JAM Packed

Packing and Jamming of Particulate Systems

15.–18. Sept. 2014
Erlangen/Germany


conference dinner
train station
conference venue
to soccer
Burgberg
Schlossgarten
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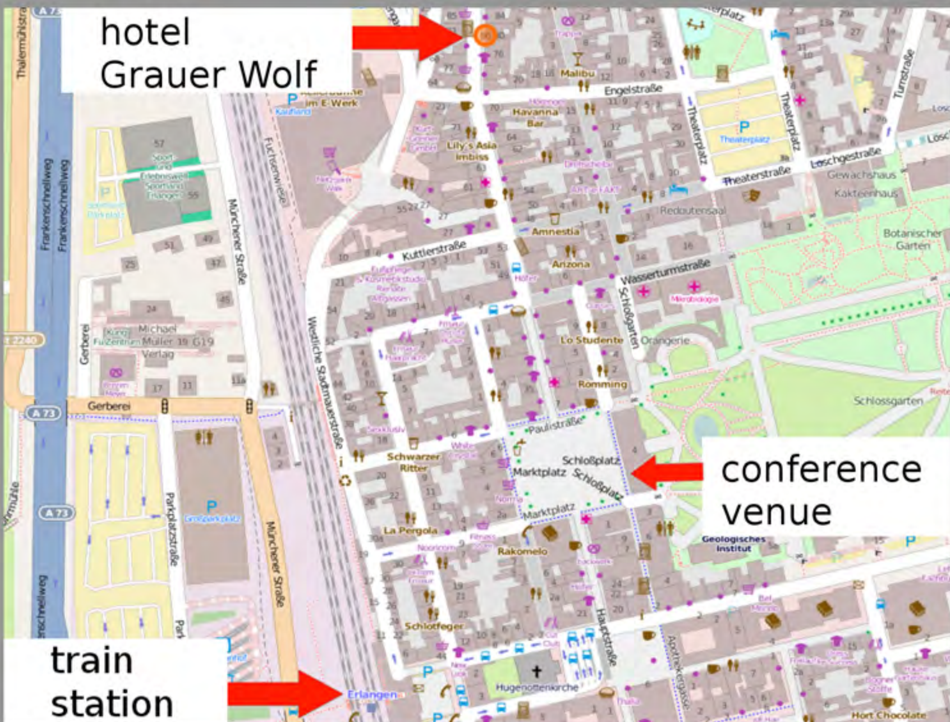
hotel Grauer Wolf
conference venue
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Jam-Packed

Erlangen, 15-18 September 2014

Packing and Jamming of Particulate Systems

Dear Colleagues,

A very warm welcome to Erlangen and thank you for joining "Jam-Packed"!

The conference follows suit from a meeting held in Dublin in September 2011, called *Packing Problems*, that addressed topics of amorphous particle packings and cellular structures in a variety of subject fields. This year's "Jam-Packed" conference attempts to continue along the same schemes, with particular emphasis to explore similarities and differences between the intimately related topics of ordering, packing and jamming.

While granular materials remain a corner stone for their study, the relevance of the concepts of jamming and packing reaches far beyond granular systems, encompassing soft matter physics and biological cellular materials amongst various other disciplines. We hope for the conference to be a lively discourse of unifying and distinct concepts in these fields, enabling discussion across the discipline boundaries.

The conference is made possible by generous support through three major DFG funding initiatives: the research group "Geometry and Physics of Spatial Random Materials", the "Engineering of Advanced Materials" Cluster of Excellence and the Collaborative Research Center for "Additive Manufacturing". We gratefully acknowledge the support of these initiatives whose diversity - covering areas from biomaterials, engineering and materials science to physics and mathematics - highlights the broad relevance of jamming and packing problems for many branches of science.

We hope you'll enjoy the conference and your time in Franconia!

Thorsten Pöschel, *Gerd Schröder-Turk*, *Adil Mughal*,
Jonathan Kollmer, *Michael Heckel*

Conference venue

The conference venue is the University Villa on the central Market square in Erlangen (**'Schloss auf dem Marktplatz'**), home to the university's central administration. It is within a few minutes walking distance of cafés and restaurants, the central train station and all conference hotels. The street address is **Schlossplatz 4, 91054 Erlangen**.

For a map of the conference venue see the inside of the front cover.

Session Format and Talk Style

Keynote lectures: 35+10 : 35 minutes talk time plus 10 minutes discussion

Contributed talks: 15+5 : 15 minutes talk time plus 5 minutes discussion

Poster Session : Tuesday 11:00-12:30

Posters are displayed for the duration of the conference. There is a dedicated **Poster Session** on **Tuesday from 11:00am to 12:30pm**.

Please take note of the **'People's Choice Best Poster Award'**. Your conference booklet contains a ballot slip for your choice of the three best posters. Please hand in your **completed ballot slip by Wednesday's afternoon coffee break**. The winners will be announced at close of the last session on Wednesday afternoon.

Wireless Internet Access : SSID "FAU-Guest"

In the conference map is a detailed instruction how to use the wireless network: Connect your mobile device to the network with SSID "FAU-Guest". Once connected open a webpage and you should see an input field for your credentials. **Your personalized username and password is provided in your registration bag.** Or you may simply try to connect via **eduroam**.

Social events

Welcome drinks – Sunday 6-8pm

Please join us for casual welcome drinks to kick off the conference on Sunday 14^{th} September from 6 to 8 pm at the conference venue, the university villa on the central market square.

Conference soccer match & bbq – Monday 6-8pm

Bring your sports gear to join us for a casual conference soccer game on Monday 15^{th} September from 6 to 8 pm. All players and all abilities welcome. We'll organise drinks and a casual bbq for the night as well. The game will take place at the 'A-Platz' of the Sports Department, at the Gebbertstraße (opposite no. 140) near the Rötelheimbad starting at 6pm. We'll get there by public transport from the conference venue, taking bus routes 286 (from the central train station, towards Bruck/Max-Planck-Str, get off at Rötelheimbad) or 287 (from the central train station, towards Sebaldussiedlung, get off at Rötelheimbad). Showers and changing rooms are available at the soccer ground.

Conference dinner – Tuesday 6pm at 'Entlas Keller'

You are cordially invited to a true-blue Franconian experience for our conference dinner, to be held at the picturesque beergarden 'Entlas Keller' at the site of Erlangen's famous May-beer festival 'The Berg'. The street address is **'An den Kellern 5-7'** which is a short 20 minutes stroll from the conference venue. This beergarden (or in case of bad weather their cellar bar) is situated on the flanks of a hill with deep horizontal cellars that were excavated for the purpose of keeping beer cool during the brewing processes of the 17th and 18th century.

The conference dinner will kick-off with a tour of the cellars starting at 6pm sharp, followed by the dinner starting at 6:30pm. While the Franconian cuisine is hearty and often meaty, vegetarian options will be available. Partners, wives & husbands all very welcome; please let us know in advance.

Please bring warm clothes as we are likely to enjoy **al-fresco outdoor dining**.

Monday

chair: Gerd Schröder-Turk

09:00 – 09:45	**Hernan Makse**	*Unifying statistical mechanics framework for packings*
09:45 – 10:05	**Alvaro Marin**	*A microfluidic hourglass*
10:05 – 10:25	**Dietrich Wolf**	*Creep near jamming*

coffee break

chair: Sidney Nagel

11:00 – 11:45	**Matthias Schröter**	*Friction with your neighbors? Think locally!*
11:45 – 12:05	**Edan Lerner**	*Marginal stability of packings of frictionless hard spheres*
12:05 – 12:25	**Mario Liu**	*Why granular media may be thermal and conventional after all*

lunch break

chair: Michael Engel

14:30 – 15:15	**Stefan Hutzler**	*Packing problems in foams*
15:15 – 15:35	**Ralf Stannarius**	*Frustrated packing of monodisperse spheres in a flat container*
15:35 – 15:55	**Massimo Pica Ciamarra**	*Jamming of deformable particles*

coffee break

chair: Denis Weaire

16:30 – 17:15	**Stefan Luding**	*Memory of jamming and shear jamming*

18:00-20:00 Conference soccer & bbq

Keynote	Hernan Makse	09:00 – 09:45

Unifying statistical mechanics framework for packings: from spherical to non-spherical particles with adhesion, friction and for any dimension.

Hernan Makse*

Levich Institute and Physics Department,
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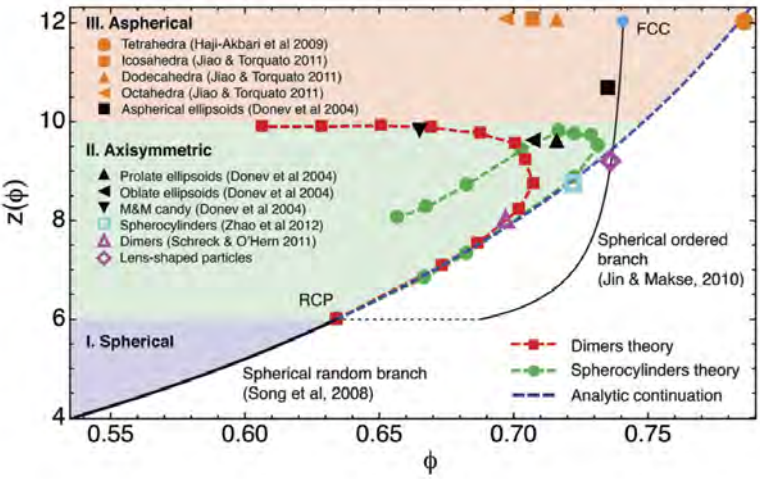
Random packings of objects of a particular shape are ubiquitous in science and engineering. However, such jammed matter states have eluded any systematic theoretical treatment due to the strong positional and orientational correlations involved. In recent years progress on a fundamental description of jammed matter could be made by starting from a constant volume ensemble in the spirit of conventional statistical mechanics. Recent work has shown that this approach, first introduced by S. F. Edwards more than two decades ago, can be cast into a predictive framework to calculate the packing fractions of both spherical and non-spherical hard particles, with or without adhesion and friction, and for any dimension [Soft Matter 10, 4423-4429 (2014)]



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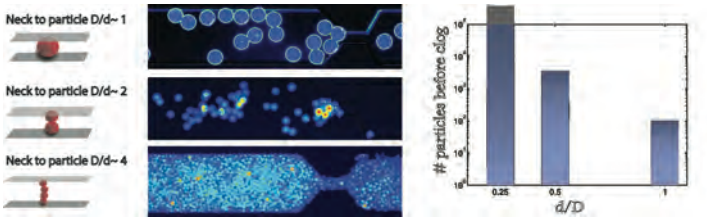
Alvaro Marin **09:45 – 10:05**

A Microfluidic Hourglass

Alvaro G. Marin,* Massimiliano Rossi, and Christian J. Kähler

Institute of Aerodynamics and Fluid Mechanics, Bundeswehr University Munich, Germany



Left figure: three cases of the microfluidic hourglass: on the top $D/d \sim 1$ and the neck gets clogged after a few hundreds particles pass the neck. As we reduce the particle size, $D/d = 2$, one needs to inject 10 times more particles to produce an arch. Finally, at a critical neck-to-particle ratio of $D/d = 4$ the system virtually does not clog, only unstable arches that break after a few instants. Right plot: Average number of particles necessary to produce an arch for the different particle-to-neck ratio d/D explored in this study.

One of the main disadvantages of microfluidic devices is their tendency to clog when a high density of particles or droplets is forced through them. The same problem is often found in classical granular flows silos and also in hourglasses. It is well-known that hourglasses work optimally when the particle-to-neck ratio is within certain ratio without interruption[1, 2], while arching occurs for particle-to-neck ratios above $d/D \approx 2$. Arching might occur in a similar way in microfluidic devices and membranes, however the topic has been treated only marginally in the literature. One good reason is that microfluidic devices normally work in regimes in which $d/D > 10$. In this regime clogging is still possible, but mainly due to the accumulation of particles at the walls, which grows until blocking the flow completely. The sticking probability has been calculated by Wyss et al. [3] in a seminal paper in which they concluded that this mechanism of clogging is triggered by single-particle events and therefore only dependent on the particle concentration, pore geometry and sticking particle-wall distance. On the other hand, clogging by arching in systems with $d/D \sim O(1)$ are expected to

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have radically different physics and statistics from clogging by deposition. In this case, collective particle dynamics and hydrodynamic interactions dominate the problem. Our results point out that the clogging of such systems have more in common with granular hoppers or silos than expected. To study these regimes, we work with microfluidic devices with a bottleneck of squared crossed section $\sim 100 \times 100$ μm through which we force polystyrene particles of 98, 50 and 25μm at packing fractions ranging from 10% up to 50%.

The microfluidic system differs strongly from a classical granular system since the dynamic of the particles it is dominated by the viscous drag of the liquid and the particle concentration is variable. In addition, particle interactions are hydrodynamic, and not frictional as in granular matter and particles feel strong stresses close to the neck. To our surprise, such a different system seems to present a clogging "transition" in the very same way as with its granular counterpart.

As we can see in the figure, the systems gets clog easily for particles of comparable size as the neck, but the clogging probability decreases exponentially as we decrease the particle size. Until we reach the case of D/d=4, in which the clogging probability is almost negligible, even at the largest particle concentrations achievable. In order to estimate the clogging probability, we calculate the number of particles that are able to pass through the neck before the clog occurs. As the figure shows, the amount of particles needed to block the neck decreases exponentially as we increase the particle-to-neck ratio d/D. Particle trajectories, packing fraction in time, and hydrocluster statistics are obtained in order to understand the reason why does a microfluidic hourglass resemble so much the clogging transition of a dry granular silo.

[1] K. To, P.Y. Lai and H. Pak. Jamming of Granular Flow in a Two-Dimensional Hopper. *Phys. Rev. Lett.*, 86,71-74, 2001.

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Dietrich Wolf **10:05 – 10:25**

Creep near jamming

A. Ries, L. Brendel, and D. E. Wolf*

University of Duisburg-Essen

When compressed between parallel, smooth walls that move in opposite directions, a cohesionless granular medium, consisting of frictional hard spheres, undergoes a transition from a jammed (at small wall velocity) to a flowing phase (at high wall velocity). In the jammed phase narrow shear bands emerge at the walls. The jammed bulk is not static, but creeps logarithmically towards increasing solid fraction. In the flowing phase there is a finite shear rate throughout the bulk leading to dilatancy. In the quasistatic limit, this dilatency is weaker than expected from a linear dependence on the inertial number. We interpret this as result of a competition between shear induced dilatency and creep compaction. The corresponding transients will be discussed.

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Keynote	Matthias Schröter	11:00 – 11:45

Friction with your neighbors? Think locally!

Matthias Schröter,[1,*] Max Neudecker,[1] N. Nirmal Thyagu,[1] Fabian Schaller,[2] and Gerd Schröder-Turk[2]

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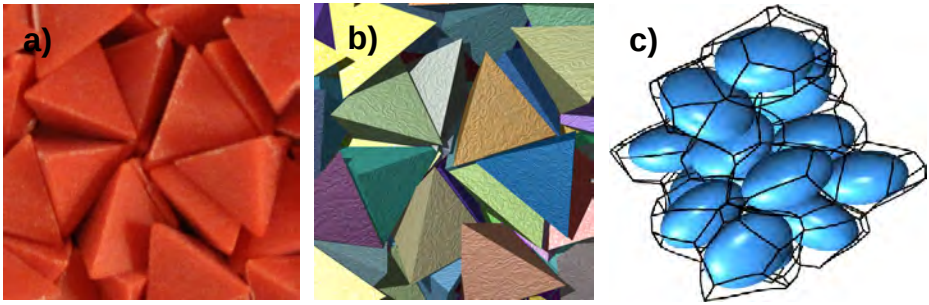
Many mechanical properties of jammed packings of particles depend on the number of contacts Z an average particle forms with its neighbors. In recent years a fair amount of research went into understanding how Z depends on the global volume fraction ϕ_g if the particles under consideration are soft and frictionless spheres. For materials such as emulsions and foams [1] this is indeed a good description because additional contacts are formed by the globally isotropic compression of the particles which also increases ϕ_g. However, in frictional granular media such as sand, salt, or sugar the control of ϕ_g is not achieved by compression but by changing the geometric structure of the sample; if we want to fill more grains into a storage container we do not compress them with a piston, but we tap the container a couple of times on the counter top.



a) Polypropylene tetrahedra with a side length of 7mm, made by injection molding. b) Raytracing of the same packing after determining particle positions and orientations from a X-ray tomography. c) Voronoi tessellation of an ellipsoid packing.

But if Z and ϕ_g are not simultaneously controlled by a globally defined parameter such as pressure, the idea of a function $Z(\phi_g)$ runs into an epistemological

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problem: contacts are formed at the scale of individual particles and their neighbors. At this scale the global ϕ_g is not only undefined; it would even be impossible for a particle scale demon to compute ϕ_g by averaging over the volume of the neighboring particles. The spatial correlations between Voronoi volumes [2, 3] would require it to gather information from a significantly larger volume than the direct neighbors. What is needed for the theoretical description of frictional particles is an ansatz which explains Z using only locally (i.e. defined on a particle level) parameters [4, 5].

This talk will present experimental results obtained by X-ray tomography of packings of two different particle shapes. For packings of frictional, oblate ellipsoids [6] of various aspect ratios α, prepared at different ϕ_g, we find that Z can be explained by a local analysis where the environment of each particle is described by its local volume fraction ϕ_l computed from a Voronoi tessellation. Z can then be expressed as an integral over all values of ϕ_l including two terms: a) the local contact number function $Z_l(\phi_l, \alpha, X)$ describing the relevant physics in term of locally defined variables only, including possible higher order corrections X. And b) the conditional probability $P(\phi_l|\phi_g)$ to find a specific value of ϕ_l given a packing of ϕ_g.

The second system are packings of frictional tetrahedra [7] which add two "complications"to the previous picture: first we go from simple point contacts between spheres and ellipsoids to four types of contacts (face-to-face, face-to-edge, edge-to-edge, vertex-to-face) which do differ in the number of mechanical constraints they impose on our packings. And secondly, tetrahedra packings show a clear dependence of Z on the preparation history. Which underlines the necessity of including a hitherto unknown parameters X into future theoretical approaches.

