Bayreuth) und Dirk Loomans und Manuela Matz (in „unserem“ Schloss in Bollschweil bei Freiburg) für das gesellige Zusammenleben, den „Familienanschluss“, und bei letzteren für die Einführung in den Square-Dance.

Schloss Bollschweil (1992-1994)

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