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[2] F. Lechenault, F. da Cruz, O. Dauchot, and E. Bertin , J. Stat. Mech. **2006**, P07009 (2006).
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Edan Lerner **11:45 – 12:05**

Marginal stability of packings of frictionless hard spheres

Edan Lerner,[1,2,*] Gustavo Düring,[3] and Matthieu Wyart[1]

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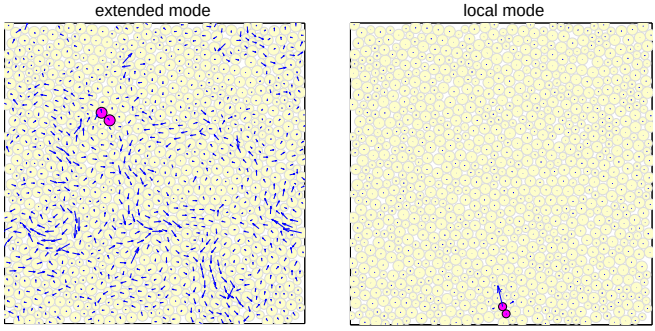

Examples of two displacement fields resulting from pushing apart a pair of particles carrying a weak contact force, represented as shaded, in a two-dimensional isostatic packing. The left panel exemplifies the case where the displacements of the rest of the particles are of the same order of the displacements of the pushed pair, and the contact force is small because the displacement field is almost orthogonal to a compressive strain. The right panel displays a different displacement field generated in the same configuration as in the left panel, by pushing apart a different pair of particles. This time the pushed pair's displacement is significantly larger than the displacements in the rest of the system. Such contacts are very weakly coupled to external stresses applied on the boundary, i.e. they are mechanically isolated.

If hard frictionless particles are compressed sufficiently rapidly deep into the glassy phase, they eventually jam into a disordered packing in which the number of contacts between the particles is exactly equal to twice the spatial dimension [1]. These so-called 'isostatic' packings have peculiar mechanical properties, as

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they dwell on the boundary between mechanical stability and instability. In my talk I will present a statistical analysis of nonlinear low energy excitations in isostatic packings [2]. I will show that isostatic packings generated by a rapid compression are *marginally stable*; this marginal stability allows us to predict a relation between the distribution of contact forces between the hard particles, and the distribution of gaps between pairs of particles that are just almost touching [3]. I will also show that only a subset of the weak contact forces – those that are strongly coupled to their surroundings – plays an important role in the mechanical response of packings under external loading, and how the statistical properties of this subset of contact forces relates to the huge increase of the viscosity of dense non-Brownian suspensions close to jamming [4].

Acknowledgments: This work has been supported primarily by the MRSEC Program of the National Science Foundation DMR-0820341, by the Sloan Fellowship, by the National Science Foundation DMR-1105387, and by the Petroleum Research Fund #52031-DNI9.

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Mario Liu **12:05 – 12:25**

Why Granular Media May Be Thermal and Conventional After All

Mario Liu*

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Taking grains as elementary building blocks interacting via the Newtonian law with an elasto-frictional force, the discrete element model (DEM) has been a success story – to the extent that it is nowadays the tool of choice for coming to terms with granular behavior.

Athermal statistical mechanics (ASM) takes this model a big step forward [1, 2]. Defining an entropy S as the logarithm of the number a granular ensemble may be stably packed, ASM assumes it is maximal in equilibrium. (The numbers are sometimes weighted.) DEM, we note, never introduces an entropy and does no need it to guide the system towards the rest state. More specifically, ASM also takes grains as athermal, elementary building blocks, same as DEM, because thermal fluctuations are so small. And it assumes in addition force equilibrium between each pair of grains at rest. Being dissipative and not conserved, energy is typically discarded as a state variable. Instead, S is taken to depend on the volume and force moment tensor.

The reason thermal fluctuations are small is because grains are macroscopically large. But there are then, by the same token, many, many internal microscopic degrees of freedom – phonons, electrons, etc. And one needs to make sure they are irrelevant. Consider the textbook example of a pendulum. Its motion is given by the Newtonian force law of a mass point including a frictional term. Yet to determine its sign, to make sure that the pendular amplitude diminishes, one needs to consider how the total entropy increases, which consists mainly of microscopic degrees of freedom: the velocity of the air molecules surrounding the pendulum, the phonons in the solid parts forming the suspension – also in the pendular weights if we have two elastic pendula colliding periodically. If this is an apt analogy for the relation between DEM and granular statistical mechanics, the internal microscopic degrees of freedom must be included when calculating S. Moreover, since the number of all these degrees vastly overwhelms that of packaging, the result of whichever version of ASM appears doubtful.

Remarkably, including the microscopic degrees of freedom, the total energy of all is conserved, and the conventional thermal statistical mechanics is again

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valid. Employing it, one finds that the grain-level energy dissipates because it is being redistributed to the microscopic degrees of freedom, and that force equilibrium holds when the total entropy is maximal [3–6]. So, thermal and athermal statistical mechanics do not disagree in this respect, and DEM agrees with both.

Summarizing the above arguments, the following conclusions seem hard to avoid:

- Granular media are not generally and naturally athermal;
- anyone taking the reduced entropy that excludes internal degrees of freedom as maximal in equilibrium bears a heavy burden of proof.

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Free download: http://www.springerlink.com/content/a8016874j8868u8r/fulltext

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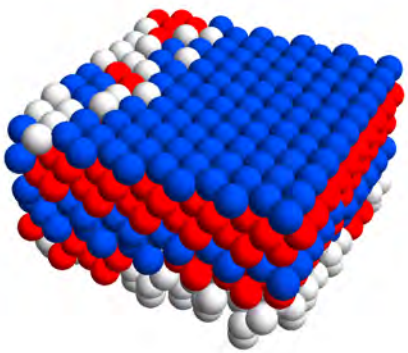
Keynote	Stefan Hutzler	14:30 – 15:15

Packing problems in foams

Stefan Hutzler*

School of Physics, Trinity College Dublin, Ireland

Foams are densely packed collections of gas bubbles surrounded by a liquid (or solid). Packing problems include the structure of fully periodic foams (the Kelvin problem), foams in confinement (e.g. in cylindrical tubes), or bubble clusters. Here we present the new analytical Z-cone model for the estimation of (surface) energy for an ordered foam in which every bubble has Z identical neighbours, as a function of liquid fraction. This confirms a Z-dependent logarithmic form for the energy-deformation relation just above the jamming transition in the wet limit [1]. We also show results from X-ray tomography for monodisperse bubbles of a few hundred microns in diameter, figure 1. Bulk ordering in these samples containing a few thousand bubbles is identified via the computation of bond orientational order parameters [2].



Example of crystallinity in the bulk of a foam consisting of monodisperse bubbles. The bubbles are coloured according to their bond orientational order classification. Red: fcc, blue: hcp, white: other [2].

Acknowledgments: The author wishes to thank co-workers in Dublin and at the Institute of Applied Materials in Berlin. Further acknowledgements: COST actions MP1106: Smart and Green Interfaces and MP1305: Flowing Matter.

[1] S. Hutzler, R. Murtagh, D. Whyte, S.T. Tobin and D. Weaire, submitted.
[2] A.J. Meagher *et al.*, in preparation.

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Ralf Stannarius **15:15 – 15:35**

Frustrated packing of monodisperse spheres in a flat container

Kirsten Harth,[1] Alex Mauney,[2] and Ralf Stannarius[1,*]

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We study the packing of monodisperse spheres in a flat vertical box with cell gap slightly larger than the particle diameter, and evaluate the statistics of the particle arrangements. After 'gravitational' filling of the container and appropriate agitation, the particles form a nearly regular triangular lattice in the cell plane. The additional freedom of a displacement of the particles normal to the cell plane places them either at the front or rear cell plate. This leads to a denser arrangement in the cell plane, but at the same time causes frustrated states (of three neighboring beads in a local triangle, two have to occupy the same side of the cell). Analogies to order in antiferroelectric Ising spin systems on a triangular lattice [1], and to colloidal assemblies in thin layers [2] are evident.

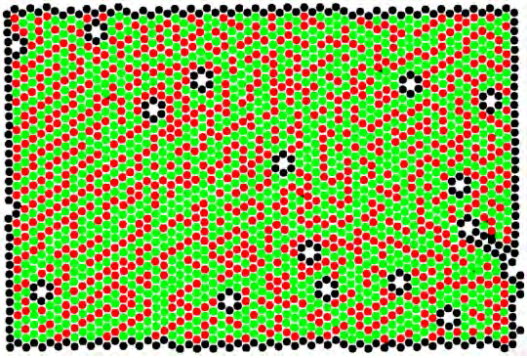

Image of a region of a flat (gap 2.9 mm) container filled with 2.2 mm glass beads, after data processing. The colors reflect three categories of beads at the borders or at lattice defects with less than six neighbors (black), beads that touch the fromt (green) and rear (red) cell plates.

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We analyse the packing properties statistically and compare them to the predictions of two models, one considering a minimum number of frustrated states to minimize packing densities, the other one assuming random uncorrelated particle positions.

When the container is tilted from the vertical, the gravitation field can mimic external forces similar to magnetic fields in spin systems. While arrangements in the vertical container adopt a frustrated state halfway between an optimal regular and a totally uncorrelated (Ising) positions of neighboring lattice sites, experimental data follow more and more the statistics of the Ising model when the cell tilt is increased. The experiment offers both insights in the influence of geometrical constraints on random packing and a descriptive example for frustrated ordering.

Acknowledgments: Andy Hirsch and Frank Rietz are acknowledged for participation in experiments and valuable discussions.

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Massimo Pica Ciamarra **15:35 – 15:55**

Jamming of deformable particles

Massimo Pica Ciamarra[1,*] and Giovanni Romeo[2]

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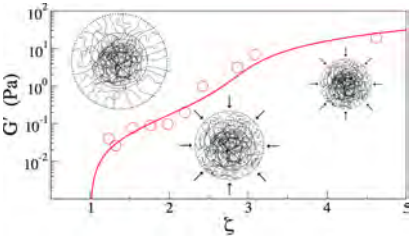
The jamming transition has been traditionally investigated in systems of stiff particles, whose deformation is small with respect to their size. Here we consider the jamming scenario of microgel suspensions. Microgels are colloidal particles made of a polymer network swollen in a solvent, whose size is commonly in the micrometer range, that so soft that they usually deform and shrink when compressed. Indeed, in these systems extremely high values of the volume fraction $\xi = \rho v_0$ can be attained [1], $\xi \gg 1$, where ρ is the number density and v_0 the particle volume in the dilute limit.



Measured (points) and predicted (full line) volume fraction dependence of the shear modulus of a microgel suspension. Note that the system reaches high value of the volume fractions, as particles shrink when compressed as schematically illustrated.

Via the analysis of experimental data and the study of a numerical model, we argue that two volume fraction characterize the response of these system to compressions: the jamming volume fraction $\xi_j \simeq \phi_j$, and the filling volume fraction $\xi_f \simeq 1$. In the volume fraction range $\xi_j < \xi < \xi_f$, most microgels appear to deform at constant volume, so that the macroscopic elasticity is set by shear modulus of the particles, which is hardly measurable [2]. At higher volume fractions, $\xi > \xi_f$, particles shrink. Despite the disordered spatial arrangement of the

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particles, in this regime microgel suspensions deform affinely upon compression, so that the bulk to shear modulus ratio becomes volume fraction independent [3, 4], at variance with the common jamming scenario. The affine response to compressions allows to develop a model connecting the macroscopic elasticity to the thermodynamic properties of the single particles [3], we describe through a combination of Flory theory for polymer gels and de Gennes theory for polymer brushes. The figure illustrates the application of this model to experimental data.

The deformation of the particle upon compression suggest that at high density microgels interact via a many–body interaction potential, as polymers and star–polymers [5–7]. We address the question of the relevance of the many–body contribution with respect to the two–body one through event driven molecular dynamics simulations of the interaction between swollen polymeric networks.

[1] J. Mattsson, H. M. Wyss, A. Fernández-Nieves, K. Miyazaki, Z. Hu, D. R. Reichman and D. A. Weitz, Nature **462**, 83 (2009).
[2] S.M. Hashmi and E.R. Dufresne, Soft Matter **5**, 3682 (2009).
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[5] P. G. Bolhuis, A. A. Louis, J. P. Hansen and E. J. Meijer J. Chem. Phys. **114**, 4296 (2001); P. G. Bolhuis, A. A. Louis, and J. P. Hansen Phys. Rev. E **64**, 021801 (2001).
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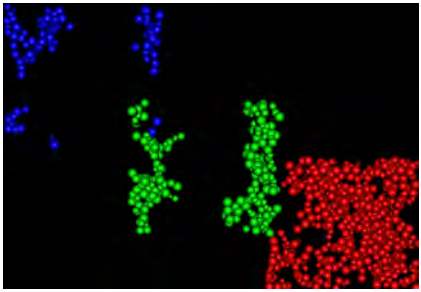
[7] A. Pelissetto, Phys. Rev. E **85**, 021803 (2012).

Keynote	Stefan Luding	16:30 – 17:15

Memory of Jamming and Shear Jamming

Nishant Kumar and Stefan Luding*

Universiteit Twente, Netherlands.



Understanding the jamming of soft matter as e.g., granular materials, found both in nature and industry, has been one of the most challenging fundamental questions for researchers in the last decade. Material behaves like a fluid below a certain volume- or solid-fraction (known as jamming density or "point") but like a solid or glass above. Various interesting, but contentious phenomena are reported near this point, like creep or shear-jamming. However, a unified model of the dynamics, statistics and rheology near jamming is still lacking. Based on the study of three-dimensional soft, frictionless, polydisperse spheres, using both isotropic and shear deformation tests, for the first time, a simple, yet quantitative model is proposed: Accepting the fact that the jamming density is not a constant, the key ingredient is the knowledge of how the jamming density changes for different deformation modes. The packing efficiency can increase logarithmically slow (creep) under gentle "tapping" or repeated compression, leading to an increase of the jamming density. In contrast, shear deformation causes anisotropy and dilatancy, and rapidly decreases the jamming density that thus represents the memory of previous deformations. A model that explains the memory of the system near jamming involves a multi- scale, fractal-type energy landscape, representing an alternative, unified picture for the multitude of phenomena reported near jamming. As major benefit, the memory of jamming shall play a significant role in altering constitutive continuum models to quantitatively explain and predict many real-world observations and applications.

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Tuesday

chair: Andy Kraynik

9:00 – 9:45	**Michael Engel**	*When and how can densest packings be achieved with nanoparticles?*
9:45 – 10:05	**Jason Gallas**	*Residual defect density in random depositions of large piles of disks*
10:05 – 10:25	**Ana-Suncana Smith**	*Dynamic packing of epithelial cells*

coffee break

11:00 – 12:30	**poster session**	

lunch break

chair: Hernan Makse

14:30 – 15:15	**Brian Tighe**	*Beyond quasistatic linear response*
15:15 – 15:35	**Günter Last**	*A class of random growth-maximal hard-core processes?*
15:35 – 15:55	**Fabian Schaller**	*Non-universal Voronoi cell shapes in ellipsoid packings*

coffee break

chair: Matthias Sperl

16:30 – 16:50	**Patric Müller**	*Granular jet impact: packing in front of finite targets*
16:50 – 17:10	**John Amend**	*Commercializing jamming-based technology - VERSABALL(R) robotic grippers*

18:00-22:00 Conference dinner

Keynote	Michael Engel	09:00 – 09:45

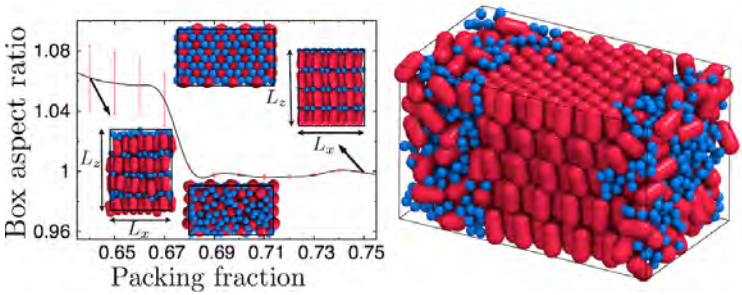
When and how can densest packings be achieved with nanoparticles?

Michael Engel,[1,*] Andres J. Millan,[2] Eric Irrgang,[2] and Sharon C. Glotzer[1,2]

[1] *Department of Chemical Engineering, University of Michigan, USA*

[2] *Department of Materials Science and Engineering, University of Michigan, USA*

Finding the densest packing of an anisotropic object is a mathematical optimization problem. Dense packings have applications in operations research, such as optimal storage, packaging, and transportation, where objects can be positioned individually. In contrast, dense packings of mesoscopic (nano- or microscale) building blocks can only be achieved via compactification, i.e. by gradually increasing the density from a fluid state. The particles can then statistically explore a subset of phase space, entropy cannot be neglected, and packing competes with self-assembly.



Binary packing and phase separation of hard spheres and hard spherocylinders [3]. (Left) Isotensile simulations show a rapid change in the box aspect ratio L_z/L_x indicative of a transition to the lamellar phase at packing fraction $\phi = 0.68$. (Right) At $\phi = 0.618$, the lamellar phase separates into the rod crystal and a mixed fluid.

Over the last years we have learned that densest packing and self-assembly results are often not identical. Nevertheless, a dense packing (candidate) is typically easy to determine [1] – easier than to self-assemble a large number of particles. It would be helpful if densest packings could serve as a first step towards understanding the phase behavior of experimental systems. Here we report computational investigations of anisotropic nanoparticles in two and three dimensions and argue that this is indeed the case in many situations.

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We use Monte Carlo simulations to reproduce and interpret observations of the self-organization of single crystalline nanoparticles in solution and at the liquid-air interface. We discuss how nanoplates can distinguish between two equally dense superlattices [2] and show how a binary system overcomes its natural entropic tendency toward macroscopic phase separation [3]. The combination of a strive towards dense packing and shape-induced entropic (and energetic) effects directs the formation and stabilization of unconventional long-range ordered assemblies not attainable otherwise [2–4].

[1] E.R. Chen, D. Klotsa, M. Engel, P.F. Damasceno, and S.C. Glotzer, *Complexity in surfaces of densest packings for families of polyhedra*, Phys. Rev. X **4**, 011024 (2014).

[2] X. Ye, J. Chen, M. Engel, J.A. Millan, W. Li, L. Qi, G. Xing, J.E. Collins, C.R. Kagan, J. Li, S.C. Glotzer, C.B. Murray, *Competition of shape and interaction patchiness for self-assembling nanoplates*, Nature Chem. **5**, 466-473 (2013).

[3] X. Ye, J.A. Millan, M. Engel, J. Chen, B.T. Diroll, S.C. Glotzer, C.B. Murray, *Shape alloys of nanorods and nanospheres from self-assembly*, Nano Lett. **13**, 4980-4988 (2013).

[4] E.M. Irrgang *et al.*, preprint.

Jason Gallas **09:45 – 10:05**

Residual Defect Density in Random Depositions of Large Piles of Disks

Nikola Topic,[1] Thorsten Pöschel,[1] and Jason A.C. Gallas[1, 2, 3, *]

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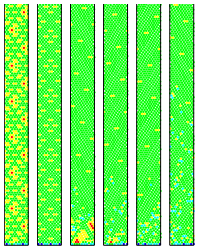
[3] *Instituto de Altos Estudos da Paraíba, Rua Infante Dom Henrique 100–1801, 58039-150 João Pessoa, Brazil*

We report a systematic characterization of the density of defects in large piles of hard disks formed by random depositions confined by channels of small to very large widths and with heights no less than 40 times those investigated previously (Fig. 1). Surprisingly, we find all piles to consistently have a residual non-zero density of defects. This is in sharp contrast to a widespread belief that the density of defects vanishes for such piles.



(a) (b) (c) (d) (e) (f)

Six representative packings illustrating typical residual defect distributions and the transients needed to reach them. All channels have widths $w = 10$ particle diameters and their height h is about $10w$. For small widths transients are usually quite short. The regular structure of voids is also visible in the channels.

Acknowledgments: The authors thank the Deutsche Forschungsgemeinschaft (DFG) for funding through the Cluster of Excellence *Engineering of Advanced Materials*. JACG was also supported by CNPq, Brazil.

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Ana-Suncana Smith **10:05 – 10:25**

Dynamic packing of epithelial cells - randomness and correlations on different length scales to avoid jamming

Sara Kaliman,[1] Jayant Pande,[1] and Ana-Sunčana Smith[1, 2, *]

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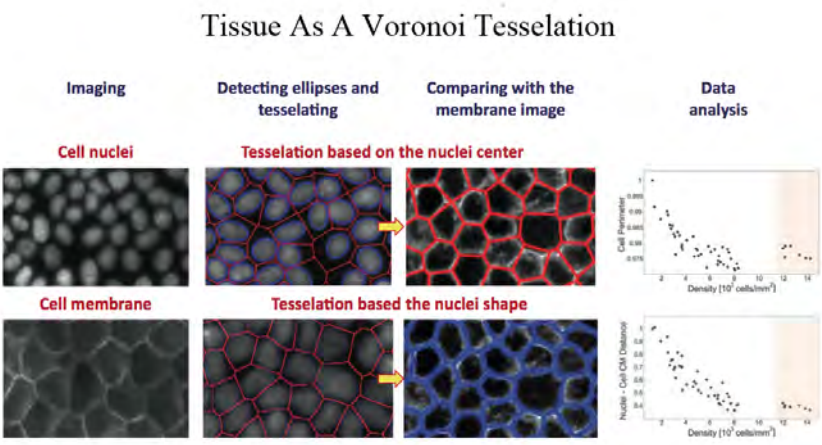

Shape based Voronoi tessellation of randomly distributed ellipses with the same size and elongation as the nuclei found in the real tissue.

Tissue growth is an inherently complex process, the details of which need to be understood not only from a biological standpoint but also in terms of the purely physical and geometrical aspects. Here we focus on epithelial tissues (made of MDCK cells) that naturally form as a single layer of cells. We grow such tissues starting from a small number of cells until millimeter large colonies are obtained [1]. We find that the developing tissue spontaneously adopts a circular shape, with a compartmentalized internal structure that self-organizes over several days. During this process a compartment of a higher density appears in the center of the colony. We characterize the morphology of the tissue as it

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develops, and show that its internal structure can be represented by the Voronoi tessellation based on the shape of the cellular nuclei (see figure). As the tissue develops, the cell organization approaches a centroidal Voronoi tessellation, which is accompanied by a decrease of the contact area between cells and the repositing of the nucleus toward the center of mass. Interestingly, we find that the average elongation of the cell does not depend on the density of the tissue which then prevents the formation of the hexagonal structure. We compare the organization of the tissue to tessellations which emerge from randomly distributed ellipses. For this purpose we analyze in detail tessellations constructed from monodisperse spheres and ellipses as a function of the filling fraction and the elongation of the constituting bodies. We find that locally, the tissue structure appears very similar to the random packing, yet this is on contrast to long range correlations that are measured. We hypothesize that such elongated shape of nuclei, and the associated tessellation, serves to avoids cell jamming at high filling fractions (0.65) that typify the growth. Consequently, the migration of cells trough the crowded environment of the tissue is enabled, both from the physical and biochemical points of view. We support this idea with simulations of the cluster growth in which we are able to reconstruct the experimentally measured compartmentalization.

We acknowledge the support of the ERC Starting Grant MembranesAct and the RTG 1962.

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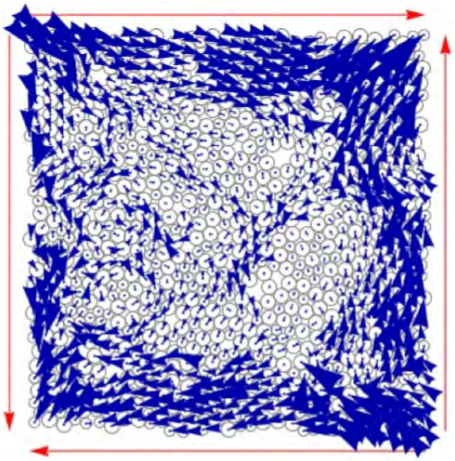
Keynote	Brian Tighe	14:30 – 15:15

Beyond quasistatic linear response

Brian P. Tighe*

Delft University of Technology, Process & Energy Laboratory, Leeghwaterstraat 39, 2628 CB Delft, The Netherlands

Mechanical response near jamming is best understood in the limit of slow and weak deformations, when damping and nonlinearity are negligible. Yet realizing these conditions can be exceedingly difficult in the laboratory, or even in the computer, because the thresholds for nonlinearity and rate dependence must vanish at point J. These thresholds can be characterized rheologically via, e.g., large amplitude oscillatory shear, stress relaxation, and flow startup tests. Using a combination of computer simulations and scaling arguments, I will demonstrate that viscoelastic solids near jamming are generically shear thinning and strain softening.



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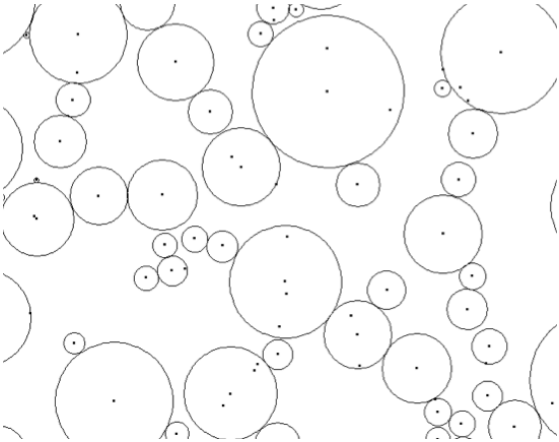
Günter Last **15:15 – 15:35**

A class of random growth-maximal hard-core processes

Günter Last* and Sven Ebert

Karlsruhe Institute of Technology

In the well-known lilypond model based on a spatial point pattern all points start growing at the same time and at the same rate. Any given ball ceases its growth as soon as it encounters any other ball. In the physics literature this is known as the touch-and-stop model. Spherical droplets grow at constant velocity and when two of them touch they stop their growth. The final configuration can be characterized by a certain growth-maximality property. In this talk we extend this model by introducing a growth-maximal hard-core model based on random convex particles arriving in time. Using a purely deterministic algorithm we prove under fairly general assumptions that the model exists (in infinite volume) and is uniquely determined by the input. Under an additional stationarity assumption we show that the model does not percolate. Our model generalizes the lilypond model considerably, even if all grains are born at the same time. In that case and under a Poisson assumption we prove a central limit theorem in a large volume scenario.



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Fabian Schaller **15:35 – 15:55**

Non-universal Voronoi cell shapes in ellipsoid packings

Fabian M. Schaller,[1,2,*] Sebastian C. Kapfer,[3] Mohammad Saadatfar,[4] Klaus Mecke,[1] Matthias Schröter,[2] Gary W. Delaney,[5] and Gerd E. Schröder-Turk[1]

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In particulate systems with short-range interactions, such as granular matter or simple fluids, the local structure plays a pivotal role in determining the macroscopic physical properties. Here, we discuss disordered packings of ellipsoidal particles which are an important model for disordered granular matter and can shed light on geometric features and structural transitions. For disordered sphere packings a great range of universality has been shown, like the random close packing limit [1] and the universal functions for contact numbers [2], free volumes [3, 4] and Voronoi cell shape measures [3, 5].

Here, we focus on jammed static ellipsoid configurations, obtained by tomographic imaging of frictional particles and by discrete element method simulations of frictional and frictionless particles with and without gravity for various aspect ratios and global volume fractions Φ_g. In addition lower density equilibrium fluid configurations from MC and MD simulations and the densest know crystal packings are analysed. We report an analysis of the structure of the Set Voronoi diagram, a generalizsation of the Voronoi Diagram for spheres [6]. The ellipsoid configurations are analysed in terms of global averages and relative to the local packing fraction Φ_l, defined as particle volume divided by Voronoi cell volume.

We find that the probability $P(\Phi_l)$ for a Voronoi cell to have a given local packing fraction is, as in spheres, only trivially dependent on Φ_g and, surprisingly, also independent of the particle aspect ratio and preparation protocol.

By contrast, the typical cell shape, quantified by the Minkowski tensor anisotropy index $\beta = \beta_0^{2,0}$, points towards a significant difference between random packings of spheres and those of oblate ellipsoids. For spheres the Voronoi Cells of spheres become more isotropic with increasing packing fraction, whereas the shape of the

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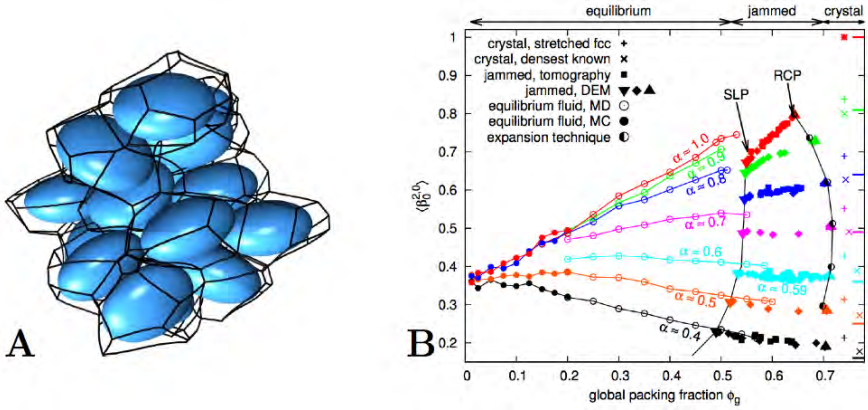

Average anisotropy index $\langle \beta_0^{20} \rangle$ of the Set Voronoi cells of the ellipsoids as function of the global packing fraction for equilibrium ellipsoid ensembles and static jammed ellipsoid packings. (MC data courtesy of Tanja Schilling, Universite du Luxembourg; MD data courtesy of Cristiano De Michele and Francesco Sciortino, University of Rome).

Voronoi cells of ellipsoids with high aspect ratio remains approximately constant or even decreases. The jammed packings are always more anisotropic than the corresponding densest equilibrium configuration.

While the average cell shape β of all cells with a given value of ϕ_l is very similar in dense and loose jammed sphere packings, the structure of dense and loose ellipsoid packings differs substantially such that this does not hold true. This non-universality has implications for our understanding of jamming of aspherical particles.

Acknowledgments: We acknowledge funding by the German Science Foundation (DFG) through the research group "Geometry and Physics of Spatial Random Structures" under grant no SCHR-1148/3-1.

[1] G.D. Scott *et. al.*, Nature **194**, 956f (1962).
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[3] F.W. Starr *et. al.*, PRL **89**, 125501 (2002).
[4] T. Aste *et. al.*, EPL **79**, 24003 (2007).
[5] G.E. Schröder-Turk *et. al.*, EPL **90**, 34001 (2010).
[6] F.M. Schaller *et. al.*, Philosophical Magazine **93**, 3993 (2013).

Patric Müller **16:30 – 16:50**

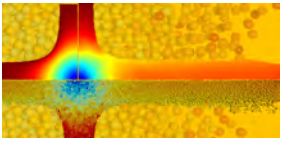
Granular Jet Impact: Packing in Front of Finite Targets

Patric Müller,[1,*] Arno Formella,[2] and Thorsten Pöschel[1]

[1] *Institute for Multiscale Simulation, Universität Erlangen-Nürnberg, Erlangen, Germany*

[2] *Department of Computer Science, Universidad de Vigo, Ourense, Spain*

We investigate the packing of a granular jet which impacts on a finite target by means of particle simulations. The resulting hydrodynamic fields are compared with theoretical predictions for the corresponding flow of an incompressible and rotation free fluid. The degree of coincidence between the fields obtained from the discrete granular system and the idealized continuous fluid flow depends on the characteristics of the granular system, such as granularity, packing fraction, inelasticity of collisions, friction, and target size. In certain limits we observe a granular-continuum transition under which the geometric and dynamic properties of the particle jet and the fluid jet become almost identical.



The lower panel of the image shows a granular jet impacting on a fixed finite target (not shown). The colors of the particles denote their absolute velocity where red corresponds to a high velocity and blue to a low velocity. The upper right panel shows the field of absolute velocity obtained from the particle data. The upper left panel shows the field of absolute velocity for the corresponding flow of an incompressible and rotation free fluid as obtained from hydrodynamic theory. The background shows a magnification of the granular jet.

Acknowledgments: We thank Marcus Bannerman, Isaac Goldhirsch, Dan Serero and Nicholas Guttenberg for discussion. The authors gratefully acknowledge the support by German Science Foundation through the Cluster of Excellence 'Engineering of Advanced Materials'.

[1] P. Müller and A. Formella and T. Pöschel J. Fluid Mech. **751**, 601-626 (2014).

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John Amend **16:50 – 17:10**

Commercializing Jamming-based Technology - VERSABALL(R) Robotic Grippers

John Amend*

Empire Robotics, Inc.

VERSABALL(R) grippers are a unique new robotics technology being developed by Empire Robotics, Inc. Based on research from Cornell University and the University of Chicago, these grippers leverage granular jamming to enable successful handling of a wide range of objects for automated tasks in industrial manufacturing. This talk will provide an introduction to the specific application of jamming materials for robotic grippers, an discussion on bridging the gap between academic research and commercial products in this field, and an industrial view on material requirements for jamming-based products.

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Wednesday

chair: Corey O'Hern

9:00 – 9:45	**Sidney Nagel**	*Jamming fronts in colliding granular clusters*
9:45 – 10:05	**Gustavo Düring**	*Analogy between strain-stiffening and jamming in dense flows*
10:05 – 10:25	**Andy Kraynik**	*Polyhedral bubble packing in sheared random foams*

coffee break

chair: Stefan Luding

11:00 – 11:20	**Jonathan Kollmer**	*Polydirectional Stability of Granular Matter*
11:20 – 11:40	**Richard Gerum**	*Traveling waves in penguin huddles*
11:45 – 12:05	**Balazs Szabo**	*Packing and ordering of particles under shear*
12:05 – 12:25	**Gary Delaney**	*Computational studies of jamming in non-spherical particle systems*

lunch break

chair: Tobias Kraus

14:30 – 15:15	**Matthias Sperl**	*Higher-order singularities at the glass transition and random-close packing*
15:15 – 15:35	**Denis Weaire**	*Phyllotaxis and the cylindrical packing of disks*
15:35 – 15:55	**Kai Huang**	*Assembly of driven wet grains: from spheres to hexagons*

coffee break – hand in your poster award ballot papers

chair: Matthias Schröter

16:30 – 17:15	**Tomaso Aste**	*Jamming matter: local geometry and global properties*

17:15 poster award presentation

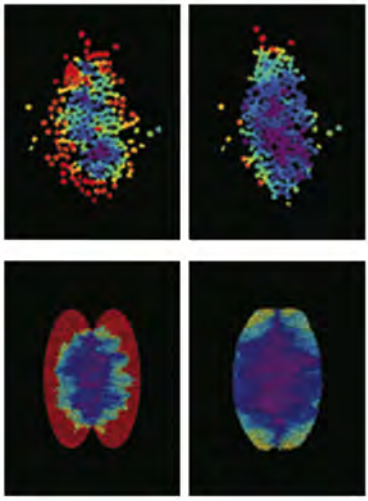
Keynote	Sidney Nagel	09:00 – 09:45

Jamming fronts in colliding granular clusters

Sidney R. Nagel*

The University of Chicago

In a granular gas, inelastic collisions produce an instability in which the constituent particles cluster heterogeneously. These clusters then interact with each other, further decreasing their kinetic energy. I will review experiments of the free collisions of dense clusters of particles in a two-dimensional geometry. The particles are composed of solid CO_2, which float with nearly zero friction on a hot surface due to sublimated vapor. After two dense clusters, each of ≈ 100 particles, collide, there are two distinct stages of evolution. First, the translational kinetic energy rapidly decreases by over 90% as a "jamming front" sweeps across each cluster [1]. In this regime the kinetic energy decays in time as $\Delta E = -Kt^{3/2}$, a form that can be predicted from kinetic arguments. Subsequently, the kinetic energy decreases more slowly as the particles approach the container boundaries [2]. In this regime, the measured velocity distributions are non-Gaussian with long tails.



Top: Photographs of the initial moments of a collision between two clusters of solid CO2 particles. A jamming front moves across the clusters after the collision. Bottom: Snapshots of a simulation of a collision between two 5000-particle elliptical clusters, showing a similar jamming front. Color indicates velocity; time increases left to right.

[1] J. C. Burton, P. Y. Lu, and S. R. Nagel, Phys. Rev. Lett. **111**, 188001 (2013).
[2] J. C. Burton, P. Y. Lu, and S. R. Nagel, Phys. Rev. E **88**, 062204 (2013).

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Gustavo Düring **09:45 – 10:05**

Microscopic theory of non-Brownian suspension flows close to the Jamming point.

Gustavo Düring,[1,*] Edan Lerner,[2] and Matthieu Wyart[3]

[1] *Universidad Católica de Chile*
[2] *University of Amsterdam*
[3] *New York University*

While the rheology of non-Brownian suspensions in the dilute regime is well-understood, their behavior in the dense limit remains unclear. As the packing fraction of particles increases, particle motion becomes more collective, leading to a growing length scale and scaling properties in the rheology as the material approaches the jamming transition where flow stops. In my talk I will present a microscopic theory for dense suspensions which connect the rheological macroscopic properties with the microscopic scale. I will show that the jamming point controls the rheology of dense suspensions and how the latter is closely related with the elasticity of amorphous materials. The theory allow to predict several critical exponents in good agreement with simple models of suspension flows.

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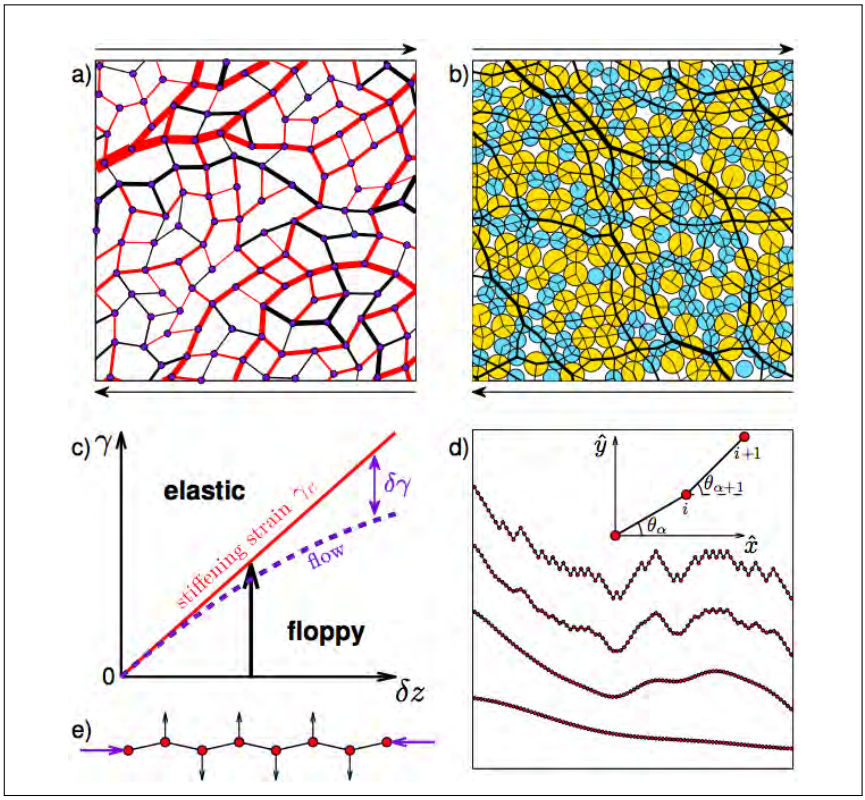

a) A random floppy network under shear deformation approaching the strain-induced jamming transition; the thickness of the lines connecting the particles are proportional to the tension (red) or compression (black). Arrows indicate the direction of the shear. **b)** Snapshot of a contact force network in the affine solvent model model of suspension flow[2], close but below the jamming threshold.

Andy Kraynik **10:05 – 10:25**

Polyhedral Bubble Packing in Sheared Random Foams

Andrew M. Kraynik,* Myfanwy E. Evans,
Klaus Mecke, and Gerd E. Schröder-Turk

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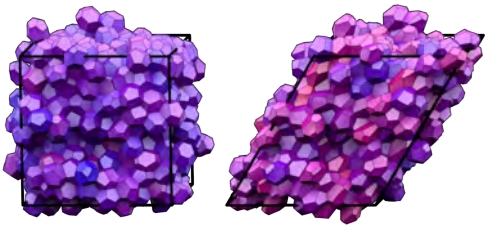
The shape and topology of polyhedral bubbles in random monodisperse soap froth [1] that undergoes quasistatic simple shearing flow is investigated by analyzing Surface Evolver simulations of spatially periodic foams [2]. Elastic-plastic behavior is caused by irreversible topological rearrangements (T1s) that occur when Plateau's law's are violated; the first T1 determines the elastic limit and frequent T1 avalanches sustain the yield-stress plateau at large strains. The stress and shape anisotropy of individual cells is quantified by Q, a scalar derived from an interface tensor that gauges a cell's contribution to the global stress. The average Q when the global stress is isotropic is a significant fraction of the average Q typical of the yield-stress plateau; however, the individual cells that are randomly oriented to achieve isotropic stress become more aligned in the stress plateau. We will also compare and contrast the topological statistics of individual cells and the entire foam during isotropic stress and yield-stress conditions.



A dry liquid foam with 512 cells per periodic unit cell at strains of 0 and 0.6 respectively. The cells are colored by Q, a scalar measure of cell distortion, where blue through red symbolizes values 0 through 1. The average Q over all cells are 0.244 and 0.425 respectively [2].

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Jonathan Kollmer **11:00 – 11:20**

Polydirectional Stability of Granular Matter

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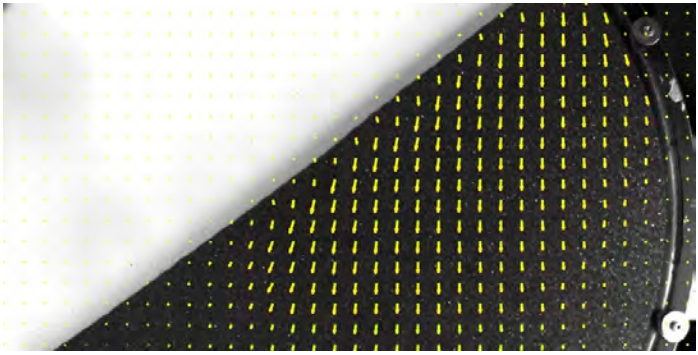

We investigate jammed granular matter in a slowly rotating drum partially filled with poly-disperse sharp-edged granular material and find a state of poly-directional stability [1]. In this state, the material responds elastically to small stresses in a wide angular interval (in our case of up to 230 degrees), while it responds by plastic deformation when subjected to small stresses outside this interval of directions. In our experiment this lead to the bulk of the material compacting by up to 6 percent. The state of poly-directional stability complements the fragile state [2], where the material responds elastically to small applied stresses only in a certain direction but even very small stresses in any other direction would lead to plastic deformations. Similar to fragile matter, poly-directionally stable matter is created in a dynamic process by self-organization.

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Richard Gerum **11:20 – 11:40**

Origin of traveling waves in an emperor penguin huddle

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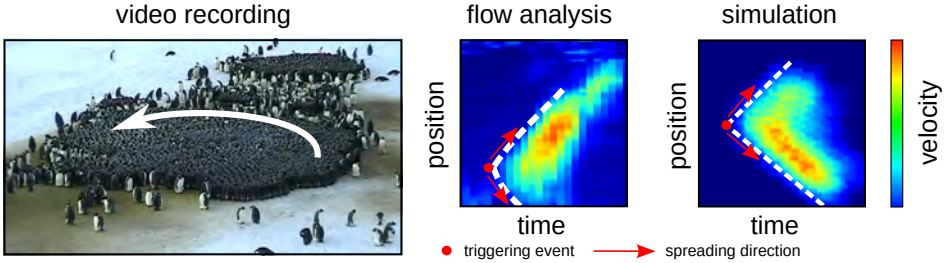
[5] *Alfred-Wegener-Institut Helmholtz-Zentrum fr Polar- und Meeresforschung, Bremerhaven, Germany*



Optical flow analysis of traveling wave dynamics. (left) Circular huddle with counter-clockwise (white arrow) rotational movements (copyright M. Beaulieu and A. Ancel, CNRS/IPEV). The flow velocity magnitude is column-wise averaged in the y direction over the lower half of the huddle. (middle) Optical flow velocities in the huddle, white lines indicate wave fronts. (right) Kymograph of huddle movements in the simulation.

Emperor penguins breed during the Antarctic winter and have to endure temperatures as low as -50°C and wind speeds of up to 200 km/h [2, 3]. To conserve energy, they form densely packed huddles with a triangular lattice structure [4, 5]. Video recordings from previous studies revealed coordinated movements in regular wave-like patterns within these huddles [6]. It is thought that these waves are triggered by individual penguins that locally disturb the huddle structure, and that the traveling wave serves to remove lattice defects and restore

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order. The mechanisms that govern wave propagation are currently unknown, however. Moreover, it is unknown if the waves are always triggered by the same penguin in a huddle. Here, we present a model in which the observed wave patterns emerge from simple rules involving only the interactions between directly neighboring individuals, similar to interaction rules found in other jammed systems, e.g. between cars in a traffic jam [7]. Our model predicts that a traveling wave can be triggered by a forward step of any individual penguin located within a densely packed huddle. This prediction is confirmed by optical flow velocimetry of video recordings of emperor penguins in their natural habitat.

Acknowledgments: Field work at Durmont d'Urville during the winter 2005 was financially and logistically supported by the Institut Polaire Francais Paul-Emile Victor and the Terres Australes et Antarctiques Francaises. We also thank Yvon Le Maho, Cline Le Bohec for encouragement, support and valuable discussions. This work was supported by DFG grant FA336/5-1.

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Balazs Szabo **11:45 – 12:05**

Packing and ordering of particles under shear

Balázs Szabó,[1,*] Sandra Wegner,[2] Ralf Stannarius,[2]
Ellák Somfai,[1] János Török,[3] and Tamás Börzsönyi[1]

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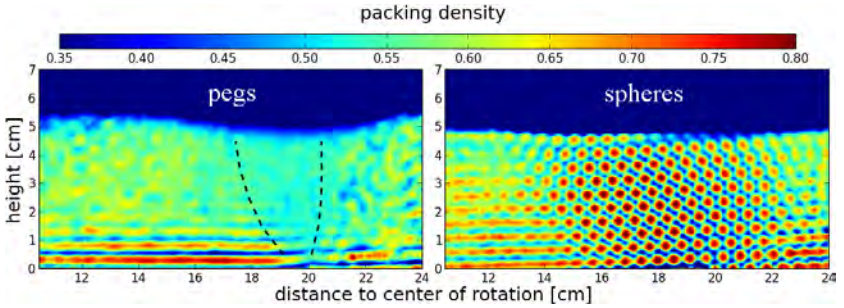

Packing densities in a split-bottom shear cell for wooden pegs (left) and airsoft balls (right) in the stationary state. For pegs the competition of the Reynolds dilatancy and the orientational ordering leads to a depression of the surface above the well oriented region (dashed lines) while neighbouring parts still show the effect of dilation in the form of heaps. For grains with isotropic shapes, the surface remains rather flat.

A granular material exposed to shear shows a variety of unique phenomena: Reynolds dilatancy [1], positional order and orientational order effects may compete in the shear zone. We study granular packing consisting of macroscopic prolate, oblate and spherical grains and compare their behaviour. X-ray tomography and optical imaging are used to determine the particle positions and orientations in a cylindrical split bottom shear cell [2]. Packing densities and the arrangements of individual particles in the shear zone are evaluated. For anisometric particles, shear induced alignment is observed [3, 4]. The preferred orientation forms a small angle with the streamlines, independent of shear rate across three decades. For a given particle shape, this angle decreases with

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increasing aspect ratio of the particles. The shear-induced alignment results in a considerable reduction of the effective friction of the granular material. Focusing on the packing density of these systems, we observe the competition of two opposite effects [5]. On the one hand, the sheared granules are dilated, on the other hand the particles reorient and align with respect to the streamlines. Even though aligned cylinders in principle may achieve higher packing densities, this alignment compensates for the effect of dilatancy only partially (left figure). Perfect monodisperse spheres crystallize in the shear zone (right figure), whereby positional order partially overcompensates dilatancy effects. However, even slight deviations from the ideal monodisperse sphere shape inhibit crystallization.

Acknowledgments: Financial support by the Hungarian Scientific Research Fund (grant no. OTKA NN 107737), and the János Bolyai Research Scholarship of the Hungarian Academy of Sciences is acknowledged.

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Gary Delaney **12:05 – 12:25**

Computational Studies of Jamming in Non-Spherical Particle Systems - Linking the Geometrical and the Physical

Gary W. Delaney,[1,*] Fabian Schaller,[2] and Gerd Schröder-Turk[2]

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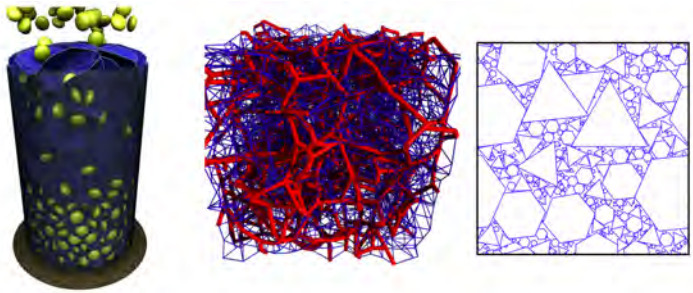
[2] *Theoretische Physik, Friedrich-Alexander-Universität, 91058, Erlangen, Germany.*



(Left) The Voronoi diagram of a sedimenting set of ellipsoids. (Middle) The force network of a set of strings at the onset of rigidity. (Right) Random Apollonian Packing of a mixture of triangles and hexagons.

We carry out a detailed study of jamming in systems of non-spherical particles in 2D and 3D, considering a range of inter-particle interaction properties, ranging from perfectly non-frictional grains up to grains with infinite inter-particle friction coefficients. Through a range of geometrical analyses and quantifications of the force network, we quantify the coupling between the geometric and the physical properties of packed jammed granular matter. The systems considered include smooth spherical particles [5], point systems with attractive forces [2] and more complex systems including 3D packings of non-spherical particles [1,3,4], and sets of Random Apollonian Packings composed of mixtures of shapes with infinite size distributions [6,7]. A range of order metrics are employed to quantify the key structural properties of these systems and determine the degree of ordering from the individual particle level up to full macroscopic scales. Correlations between the structural characteristics of the Voronoi diagram for jammed

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ellipsoid packings [8] and the physical forces within the system are investigated.

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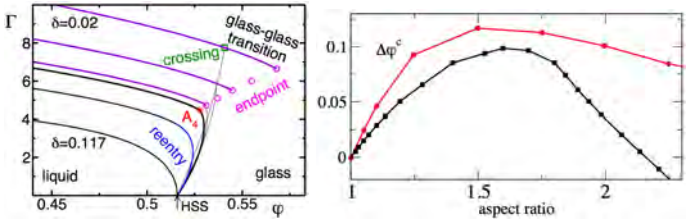
Keynote	Matthias Sperl	14:30 – 15:15

Higher-Order Singularities at the Glass Transition and Random-Close Packing

Matthias Sperl*

Institut für Materialphysik im Weltraum,
Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany

Higher-order glass-transition singularities are implications of the competition between different mechanisms of glassy arrest. Beyond simple liquid-glass transition singularities, higher-order singularities involve transitions between different glassy states. Such transitions are known for attractive [1] (see figure) and repulsive systems [2], as well as for mixtures [3].



Glass-transition diagram of the square-well system (left). The interplay between attraction and repulsion causes glass-glass transitions [1]. Increase of the transition packing fraction beyond the hard-sphere value for ellipsoids (right) at the glass transition (squares [5]) and random-close packing (circles [6]). For increasing aspect ratios, rotational motion arrests for glasses and contact numbers saturate for packings.

When treating the singularity at the transition into random-close packing [4] as the analog of the liquid-glass transition, one can interpret changes in mechanical moduli and in the contact number as indication for higher-order singularities for packings. Such higher-order packing singularities are found in asymmetric binary mixtures where large jumps in mechanical moduli are measured by stress birefringence and sound. Additional glass-glass transitions are found for ellipsoids where on top of already arrested translational motion also the rotation of the ellipsoids arrests for higher aspect ratios. Monitoring the packing of ellipsoids [6], one identifies the saturation of the contact number at aspect ratios corresponding to the glass-glass transition line.

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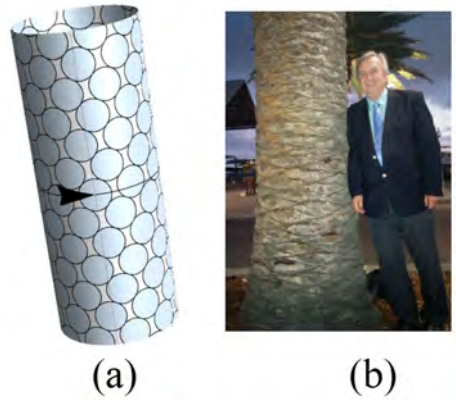
Denis Weaire **15:15 – 15:35**

Phyllotaxis and the cylindrical packing of disks

Denis Weaire[1] and Adil Mughal[2,*]

[1] *School of Physics, Trinity College Dublin & Gledden Fellow, UWA, Spring 2014*
[2] *Theoretische Physik, Fried.-Alex.-Universitat Erlangen-Nurnberg & Institute of Mathematics and Physics, Aberystwyth University*

Phyllotaxis (the growth pattern of plants) has a long and confusing history. The common occurrence of the Fibonnaci numbers (1,1,2,3,5,8,15...) in the analysis of the spiral arrangements of buds and branches along a stem has proved irresistibly attractive to biologists, mathematicians and even physicists. (They rarely understand each other and have different ideas of what constitutes an "explanation".) Despite hundreds of publications, it is doubtful whether the phenomenon is well understood: many websites still speak of "mystery". We review some of this history and offer yet another "straw in the wind" to the never-ending debate. It is based on our theory and simulations of optimal hard-disk packings on a cylinder [1].



(a) Wrapping of a regular lattice onto a cylinder which can be described using phyllotactic principles (b) Phyllotaxis in Perth

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Kai Huang **15:35 – 15:55**

Assembly of Driven Wet Grains: From Spheres to Hexagons

Kai Huang,* Christopher May, Michael Wild, and Ingo Rehberg

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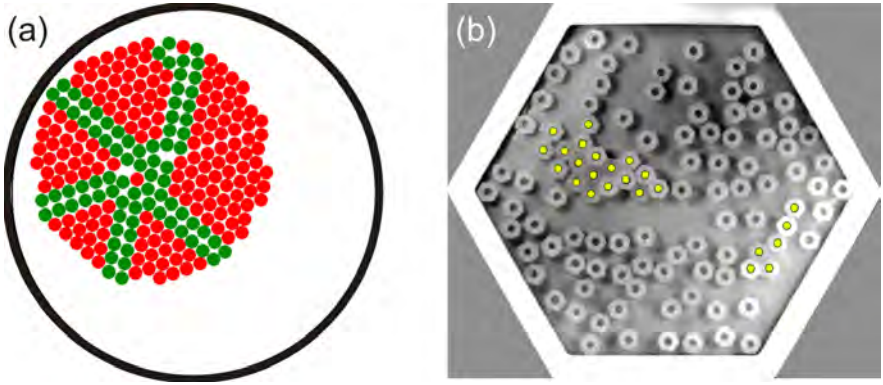
Agitated wet granular matter can be considered as a nonequilibrium model system for phase transitions, where the macroscopic particles replace the molecules and the capillary bridges replace molecular bonds. Using such a model system, we would like to address experimentally the influence from shape on the self-organization of particles into ordered states: A universal phenomenon appearing widely in nature, ranging from thermally driven molecules or colloids [1, 2] to athermal systems such as animal groups [3].

Starting from spherical particles, we demonstrate that a mono-layer of wet granular crystal under horizontal swirling motion melts from its free surface, preceded by an amorphous state. The transition into the surface melting state, as revealed by the bond orientational order parameters, behaves like a first order transition, with a threshold being traceable to the rupture energy of a single capillary bridge [4]. In the amorphous state, the fluctuations of the effective length of the



a) A wet granular crystal of spheres driven by horizontal agitations. The particles are color coded by their local orientational order. b) Clustering of wet granular hexagons under vertical agitations. The particles marked with yellow are bonded with each other via the formation of liquid bridges at the contact surfaces.

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'cracks' inside the wet granular assembly, as shown in Fig. 1a, exhibits a '1/f' noise, suggesting that self-organized criticality (SOC) may take place before the surface layers start to melt.

Continuing with hexagonally shaped particles under vertical agitations, we demonstrate how the shape influences the collective motion. The particles are covered with a thin liquid film so that short ranged cohesive force may arise from the formation of capillary bridges between contacting surfaces. In contrast to agitated spherical particles, the hexagonal shaped particles exhibit a strong tendency to spin around its vertical axis, i.e., acting as self-propelled rotors. This type of self-propelled motion is found to hinder the binding of particles through the formation of capillary bridges and hence give rise to dramatically different dynamics towards clustering and crystallization of the particles, as shown in Fig. 1b. The time evolution toward various non-equilibrium steady states of such a granular system will be presented.

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Keynote	Tomaso Aste	16:30 – 17:15

Jamming matter: local geometry and global properties

Tomaso Aste,[1,*] Antonio Coniglio,[2] Gary W. Delaney,[3] and Tiziana Di Matteo[4]

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There are many systems, such as molecular liquids, colloids, granular materials, foams and others that by changing the control parameters exhibit a very slow dynamics followed by a structural arrest or quasi structural arrest into a 'jammed' state [1–3]. Understanding the origin of this glass transition –or jamming– from a fluid/soft phase to a rigid/solid state is a major and still unsolved challenge [1].

In [4–6] we introduced a 'cell theory' that combines the ideas of inherent structures, free-volume theory and geometrical packing properties to derive a general theory to understand the complex dynamics of glass-forming liquids, granular packings and amorphous solids. The main feature of this theory is the demonstration that thermodynamical properties of these systems can be retrieved from the study of geometrical and topological properties of their local configurations only.

The original cell theory predicted the local volumes around each particle to be distributed exponentially. However, experimental observations and simulations reveal that the Voronoï volumes around each particle are distributed accordingly with a k-Gamma distribution [7–9]

$$p(v) = \frac{k^k}{\Gamma(k)} \frac{v^{k-1}}{\bar{v}^k} \exp\Big(- k\frac{v}{\bar{v}}\Big) \quad . \tag{1}$$

We recently discovered that by extending the original cell theory considering that only a fraction $1/\lambda$ of grains/particles can participate to the internal rearrangement of the material, we can retrieve the k-Gamma distribution for the Voronoï volumes. The parameter k in Eq.1 is related to the portion of jammed grains/particles: $k = k_0 + \lambda$ with k_0 a small constant.

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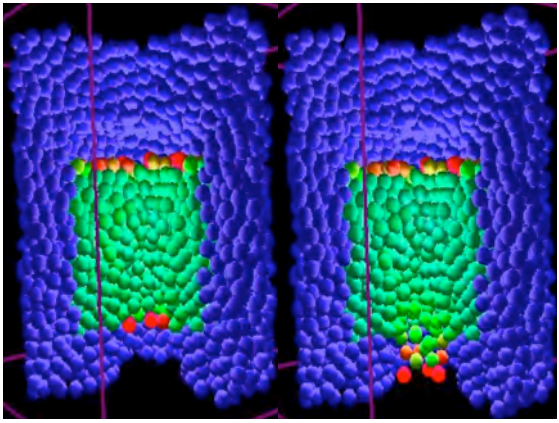

Representation of local Voronoï volumes changes occurring when a jammed granular packing starts unjamming. This is a DEM simulation from a tomographic image of a real experimental packing.

This provides us a very significant insight on the origin of the k-Gamma distribution and links together the properties of granular materials with the ones of glasses. The idea being that in both systems, when density increases, larger and larger regions must cooperate in order to have the structure rearranged. Ultimately, when the region becomes infinitely large (larger than the container), this leads to a structural arrest into a jammed state. We investigate these ideas both by comparing our prediction for relaxation times in structural glasses with experimental data and by looking at simulations of granular flow and jamming/unjamming experiments [10] (see figure).

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chair: Tomaso Aste

9:00 – 9:45	**Tobias Kraus**	*Order and disorder, mobility and interaction in nanoparticle agglomeration*
9:45 – 10:05	**Claus Heussinger**	*Shear thickening and jamming at finite stress: frictional vs frictionless particles*
10:05 – 10:25	**Jeffrey Aguilar**	*Jamming and added mass effects enable high jumps on granular media*

coffee break

chair: Gary Delaney

11:00 – 11:45	**Corey O'Hern**	*Hypocoordinated solids in particulate media*
11:45 – 12:05	**Yujie Wang**	*X-ray tomography study of the random packing structure of ellipsoids*
12:05 – 12:25	**Takenobu Nakamura**	*A characterization of the amorphous silica structure by persistent homology*

lunch break

chair: Yujie Wang

14:30 – 15:15	**Hans Herrmann**	*Rolling and synchronization in dense packings of spheres*
15:15 – 15:35	**Nick Rivier**	*Getting out of a (deep) jam*
15:35 – 15:55	**Jens Boberski**	*Local elastic fields in sheared solids*

Closing remarks

Keynote	Tobias Kraus	09:00 – 09:45

Order and disorder, mobility and interaction in nanoparticle agglomeration

Tobias Kraus*

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Microscopic solid particles tend to agglomerate. Molecular ligands can stabilize their liquid dispersions, but agglomeration frequently occur during processing. Can we understand and control agglomeration? Can we use it to structure particle-polymer composite materials? I will discuss experiments in which we observe the agglomeration of particles with diameters below 10 nm in organic solvents, analyse agglomerate structures, and bias particle arrangement systematically.

The particles that we use are Brownian and very uniform, often with standard deviations of the mean diameter below 5%. And yet, their agglomerates are usually disordered. Short-range interactions prevent the particles from reaching dense packings. Crystalline agglomerates form only when the mobility of particles in the agglomerates is sufficient. If ligands do not provide at least some mobility, crystalline arrangements do not occur.

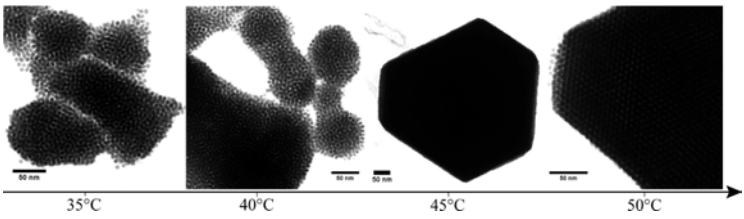

Fig. 1: Temperature-dependant agglomerate morphologies. Gold spheres with a diameter of 6 nm with a dense coating of hexadecanethiol form crystalline agglomerates above a certain temperature when their dispersion is destabilized by a polar solvent.

For example, we used gold spheres with diameters of 6nm that we coated with alkylthiol ligands [1]. The ligands form dense layers on the particle surfaces in which the alkyl chains interact. Their agglomerates were amorphous unless

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we increased the temperature until the ligand layer became liquid. Above this melting temperature, crystalline bodies formed (Figure 1).

Crystalline agglomeration at high temperatures seems to be driven solely by the lower energy of dense packings. We suggest that solid ligand layers prevent crystalline particle arrangement because they create local traps in the energy landscape [2]. Other experiments suggest that incomplete ligands shells generate traps that cannot be ameliorated via temperature: in particles where parts of the ligand shell had been removed, no crystalline agglomerates were formed at any temperature.

Agglomeration experiments in bulk are inherently complex. Agglomerates form in a wide size range, they coalesce and sediment. A new experimental system, inspired by classical experiments on homogeneous nucleation in droplets, relies on oil-in-water emulsions where small particles are confined inside the oil droplets (Figure 2). The oil phase consists of an organic solvent (for example hexane) with a partial pressure that is sufficient to slowly evaporate it while staying in emulsion. Optical spectroscopy and x-ray scattering can follow the agglomeration processes in the emulsion droplets [3].

Inside the droplets, agglomerates form. We found conditions at which the agglomerates had neither random dense nor crystalline structure (Figure 3). The particle arrangement reminded of argon or noble metal clusters. Such supraparticles only formed in emulsion stabilized by suitable surfactants. I will discuss the role of the liquid-liquid interface on the mobility of the particles.

If particles move inside agglomerates, do they also move in layers and materials? We use variants of dynamic light scattering to estimate the (slow) motion of particles in dry layers. Coherent light that has been reflected from a dense particle layer carries information on overall mobility, and we study the slow correlations that exist in dry particle films. Optically anisotropic particles such as metal nanorods depolarize light. Their dynamic depolarization is a probe to rotation. We use it to observe the freezing of particles during material formation [4].

Mobility and interaction of nanoparticles are closely linked to their microscopic arrangement in agglomerates and in materials. The link between particle (including ligand) structure and this mobility is subtle. Investigating it is fundamentally interesting and helps understand the long-term stability of particle-based materials.

The author acknowledges crucial contributions from members of the Structure Formation Group at INM, in particular Johann Lacava and Philip Born, funding from the Deutsche Forschungsgemeinschaft, BMBF, DAAD, and INM. The continuous support of Prof. Eduard Arzt is gratefully acknowledged.

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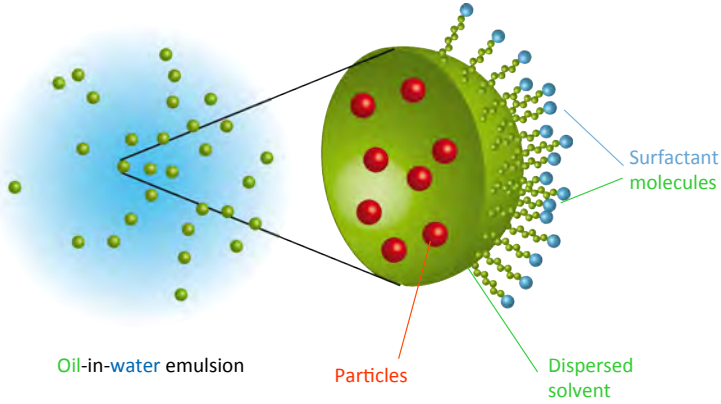


Fig. 2: Particles confined in an emulsion droplet. The particles are stabilized by ligands (not shown), the droplets of the emulsion are stabilized by surfactant molecules.

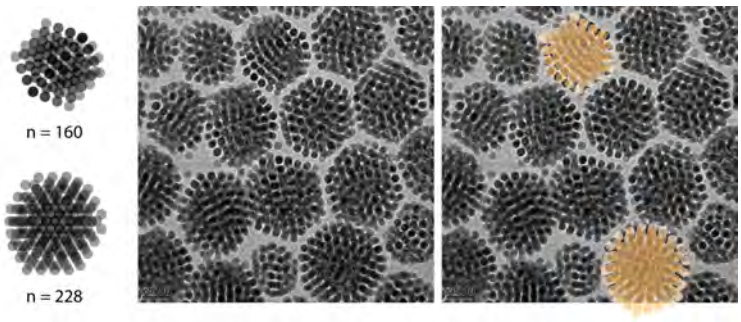


Fig. 3: Gold nanoparticles confined inside the droplets of an oil-in-water emulsion form supraparticles under certain conditions. The figure shows electron micrographs of a dense monolayer that the supraparticles formed on a surface. Two supraparticles are compared to theoretical structures shown on the left side.

Claus Heussinger 09:45 – 10:05

Shear thickening and jamming at finite stress: frictional vs frictionless granular particles at the fluid-to-solid jamming transition

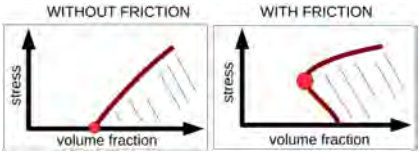
Claus Heussinger*

Institute for Theoretical Physics, University Göttingen

The jamming paradigm for fluid-to-solid transitions aims at providing a unified view for the elastic and rheological properties of materials as different as foams, emulsions, suspensions or granular media. The usefulness of such a unifying concept hinges on the presence or absence of phenomena that are in some sense universal.

In this contribution, we will approach the jamming transition from the fluid side, by monitoring the flow properties as the jamming transition is approached.

In particular, we will be concerned with the effect of frictional forces and show how the jamming phase diagram has to be modified as compared to the frictionless scenario (see figure). Essential findings are a discontinuous and hysteretic jamming transition that features jamming at finite stress as well as re-entrant fluid flow. All these features are absent in frictionless systems. Finally, in the fluid phase the frictional system displays a pronounced shear-thickening regime, where frictionless particles are generically shear thinning.



Jamming phase diagram (shear stress vs. particle volume fraction) as determined from simulations of steady shear flow. In the jammed phase non-flowing states with finite shear stress exist. Without frictional interactions between the particles a jammed state can be unjammed by increasing the stress. In contrast, with frictional interactions a flowing state can be brought to jam by increasing the stress.

Acknowledgments: Financial support from the DFG via the Emmy Noether group He 6322/1-1 is acknowledged.

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Jeffrey Aguilar 10:05 – 10:25

Jamming and added mass effects enable high jumps on granular media

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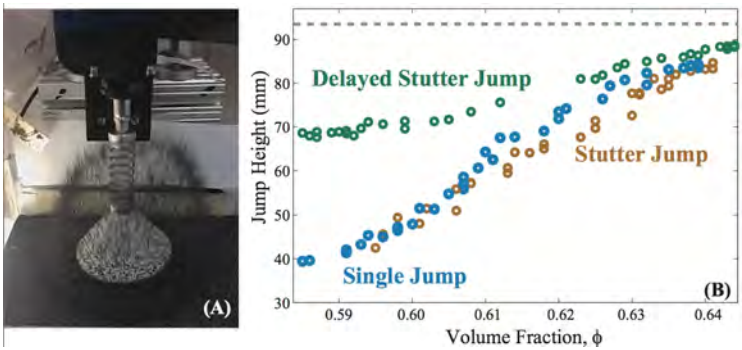
[2] *Georgia Tech School of Physics*



(A) Experimental jumping robot apparatus. (B) Experimental jump heights of 3 different jump types at a sweep of volume fractions from loose to close-packed. Gray dashed line represents the hard ground jump height for all jump types.

Various animals exhibit locomotive behaviors (like sprinting and hopping) involving transient bursts of actuation coupled to the ground through internal elastic elements. The performance of such manoeuvres is subject to reaction forces on the feet from the environment. On substrates like dry granular media, the relationships that govern these forces are not fully understood, and can vary with foot size and shape, material compaction and kinematics of intrusion. To gain insight into how such interactions affect jumping on granular media, we study the performance of a self-actuated spring mass robot with a 7.62 cm flat circular foot. We compare performance between two jump strategies: a single-cycle sine-wave actuation (a single jump) and a counter-movement pull-up phase proceeded by a single jump (a stutter jump); on hard ground, both jump methods perform comparably, and the rapid single jump requires greater peak power than the slower stutter jump [1]. We use an air fluidized bed to systematically vary volume fraction ($0.58 < \phi < 0.63$) at fixed actuation parameters for both strategies,

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and find that both of these jumps perform similarly poorly in loose-packed granular media, reaching only 44% of the close-packed jump height. Introducing a delay time between the pull-up phase and the push-off phase of the stutter jump (the delayed stutter jump) results in significantly improved jump heights at low volume fraction, achieving 77% of the close packed height (Fig. 1). A simulation of the robot reveals that a depth and velocity dependent model of granular intrusion force [2][3] is insufficient to reproduce experimental jump heights. To gain insight into the behaviour of the granular media during these impulsive events, we record high speed video of the particle flow around a foot through a transparent sidewall. To monitor grain flow, we adapt particle image velocimetry (PIV) techniques to perform a 2D particle tracking velocimetry (PTV) analysis on these images. This analysis reveals that an approximately conical region of grains below the foot, similar in radius to the foot with a 12° half-angle, moves downward with comparable speed to the foot. The flow field is reminiscent of observations of a jammed flowing region in a suspension of corn starch in water [4], which leads to impulsive interaction forces dominated by added mass effects. When this physics is included in the model, agreement between experiment and theory improves for all jump methods.

Acknowledgments: This work is funded by NSF POLS CAREER, Burroughs Wellcome Fund, and ARO. Special thanks to Paul Umbanhowar, Nick Gravish, Yang Ding, Professor Harvey Lipkin, and Andrei Savu.

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Keynote	Corey O'Hern	11:00 – 11:45

Hypocoordinated Solids in Particulate Media

Thibault Bertrand,[1,2] Carl F. Schreck,[3] Corey S. O'Hern,[1,2,3,4,*] and Mark D. Shattuck[1,5]

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The vibrational response of conventional solids, such as metals, ceramics, and minerals, can be described by the harmonic approximation at sufficiently low temperatures compared to the melting points. Nonlinearities stemming from weak structural disorder and the shape of the interaction potential explored at low temperatures can be treated as small perturbations. Particulate systems, such as granular media and colloids, can also exist in solid-like states in the limit of weak driving or thermal fluctuations. However, in contrast to molecular-scale solids, where interactions extend beyond one atomic diameter, the interactions in many particulate solids are purely repulsive and vanish when particles come out of contact.

Even small changes in the contact network in purely repulsive particulate solids (both crystalline and disordered) can give rise to strong nonlinearities in the vibrational response [1, 2]. This occurs whenever the number of instantaneous contacts between particles is less than the number of degrees of freedom in the system, which causes zero eigenvalues in the dynamical matrix. Such contact-breaking nonlinearities do not occur in conventional solids with interactions that extend well beyond a particle diameter because there are significantly more interactions in these systems than degrees of freedom.

We propose a 'phase diagram' for particulate systems with purely repulsive contact forces, such as granular media and colloids[3]. We identify two classes of behavior in the $\Delta\phi$ and T_0 plane near jamming as shown in Fig. 1: iso- and hypocoordinated solids (ICS and HCS), which are distinguished by the time-averaged

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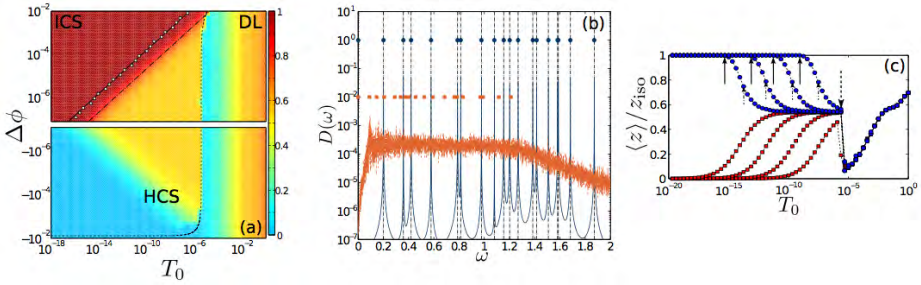

(a) 'Phase diagram' for the vibrational response of MS packings versus $\Delta\phi$ and T_0 illustrated by heating and compressing (or decompressing) a single, illustrative $N = 10$ packing at $\Delta\phi = 0$ and $T_0 = 0$. The shading gives the time-averaged contact number $\langle z\rangle/z_{\rm iso}$. For $0 < \Delta\phi < \Delta\phi_c(T_0)$ (data and scaling curve given by open squares and solid line), the contact network for the 'ICS' does not change from that at $T_0 = 0$ and the vibrational response is strictly harmonic. The midpoint T_0 at which $\langle z\rangle/z_{\rm iso}$ crosses over from 1 to 0.5 defines the boundary $\Delta\phi_+(T_0)$ (dot-dashed line with slope 0.5). In the 'HCS', the contact network fluctuates with $\langle z\rangle/z_{\rm iso} < 1$, but there are no particle rearrangements as in the 'DL' regime with $\Delta\phi < \Delta\phi_{cb}(T_0)$ (dashed line). (b) $\langle z\rangle/z_{\rm iso}$ versus T_0 for a single, illustrative $N = 10$ packing compressed (decompressed) to $\Delta\phi = \pm 10^{-7}$, $\pm 10^{-6}$, $\pm 2 \times 10^{-5}$, and $\pm 2 \times 10^{-4}$ (circles and squares) from left to right. The solid, dot-dashed, and dashed arrows indicate $\Delta\phi_c(T_0)$, $\Delta\phi_+(T_0)$, and $\Delta\phi_{cb}(T_0)$. (c) Comparison of portions of the density of vibrational frequencies $D(\omega)$ from the Fourier transform of the velocity autocorrelation function (lines) and associated with the dynamical (vertical dot-dashed lines) and displacement correlation matrices (symbols) for ICS at $\Delta\phi = 2 \times 10^{-7}$ and $T_0 = 4 \times 10^{-19}$ (blue solid lines and circles) and HCS at $\Delta\phi = 2 \times 10^{-7}$ and $T_0 = 2 \times 10^{-11}$ (orange dashed lines and squares) for $N = 10$

contact number $\langle z\rangle$ and density of vibrational modes $D(\omega)$. For the ICS, with $\Delta\phi > \Delta\phi_c(T_0) > 0$, the contact network does not change from that at $T_0 = 0$, the contact number remains at the isostatic value, $\langle z\rangle = z_{\rm iso}$, and the vibrational response is harmonic with strong peaks in the Fourier transform of the velocity autocorrelation function at the dynamical matrix eigenfrequencies. HCS occur both above and below ϕ_J in the region defined by $\Delta\phi_+(T_0) > \Delta\phi > \Delta\phi_{cb}(T_0)$. In HCS, the network of interparticle contacts fluctuates with $\langle z\rangle/z_{\rm iso} < 1$, the vibrational response is strongly nonharmonic, and the form of $D(\omega)$ depends on the measurement method. In the regime $\Delta\phi < \Delta\phi_{cb}(T_0)$, cage-breaking particle rearrangements occur and $D(\omega)$ resembles that for dense liquids (DL).

Acknowledgments: We acknowledge support from the National Science Foundation (NSF) Grant No. CBET-0968013 (MS), Defense Threat Reduction Agency Grant No. 1-10-1-0021 (CO and TB), and seed funding from NSF MRSEC DMR-1119826 (CO and TB).

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Yujie Wang **11:45 – 12:05**

X-ray tomography study of the random packing structure of ellipsoids

Chengjie Xia,[1] Yixin Cao,[1] Binquan Kou,[1] Jindong Li,[1] Xianghui Xiao,[2] Kamel Fezzaa,[2] and Yujie Wang[1,*]

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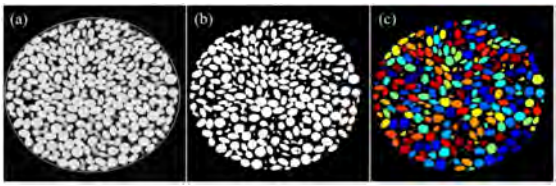

Cross-sections of (a) a raw image, (b) a binary image, and (c) a segmented image.

We study the random packing of ellipsoids using X-ray tomography. The local structure of the ellipsoid packing displays short-range correlations. In addition to the contact number Z, we introduce ρ_{shell}, the average contact radius of curvature for contacting neighbors, as an additional parameter to characterize the local orientational geometry. In general, we find that the local free volume w is affected by both Z and ρ_{shell},. We believe that the particle asphericity induces a polydispersity effect to influence the packing properties. We finally introduce a model which can explicitly map the ellipsoid packing onto a polydispersed sphere one, and it reproduces most of the experimental observations. Additionally, we will present results on the structural differences between dry and wet granular packings witch suggests different dynamic arrest mechanism for system with and without attractive interactions.

The use of the APS was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357, and the work is supported by the Chinese National Science Foundation no. 11175121, and the National Basic Research Program of China (973 Program; 2010CB834301).

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Takenobu Nakamura 12:05 – 12:25

A characterization of the amorphous silica structure by persistent homology

Takenobu Nakamura,[1,*] Yasuaki Hiraoka,[2] Akihiko Hirata,[1]
Emerson Escolar,[2] Kaname Matsue,[3] and Yasumasa Nishiura[1]

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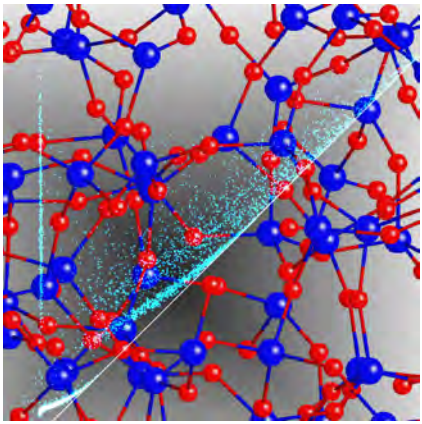
[2] *IMI Kyushu University, Japan*
[3] *The Institute of Statistical Mathematics, Japan*

Different from the perfect crystal, the amorphous material is difficult to characterize an atomic structure by the structure factor or the pair correlation function. This is because amorphous does not show long-range order seen in perfect crystal. Even though amorphous material shows isotropic and uniform structure similar with the liquid in macroscopic scale, it also shows rigidity that is usually accompanied with the atomic-scale order. To extract nontrivial order from the amorphous material, we adapted persistent homology [3] analysis to the atomic configuration of amorphous silica obtained by molecular dynamics simulation [1]. In the presentation, we will show the characteristic of persistent diagram (PD) for the amorphous silica (see figure), which is completely different from the perfect crystal (periodic), or liquid (random), and explain the relation to the medium- and short-range order.



The configuration of amorphous silica obtained by molecular dynamics and the persistent diagram for $d = 1$ (ring).

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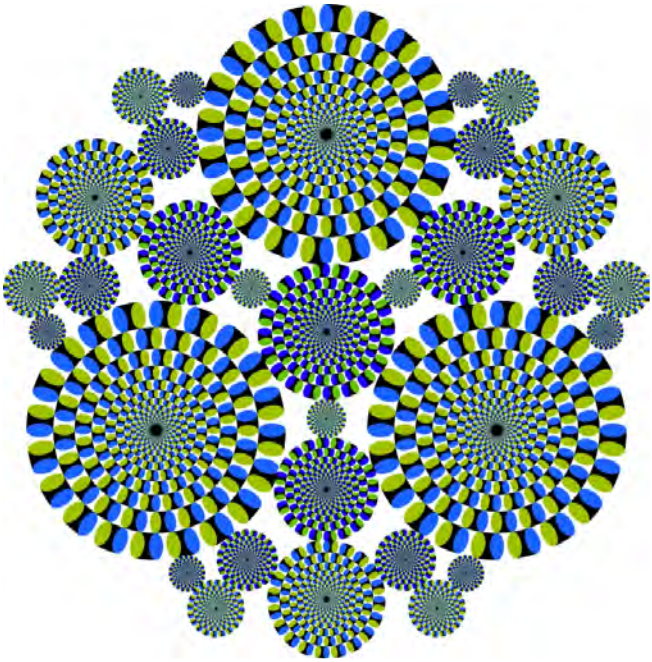
Keynote	Hans Herrmann	14:30 – 15:15

Rolling and Synchronization in Dense Packings of Spheres

Hans Herrmann*

ETH, Zürich

A large family of packing topologies allows for slip-less rotations between touching disks or spheres and thus form systems of bearings. I will discuss their construction and their fractal dimensions. Bearings are mechanical dissipative systems that, when perturbed, relax toward a synchronized (bearing) state. In fact bearings can be perceived as physical realizations of complex networks of oscillators with asymmetrically weighted couplings. Accordingly, these networks can exhibit optimal synchronization properties through ne tuning of the local



Static illusory-motion image of a bearing of 31 discs. Every two touching disks always have opposite senses of rotation.

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interaction strength as a function of node degree. I show that, in analogy, the synchronizability of bearings can be maximized by counterbalancing the number of contacts and the inertia of their constituting rotor disks through the mass-radius relation, m r, with an optimal exponent which converges to unity for a large number of rotors. Under this condition, and regardless of the presence of a long-tailed distribution of disk radii composing the mechanical system, the average participation per disk is maximized and the energy dissipation rate is homogeneously distributed among elementary rotors. The synchronization of rotations occurs in avalanches following a broad size distribution. The bearing configurations also fulfill Kolmogoroff scaling and display Richardson's diffusion law in the limit of small Stokes numbers and constitute also an interesting toy model for turbulence.

Nick Rivier **15:15 – 15:35**

Getting out of a (deep) jam

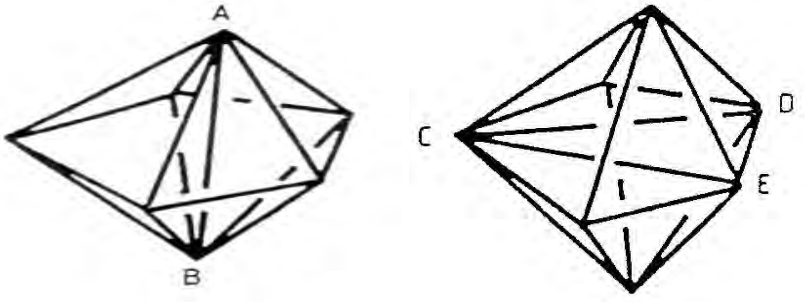
Nick Rivier*

IPCMS, Université de Strasbourg

How? By using (Poisson) shear, dilatancy and dislocation glide.

The densest packing of a hard, dry granular material (modelled as hard spheres of equal radius and infinite tangential friction that forces the grains to roll without slip on each other, or to lose contact) is a geometric, many-body optimisation problem with solutions on the boundary of configuration space:

Physical contacts between grains are struts of minimal length. The boundary is made of smooth regions (one grain rolling on another), separated by (Pareto) points where the grains are stuck. The optimisation problem consists therefore in identifying the Pareto points in an arbitrary disordered packing and in exploring physically (by shearing) the configuration space in order to reach another Pareto point.



Let us begin with the configuration space of one tetrahedron. Dilatancy (the "paradox" of the wet footprint on the beach, O. Reynolds 1885) is explained simply in a minimal model of the granular material ("sand") packed together as tetrahedra (Delaunay tessellation, the dual of Voronoi's) and making up a graph. Upon external stress, the spheres can either roll on each other without slip - impossible in circuits of odd numbers of grains in contact -, or lose contact with each other. Macroscopic uniaxial stress (the foot's pressure) shears the granular material; it forces the grains to roll on each other and the odd circuits to open up. Each tetrahedron of spheres is distorted into a gauche circuit of

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four contacts (struts) and two opposite and orthogonal extended edges (three possibilities). This distortion of the tetrahedron breaks minimally the triangular circuits of grains in contact, thereby increasing its volume and letting in water that is expelled in the wet footprint left behind.

How do the tetrahedra pack together? Initially with n tetrahedra sharing an edge (n = 3,4,5). Is the distortion consistent throughout the tessellation? Yes (essentially because the dual Voronoi foam is an Eulerian graph). Can disorder be accommodated? Yes (automatically through the Voronoi-Delaunay tessellation). The packing has then only even circuits of struts and each grain can thus roll on its neighbor(s) without slip and explore freely the (boundary of the) configuration space.

For four tetrahedra sharing an edge (the diagonal of an octahedron), the Pareto points are readily identified as local, cubic or hexagonal close-packed configurations (Kepler-Hales). Shear may force an elementary local topological transformation that flips the diagonal and changes neighborhood.

Five tetrahedra sharing an edge constitute a pentagonal dipyramid (see figure). If top and bottom grains are in contact (AB), there is one single, vertical diagonal, a strut that supports the physical contact. Shear forces disconnection and imposes a horizontal, pentagonal circuit with two diagonals (CD and CE), a dislocation that can glide under further shear. (topological annealing). This explains why, in the random close-packed state, 5-rings (in the dual Voronoi foam) are predominant [1].

[1] N. Francois, M. M. Saadatfar, M. Hanifpour, R. Cruikshank, A. Sheppard *Powders and Grains, AIP Conference Proceedings*, **1542**, 369, 2013.

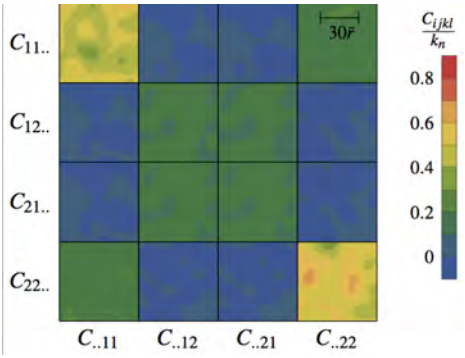
Jens Boberski **15:35 – 15:55**

Local elastic fields in sheared solids

J. Boberski* and D. E. Wolf

University of Duisburg-Essen

Modeling the elastic properties of disordered or granular solids requires a theory of elasticity that takes non-affine deformations into account. The shown method manages this by linearizing the forces around the initial state and calculating the elastic deformations due to an external pertubation. Based on the coarse grained expressions for the local, linear strain and stress fields, a way to calculate maps of the local linear elastic constants for fictional granular packings is presented. This method is used, to study jammed and sheared systems.



Map of elastic tensor components in a jammed packing of frictional disks.[1]

[1] J. Boberski, L. Brendel, D. E. Wolf AIP Conf. Proc. **1542**, 433-436 (2013).

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Poster Contributions

Posters are displayed for the duration of the conference. There is a dedicated **Poster Session** on Tuesday from 11:00am to 12:30pm.

Please take note of the "People's Choice Best Poster Award". Your registration bag contains a ballot slip for your choice of the three best posters. Each poster can be identified by its number on the poster board. Note that you can only vote once for each poster. Please hand in your completed ballot slip by Wednesday's afternoon coffee break. The winners will be announced at close of the last session on Wednesday afternoon.

Poster 1 **Rubitha Srikantharajah**

Defined deposition of anisotropic nanoparticles from liquid phase by a drying process

Rubitha Srikantharajah,* Stefan Schäfer,
Martin Klaumünzer, and Wolfgang Peukert

Institute of Particle Technology, University of Erlangen-Nuremberg,
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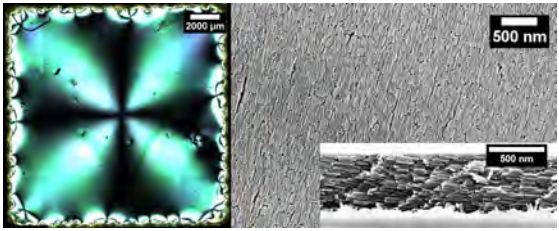

Particulate layer formed by controlled self-assembly of ZnO nanorods (SEM image).

Drying processes are important process steps in liquid phase based methods for the deposition of nanoparticulate thin films [1]. However, heat flux and mass transport during drying of dispersions are complex and, thus, hard to control. The aim of this study was the preparation of densely packed films composed of zinc oxide (ZnO) nano rods. Due to the anisotropic habitus of the ZnO material applied low porosities can be achieved. Minimization of the interparticle distances during drying leads to a maximization of contact area and, thus, to an increase in conductivity of the semiconducting layers formed. To circumvent premature agglomeration the ZnO nano rods showing an aspect ratio of about 15 and a total length of (90 ± 30) nm colloidal stabilization is necessary. Long-term stability over several weeks can be achieved [2]. Deposition of the particles onto substrates is done by two methods: direct deposition from a dispersion droplet and dip-coating. In order to optimize the deposition process the development of an appropriate method to assess the quality of the layers was necessary. The degree of order is determined quantitatively by polarization microscopy as well as scanning electron microscopy (SEM) with subsequent image analysis. The drying rate is varied by controlling temperature ($10°C \ldots 40°C$) and relative humidity ($10\% \ldots 80\%$) using a climate cabinet. Other influencing factors like

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particle-particle and particle-solvent interactions, flow patterns within the film upon formation as well as interfacial energies are studied to tailor and optimize the self-organization process. Quantitative assessment of the aforementioned process parameters allows for reproducible production of self-organized structures in the order of magnitude of cm^2 with high potential for optoelectronic applications [3].

Acknowledgments: The authors gratefully acknowledge the Erlangen Research Training Group 1161 "Disperse Systems for Electronics" and also funding of the German Research Council (DFG), which, within the framework of its 'Excellence Initiative' supports the Cluster of Excellence 'Engineering of Advanced Materials' at the University of Erlangen-Nuremberg.

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Poster 2 **Jochen Schmidt**

A novel process route for the production of LBM polymer powders of small size with good flowability

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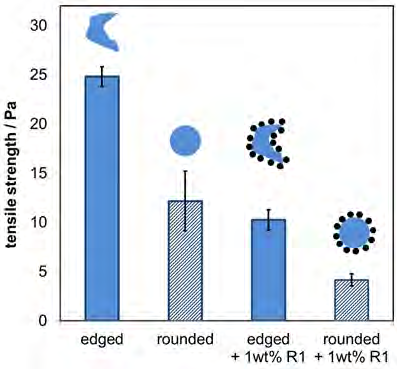
In recent years an increasing demand to widen the field of application has been noticeable: rapid prototyping gradually is transferred to additive manufacturing. Especially laser beam melting processes (LBM) applying polymer powder systems are promising. In the case of LBM basically only polyamide is available as an optimized powder material showing satisfying behavior during processing. In fact, it is challenging to produce powder materials for LBM processes with small particle size, good flowability and processability.



Influence of particle shape and surface functionalization on powder tensile strength: tensile strength of PS particles decreases (flowability increases) with rounding and dry particle coating with silica R1.

In order to expand the variety of materials and the applicable particle size range wet grinding at reduced temperatures is a promising approach [1]. The comminution product consists of microparticles of irregular shape and typically shows

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poor powder flowability resulting in poor device qualities. Within this contribution a novel process route for the production of spherical polymer micron-sized particles of good flowability is discussed [2]. In a first step polymer microparticles are produced by a wet grinding method. The mean particle size and the particle size distribution can be tuned between a few microns and several 10 microns and adapted to specific needs. The micron-sized polymer particles obtained by grinding as intermediate products are cohesive and thus will show poor LBM processability. In a second step the irregular shaped ground product is rounded in a heated downer reactor. It will be demonstrated that the degree of rounding can be controlled by changing the temperature profile or the residence time. The flowability of the spherical polymer microparticles is further improved by a unique nanocoating on the microparticles' surface as a third step.

The increase of powder flowability after the consecutive process steps has been monitored using a tensile strength tester. The improvement of powder flowability after the consecutive process steps is remarkable: rounded and dry-coated polystyrene (PS) powders exhibit a strongly reduced tensile strength (by a factor 5) in comparison to the tensile strength of the edged PS comminution product. Improved product qualities in the LBM process result [3]. The influence of particle habitus, particle size distribution and surface functionalization on powder flowability and properties of the products after the LBM process is discussed.

Acknowledgments: This study has been supported by Deutsche Forschungsgemeinschaft (DFG) within the framework of the collaborative research center SFB 814 "Additive Fertigung" (A1, A2, A3). Financial support is gratefully acknowledged.

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Poster 3 **Moumita Maiti**

Structural aspects of nearly jammed sheared suspensions and comparison with jammed-packings.

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Structural information of nearly jammed – and sheared – suspensions is extracted from the free volume distribution. The free volume of a particle is defined as the geometrically available space to the centre of the particle keeping its' neighbours fixed. At densities not far below close packing, the free-volume distribution has a strong delta peak at zero free volume and a power law tail for 5-10% particles (rattlers). Interestingly, we find that shearing, on average, destroys free volume by comparing with configurations of the same density but decompressed from jammed-packings. In fact, by shearing the structure approaches that of jammed-packings also by comparing the radial distribution function. In this context we further explore the role of rattlers in preserving the structure of sheared configurations due to weak thermalization.

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Poster 4 Patric Müller

Epitaxial Growth of Patchy Coatings on Nanospheres

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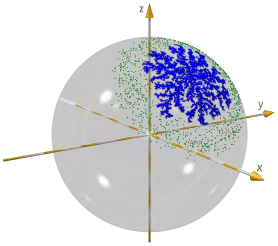
Patchy nanoparticles are characterized by heterogeneous surface properties. The resulting anisotropic chemical and physical behavior makes them interesting for novel applications. Recently a one-pot colloidal method for the facile synthesis of gold and silver patches on silica and polystyrene nanospheres has been described [1–3]. We show that the corresponding patch growth process may be described by diffusion limited epitaxial aggregation on the curved surface of the core particle. The experiments display fast diffusion limited and slow integration limited aggregation leading to either dendritic or continuous cup-like structures. Depending on the parameters our model is able to describe both regimes of aggregation and the associated patch morphology.



Diffusion limited epitaxial aggregation on a spherical surface as a model for the growth of patchy coatings on nanospheres. Preliminary simulation results of a dendritic patch morphology.

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Poster 5 **Ignacio Tejada**

Ensemble theory for deformable granular matter

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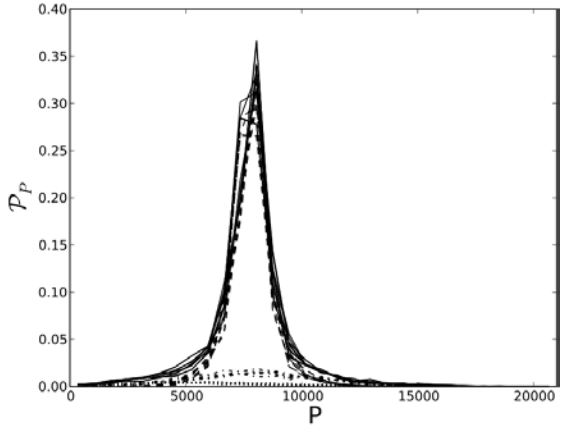
A development of the original athermal statistical mechanics theory proposed by Edwards and co–workers for granular matter is presented. The formalism is useful to compare static and jammed packing of a granular system made of slightly deformable particles. These microstates are seen as statistical distributions in a force-moment (stress multiplied by volume) space. Both the internal and external constraints of the system are considered to explain such distributions.



Statistical distribution of the mean force–moment of ten different packings compressed at the same force–moment state. Solid lines represent the total distribution while dotted lines represent the contribution of configurations having the same number of forces: six (−−), five (−.) and four (..) .

The internal constraints are the intrinsic features of the system (*e.g.* size distribution, friction, cohesion) together with the force–balance condition. In the end, they determine which the possible local states of equilibrium of each particle

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are. Following a principle of equal a priori probabilities, it can be assumed that, when no other constraints are imposed, particles are equally likely to be in any one of these local states of equilibrium. Then a flat sampling over all these local states leads to a non–uniform distribution in the force–moment space. To take into account this fact, density of states functions are used. These functions can be measured, but some of their features can be explored. For instance, the number of states increases monotonically with the mean force–moment value, while the limitations imposed by the intrinsic features often do not depend on it. Furthermore, the possible local states of equilibrium can be classified into configurations to separate the density of states functions, what makes it possible to get more information about the expected features of the system.

The external constraints are those macroscopic quantities controlled by the protocol that explore the microstates. Those ensembles that use quantities which can be expressed as functions of the force-moment, can be analyzed in this space (*e.g.* the force–moment itself, the volume, the elastic energy or the stress). Some assumptions have to be made in order to relate, for instance, the volume or the elastic energy to the equilibrium state, and some symmetries are useful: for instance, the volume depends exclusively on the mean force–moment or, in the case of isotropic stress fields, the statistical weight is independent from the orientation of the field.

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Poster 6 **Roel Baars**

Simulating dense random packings of superquadric particles by the mechanical contraction method

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We investigate random dense packings of non-spherical particles with the mechanical contraction method [1]. Our motivation is the description of packings of anisometric colloidal particles, for example colloidal silica cubes [2]. We employ a superquadric particle shape, allowing for various geometries, e.g. spheres, cuboids, ellipsoids and platelets. In this work in progress, we demonstrate our algorithm, and discuss particle contact detection. We compare our packings, in particular the obtained packing fractions ϕ, with available literature data for well known particle shapes (spheres, ellipsoids, superellipsoids, spherocylinders and platelets) to validate our approach.

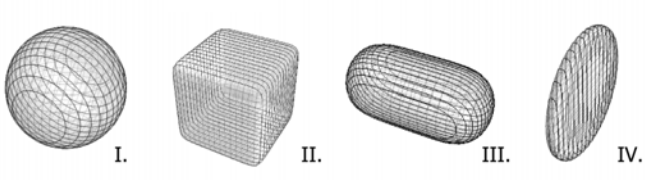

Fig. 1: Several possible superquadric shapes. I. Sphere ($a_1 = a_2 = a_3$, $\gamma_1 = \gamma_2 = \gamma_3 = 2.0$), II. 'Cuboid' ($a_1 = a_2 = a_3$, $\gamma_1 = \gamma_2 = \gamma_3 = 10.0$), III. 'Spherocylinder' ($2a_1 = a_2 = a_3$, $\gamma_1 = 5.0, \gamma_2 = \gamma_3 = 2.0$), IV. 'Platelet' ($a_1 = 10a_2 = 10a_3$, $\gamma_1 = 10.0, \gamma_2 = \gamma_3 = 2.0$)

The superquadric shape is defined by the implicit surface

$$F = \left|\frac{x}{a_1}\right|^{\gamma_1} + \left|\frac{y}{a_2}\right|^{\gamma_2} + \left|\frac{z}{a_3}\right|^{\gamma_3} = 1. \quad (1)$$

The values of a_i scale the particle along its principal axes and γ_i determines the shape of the particle. Figure 1 shows several possible superquadric particle shapes. We restrict ourselves to convex particles, because of the available contact

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detection algorithms. No analytical expression is known for the shortest distance between two superquadrics, so that a non-linear numerical optimization scheme is required (e.g. [3]).

Figure 2 shows a typical simulation result for cuboid-like shape ($N = 1000$ particles) and a comparison with earlier simulations by Jiao [4], showing only a slight discrepancy to lower ϕ.

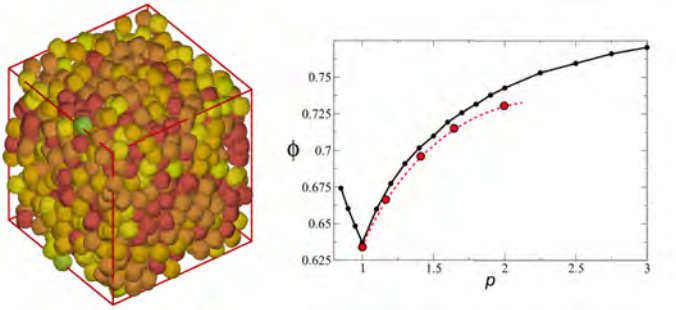

Fig. 2 : (Left) a typical result from the mechanical contraction method of superquadric particles. (Right) a comparison with data from [4] ($p = \gamma/2$). The dotted line is added as a guide for the eye.

Acknowledgments: This research is supported by the Dutch Technology Foundation STW, which is part of the Netherlands Organisation for Scientific Research (NWO), and which is partly funded by the Ministry of Economic Affairs. "SMART Separations for complex system" programme.

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Poster 7 **Fengxian Fan**

Numerical Simulation of Hydrodynamic Effects on $PM_{2.5}$ Interactions in Acoustic Agglomeration

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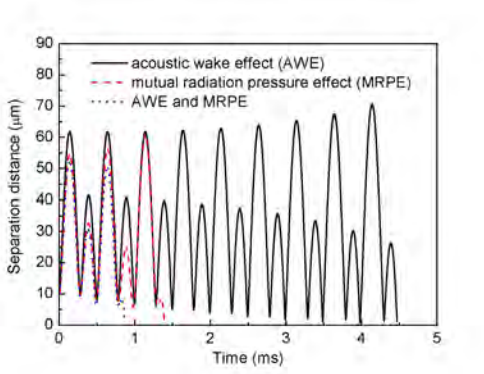

Separation distances in $PM_{2.5}$ interaction processes

Increasing attention has been paid on $PM_{2.5}$ due to their adverse effects on human health and the environment. Since the existing particulate separation devices are still not efficient enough in capturing these particles, a large amount of $PM_{2.5}$ from power plants and industrial sources are emitted into atmosphere. It has been expected that the collection efficiency of $PM_{2.5}$ particles can be improved by means of acoustic agglomeration. The particle interaction mechanisms in acoustic agglomeration consist of the gravitational effect induced by the difference in settling velocity of the particles, the orthokinetic effect due to the viscous entrainment of the incident wave, and hydrodynamic effects which include the acoustic wake effect generated by the disturbance of the flow field due to the presence of the particle and the mutual radiation pressure effect caused by the scattered wave [1,2]. Theoretical studies show that the acoustic wake is much

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more important than the mutual radiation pressure effect [3]. However, the particles used in the studies are greater than 4 μm, which are too big to represent the $PM_{2.5}$ particles. Recently Zhang et al [4] numerically simulated the interaction of $PM_{2.5}$ particles, but in their work only the hydrodynamic interaction due to the acoustic wake effect is considered. Thus studies on $PM_{2.5}$ interaction under both the acoustic wake and the mutual radiation pressure effect are necessary.

In this work we modelled and simulated the interaction of two $PM_{2.5}$ particles in a horizontal standing-wave acoustic field. The separation distances between the particles under the influence of different hydrodynamic effects are given in the figure. The results show that the time needed for particle collision is 4.5, 1.4 and 0.86 ms under the acoustic wake effect, the mutual radiation pressure effect and the above two effects, respectively. It indicates that the mutual radiation pressure effect is much more significant than the acoustic wake effect in the simulation case (particle density: 2400 kg/m^3; particle diameters: 0.5 μm and 2 μm; acoustic intensity: 150 dB; frequency: 2000 Hz; orientation angle: 90^o). The combination of the hydrodynamic effects effectively promotes the interaction and collision of $PM_{2.5}$.

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Poster 8 **Ellen Fischermeier**

Dynamical States in Driven Colloidal Liquid Crystals

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The driving of liquid crystals by external potentials is a common phenomenon in many electro-optical applications [1]. Those Liquid crystals can be either comprised of anisotropic molecules or colloidal particles. The advantage of the latter is the fact that they can be experimentally studied by direct observation in real space. In theoretical studies computer simulations have been established as a useful tool to evaluate such complex systems.
In this work we investigate a system of hard spherocylinders with a Langevin dynamics simulation using the pe-physics engine [2]. The bulk phase behavior of this simple model system for rod-like colloidal liquid crystals depends solely on packing fraction and aspect ratio of the particles [3]. We choose a length to diameter ratio of five and evaluate the response of the system at different packing fractions to an aligning potential V_{ext}. It defines a preferred direction of alignment u_0 that rotates in the x-y-plane at a frequency ω_0: $\vec{u}_0(t) = (\cos\omega_0 t, \sin\omega_0 t, 0)$. This potential acts on the orientation of each spherocylinder j individually depending on its orientation $\vec{e}_j$:

$$V_{ext}(t, \vec{e}_j) = -V_0 \left\langle \vec{u}_0(t), \vec{e}_j \right\rangle^2 = -V_0 \cos^2(\omega_0 t - \varphi_j) \sin^2(\vartheta_j)$$

For infinite driving frequency the particles feel the time averaged potential $-V_0 \sin^2(\vartheta_j)/2$. At low packing fractions this potential leads to a paranematic state in which the particle orientations $\vec{e}_j$ are isotropically distributed in the x-y-plane. For higher packing fractions an additional alignment within that plane becomes favorable leading to a nematic state [4].
These two regimes in the static limit also exhibit a distinct behavior at finite driving frequencies ω_0. In the high packing fraction regime at low ω_0 the nematic director follows the external field at a constant offset as each particle is turning synchronously with the external field (towing). At higher driving frequencies a complex behavior develops due to the interplay between excluded volume interactions between particles, friction with the fluid and the externally imposed torque. At first the height of the peak in the angular distribution that arises from the alignment of the particles along the director starts to oscillate (breathing).

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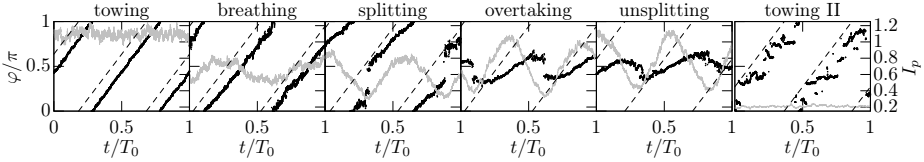
At even higher driving frequencies this peak splits into two, with intensity shifting from one peak to another emerging at higher azimuthal angle φ (splitting). For ω_0 above a certain threshold the phase shift between the two peaks surpasses $\pi/2$ corresponding to a backwards jump (overtaking). Finally, at the highest frequencies the two peaks merge again to one peak which cannot follow the external field anymore but switches its turning direction periodically (unsplitting) (see figure). These results agree qualitatively very well with findings of dynamical density functional theory [5]; however, we find the boundaries between different states to lie at lower driving frequencies.
A system prepared in the paranematic packing fraction regime behaves in a significantly different manner. While for low frequencies also in this regime a nematic state is induced where each particle turns with the same frequency as $\vec{u}_0$ (towing) we find after a narrow breathing regime a towing like behavior for all frequencies above a certain threshold (towing II) (see figure). Here the peak in the angular distribution, that is towed by the external potential minimum, originates from a short time alignment of individual particles with the direction $\vec{u}_0$ while the majority of particles provides an isotropic background of orientations in the x-y-plane. This distinction between the different types of towing has not yet been reported.



Dynamical states: Polar angle φ_0 of the potential minimum (dashed line) and of the maximum peak in the angular distribution φ_p (black dots) as well as the height I_p of this peak (grey line) over one period of V_{ext}.

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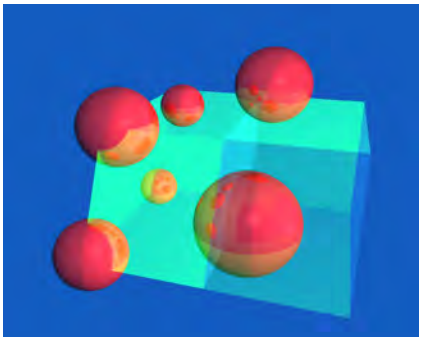
Poster 9 **Arno Formella**

Approximate and exact solid fraction fields: improved and new methods

Arno Formella*

Universidade de Vigo, Departamento de Informatica



Spheres intersecting different polyhedras. Only some cells of the space subdivision are shown in a semi-transparent manner.

Computing solid fraction fields is an important subtask in many applications of particle simulations and package analysis, where the ususally small particles are scattered in a volume (or area) that is subdivided conveniently into cells. Special care must be taken on boundaries not to distribute mass to the wrong side of the border whenever approximate methods are used.

We describe and compare different solid fraction field computation methods extending the work of [2] by reducing the computional cost of the methods and dealing with certain special cases not handled there.

Further we present a new approximative calculation that can deal with any polyhedral subdivision of the simulation volume with equally shaped cells. The approximation may distribute the fractions with a small error among neighboring cells, however, the approximation is exact in the sense that the overall sum of all mass fractions distributed over different cells is equal to the total mass of the particle which can always be achieved by renormalization of the fractions.

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The approximation is based on solid angle calculation (see [1]) combined with a simple computation scheme adding and subtracting appropriate partial fractions. The method is shown for the 2D case, where it appears to be exact, and the 3D case, where we give an analysis of the relative error introduced by the approximation.

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Poster 10 **Michael Heckel**

Hysteretical behavior of a jam-packed granular monolayer

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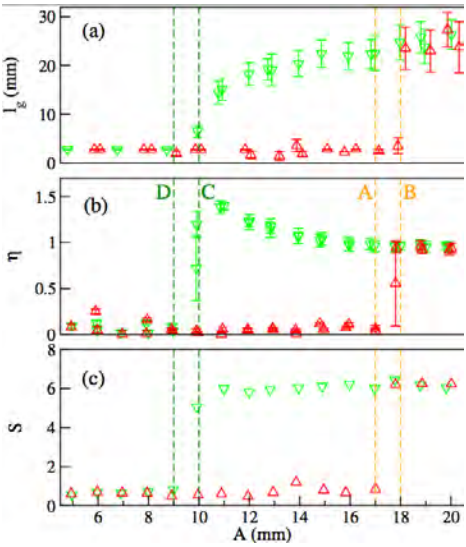

Characterization of the solid-3d gas transition, using a) the gap size, l_g, b) the dissipation rate, η, and c) the sound emission, S. Error bars indicate the standard deviation of independent measurements. Red symbols indicate increasing amplitude, green symbols stand for decreasing amplitude. Vertical dashed lines labeled $A - D$ correspond to the transition points.

When a granular (sub-)monolayer is subjected to horizontal vibrations, three different states are observed, depending on the parameters of driving: 1) a two-dimensional gas-like state where the particles move incoherently in the entire container by undergoing occasionally collisions; 2) a state where the particles still move in contact with the floor (that is, in two dimensions) but part of the system is found in condensed (frequently crystalline) state; and 3) a state of

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high energy which we call a three-dimensional gas where the particles experience violent collisions and the system expands in the third dimension.

Here, the transition between a jam-packed monolayer state and a 3d gas state is discussed: For fixed frequency, ω, by slowly varying the amplitude, A, of the oscillation, we observe a sudden change of the system's dynamical state where the system expands to the vertical dimension. The transition is characterized by abrupt changes of several measurable quantities, such as energy dissipation rate, η, sound emission characteristics, S, and a gap size, l_{g}, which quantifies the sloshing motion of the material (see figure). We find a well defined hysteresis of the transition which can be explained by considering the energy of the collective motion of the particles relative to the container. Looking to the full parameter space, (A, ω), we find both transitions forward and backward on lines where $A \propto \omega^{-1}$ also indicating that the transitions occur at critical energies. For a submonolayer, the transition occurs gradually and the hysteresis vanishes which also supports the energy argument for the explanation of the transition.

Acknowledgments: We acknowledge funding by Deutsche Forschungsgemeinschaft (DFG) through the Cluster of Excellence "Engineering of Advanced Materials" and the Collaborative Research Center SFB814.

Poster 11 Thomas Müller

Vertically Agitated Granular Rods: Tetratic or Nematic?

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Although many laboratory experiments use spheres to represent granular particles, nature and technical applications provide more complex shapes. Concerning products like wood pellets, medicine capsules, rice, etc., rod-shaped granular particles of cylindrical symmetry are worthwhile to be investigated. Due to their elongated shape, they share many properties with rod-like liquid crystals, such as a transition from an isotropic to a nematic phase. However, continuous energy injection is needed for the self-organization of granular particles due to the dissipative particle-particle interactions, which characterizes agitated granular matter as a system far from thermodynamics equilibrium.

We experimentally study a single layer of monodisperse polyvinyl chloride rods confined in a circular cavity which is vertically driven with a sinusoidal vibration. With increasing packing fraction of the elongated circular cylinders, a transition from an isotropic angular distribution to an alignment of the rods can be observed. Depending on the aspect ratio of the cylinders, either a tetratic ordering of fourfold symmetry or a uni-axial nematic one of twofold symmetry can be found. We experimentally explore the phase diagram by varying the aspect ratio and packing fraction of the rods. Moreover, we compare our experimental results with theoretical density-functional studies and Monte Carlo simulations of hard rectangles.

Illustration of a tetratic alignment of rod-like particles with an aspect ratio of 3.3. The color of the rods indicates their orientation angle with respect to some laboratory axes.

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Poster 12 **Weiwei Jin**

New Findings in the Packing of Tetrahedral Particles

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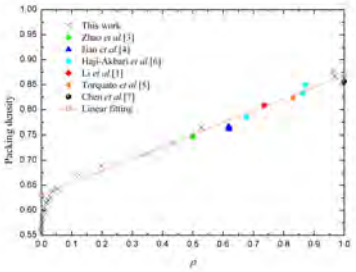
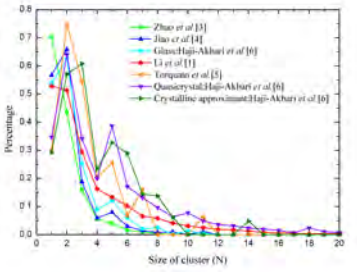


The distribution of clusters is obtained from six different packing samples. Two main peaks at N=2 and N=5 (N denotes the size of cluster) are observed. Dimer and wagon wheel are the dominant cluster topologies in tetrahedral particle packings, especially in the ones produced by Monte Carlo simulations.Dimer here denotes two tetrahedra with strict face-face contact, and wagon wheel denotes five tetrahedra packed around a common edge.



A relative ratio ρ is introduced to evaluate the amount of particles in clusters, i.e. ρ = Njp/Np, where Njp is the number of jointed particles and Np is the total number of particles in the packing.The relationship between the relative ratio ρ and packing density presents a strong linear correlation for various tetrahedral particle packings. The upper bound density of the fitting line is about 0.8687, and the lower bound is around 0.6315.

We present several new findings in the packing of tetrahedral particles in this work. Cluster analysis method is applied to explore the micro structure of tetrahedral packing. A cluster here is defined as assembled particles with continuous face-face joints (strict face-face contacts). Two main peaks at N=2 and N=5 (N denotes the size of cluster) are observed in the cluster distribution curves. It demonstrates that cluster dimer (N=2) and wagon wheel (N=5) are two special and dominant cluster topologies in tetrahedral particle packings. The excluded volumes of clusters in tetrahedral packing are investigated. We find that the excluded volumes of dimer and wagon wheel are relatively lower than other cluster

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forms, which explains the existence of peaks in cluster distribution curves. The proportion of particle amount in clusters is observed to have a strong linear correlation with the packing density, and the parameter is suggested as a new order metric for tetrahedral particle packings. The findings reveal that the density and order disparities in tetrahedral particle packings are induced by the amount of jointed particles. We also find that the nematic order of clusters can be used to classify the ordered and disordered packing of tetrahedra. Furthermore, the effect of rounded corner for dense packing of tetrahedral particles is studied. We find that packing of spherotetrahedra with small rounded corner could reach a significantly higher packing density (0.87636).

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Poster 13 **Pablo Ramos**

Packing of athermal polymers in the bulk & under confinement

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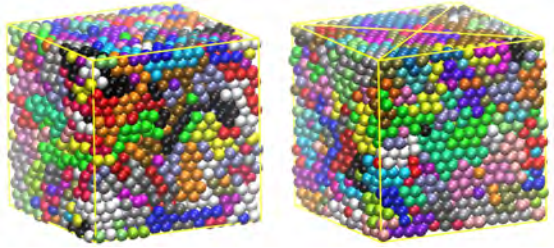
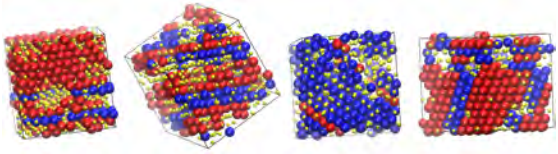


Snapshots of a 48-chain $N = 100$ system at a packing density $\varphi = 0.60$, (left) in the bulk and (right) under confinement in one dimension. Hard spheres are colored-coded according to the parent chain.



Snapshots of a 100-chain $N = 12$ system in the bulk at $\varphi = 0.5575$ with varied softness of bond lengths. Hard spheres are color coded according to the local structure: red, blue and yellow correspond to fcc, hcp and amorphous structures, respectively. Amorphous (yellow) sites are shown with reduced radii for clarity.

Polymers constitute a distinct class of anisotropic particles with unique dynamical, rheological and mechanical properties[1]. Thus, it is not surprising that during the last decades they have been under the spotlight of intense scientific research. Macromolecular systems, even in dilute solutions and high-temperature

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melts, present a formidable challenge from the modeling perspective as they are characterized by a wide range of characteristic length and time scales.

From the packing aspect, polymer chains are highly anisotropic entities, with the additional characteristic of having shape and size constantly fluctuating over time and with global and local structure being affected by a plethora of factors and conditions. Thus, packing trends and principles, valid and well-established for monomeric counterparts remain under question when it comes to polymer assemblies.

In the present contribution we study the packing properties of athermal polymers through extensive Monte Carlo simulations on freely-jointed chains of hard spheres of uniform size [2]. We examine in detail how factors like volume fraction (packing density), chain length, bond constraints and spatial confinement affect the packing ability of polymeric systems and their phase behavior (crystallization).

We find that the degree of softness of bond lengths has a profound effect on the ability of chains to crystallize, on the structure of the ordered morphologies and on the crystallization rate. Near the melting transition (of monomeric analogues[3]) and below a critical value of bond softness, chains remain amorphous reaching eventually the maximally random jammed (MRJ) state[4].

Confinement is realized through the presence of flat, planar, impenetrable walls in (at least) one dimension. We investigate how chain and monomer packing are affected by confinement, near and far from the surface walls and we compare the established confined polymer morphologies against the ones in the bulk[5].

Present modeling results can be used to aid the design of model polymers (granular/colloidal) with tailored phase behavior and packing properties.

Acknowledgments We acknowledge support through projects "Ramon y Cajal" (RYC-2009-05413 and RYC-2010-06804), "MAT2010-15482" and "MAT2011-24834" of the Spanish Ministry of Economy and Competitiveness (MINECO). Authors thankfully acknowledge the computer resources, technical expertise and assistance provided by the Centro de Computacion y Visualizacion de Madrid (CeSViMa).

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Poster 14 **Nishant Kumar**

Effects of polydispersity and deformation paths on the micro-macro behavior of granular assemblies

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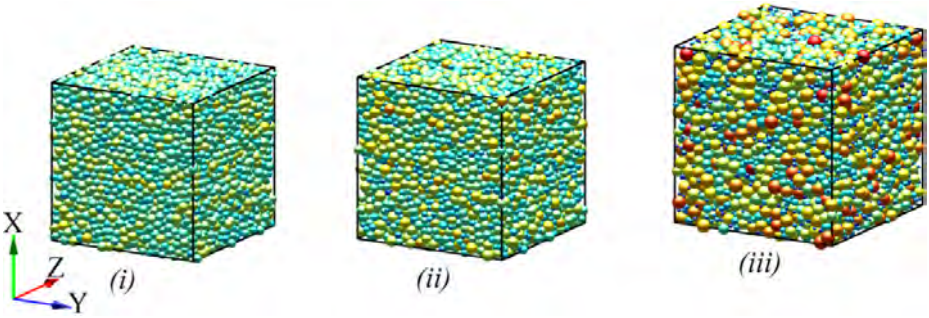

Fig. 1: Snapshots of three systems with polydispersity (*i*) 1.5, (*ii*) 2 and (*iii*) 5 respectively with the same volume fraction $\nu = 0.82$ [1]. The color code indicates the contacts of the particles : (red: big contacts, blue: no contacts).

The micromechanical and macromechanical behavior of idealized granular assemblies, made by linearly elastic, frictionless, polydisperse spheres, are studied in a periodic, triaxial box geometry, using the Discrete Element Method (DEM) as a viable tool. Emphasis is put on the effect of polydispersity (ratio of large/small particles) on the micro- mechanical behavior of granular assemblies when they are subjected to isotropic, deviatoric (volume-conserving) and uniaxial deformation. As an example, we show in Fig. 1 isotropic samples with three different uniform polydispersity distribution (with the same average particle radius for the three cases) and at the same volume fraction. Note that for the same volume fraction, the volume of the box is higher for higher polydispersity, since mean volume of the particles increases with polydispersity (see Ref. [1] for more details).

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On the macroscopic side, we observe that scaled pressure, coordination number and fraction of rattlers behave in a very similar fashion as functions of volume fraction, irrespective of the deformation path applied. Interestingly, they show a systematic dependence on the deformation mode and polydispersity via the respective jamming volume fraction, as seen in Fig. 2. This confirms that the concept of a single jamming point has to be rephrased to a range of variable jamming points, dependent on microstructure and history of the sample, making the jamming volume fraction a state-variable [1].

This behavior is confirmed when a simplified constitutive model involving structural anisotropy is calibrated using the purely isotropic and deviatoric simulations. The basic model parameters are found to depend on the polydispersity of the sample through the different jamming volume fractions. The predictive power of the calibrated model is checked by comparison with an independent test, namely uniaxial compression.

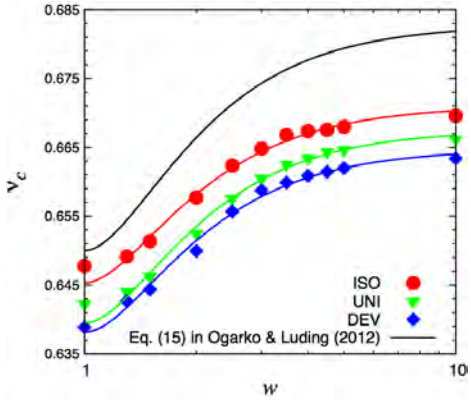

Fig. 2: Evolution of jamming point ν_c with polydispersity w for the deformation modes considered. Corresponding solid lines are the theoretical predictions for different modes [1]. Note that the fit is applied only to $w > 1.2$, since local crystallization [2] might happen at lower polydispersity causing ν_c values much higher than the disordered, random prediction.

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Poster 15 **Lucie Jezerska**

Experimental determination of the powdered coal storage parameters

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Powders are used to produce a lot of products. A good understanding of powder behaviour is therefore basis for optimization processes, developing a high quality product, innovation processes and for selecting suitable powder characterisation methods. The Laboratory of bulk materials at VSB Technical University of Ostrava solves many problems of flow failure in different technologies and processes with particulate materials. It has been clearly demonstrated that knowledge of mechanical and physical properties of powders and bulk solids is necessary when designing a new silo/bin/hopper, stockpile, feeder, chute, conveyor or other material handling equipment to improve functionality which we require [1, 2].

The present work shows, which mechanical-physical properties of three powder coal samples are important for their storage. These samples are frequently used in energy and metallurgical industries. Electron microscopic photos of tested samples are illustrated in the figure. The sample called A showed satisfactory process behavior unlike the other samples which caused process fluctuations and operational issues. Cilas Particle Size Analyzer was used for particle size distribution.

Experimental work was performed on the powder Rheometer Freeman FT4 [3]. The device allows obtaining a considerable amount of information about powder behavior from basic bulk density until friction or mechanical interlocking. It was found that dominant parameter in storage process is compressibility. Dependence between compressibility and the ratio of the microparticles and nanoparticles was observed, see the figure (A). Compressibility differences between similar samples were up to 6.5 percent at normal stress 22 kPa. Some relationships were found between the parameters of compressibility and angle of internal friction too. The measured flow functions of samples have been used to determine the cohesion and flow regime. The flow functions of the samples passed from easy-flowing to free flowing materials regime.

Goal of the presented paper is an opinion of prediction process behavior of

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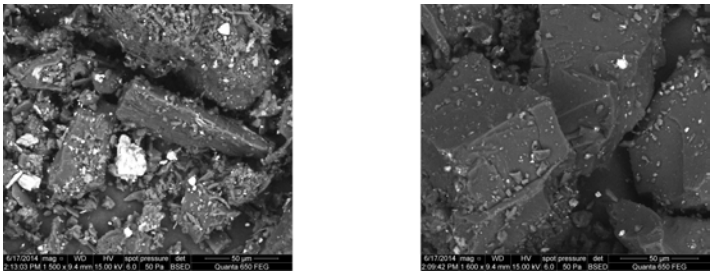
new batches in different industrial plants based on specific mechanical-physical properties which were identified. The tested samples of coal showed changes of its flow properties, compressibility, angle of internal friction, etc. This fact might have an impact on functionality of mechanical equipment and storage processes.



SEM photos (A and B coal samples with various process characteristics).

Acknowledgments: This paper was elaborated in the framework of the New creative teams project in priorities of scientific research, reg. no. CZ 1.07 / 2.3.00/30.0055, supported by Operational Programme Education for Competitiveness and co-financed by the European Social Fund and the state budget of the Czech Republic and by research projects of the Ministry of Education, Youth and Sport of the Czech Republic: the Centre ENET CZ.1.05/2.1.00/03.0069

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Poster 16 **Hideyuki Mizuno**

Shear Modulus Fluctuation and its Length Scale near the Unjamming Transition

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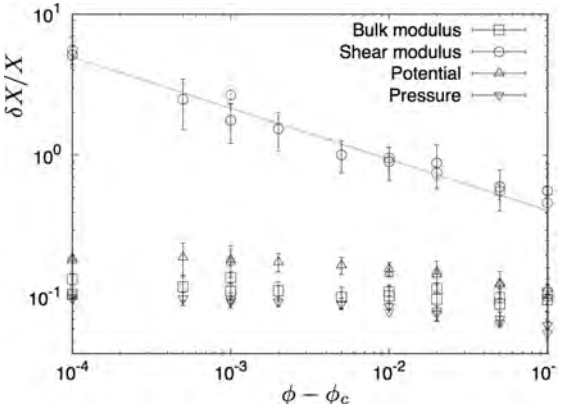
The jamming to unjamming transition shows a mixed character of the first-order and the second-order phase transitions [1]. As we approach the transition point ϕ_c from the jammed phase, the average contact number Z discontinuously goes to zero. Despite this first-order-like behavior, some other quantities, e.g., the pressure, the shear modulus, exhibit the power-law scaling behaviors, as in the second-order transition. The early work [2] extracted a length scale ξ_T from the vibrational properties in the jamming system. The length ξ_T physically represents a criteria for the propagation of the plane wave: the waves with larger wave lengths than ξ_T propagate in the granular medium, as in the elastic medium. At the length scales above ξ_T, the granular medium can be considered as the elastic medium, whereas the "disorder" nature appears below ξ_T. It has been demonstrated that the value of ξ_T diverges as the power law behavior, $\xi_T \sim (\phi - \phi_c)^{-\nu_T}$



The relative fluctuation $\delta X/X$ is plotted as a function of the packing fraction, $\phi - \phi_c$. The values are shown for the bulk modulus, the shear modulus, the potential, and the pressure.

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($\nu_T = 0.24$), with $\phi \to \phi_c^+$ [2].

In the present work, we will show that such a growing length scale can be extracted directly from the spatial fluctuation of the shear modulus. It has been well established that the elastic modulus spatially fluctuates in disordered solids, such as glasses, granular materials [3,4]. By using the numerical simulation and the fluctuation formulas [4], we measure the "local" elastic modulus in the jamming system, composed of the mono-disperse, soft spheres interacting through the harmonic potential, and then obtain the probability distribution function of the local modulus, which is well-fitted to the Gaussian distribution with the average value X (macroscopic value) and the standard deviation δX. In the figure, the relative fluctuation $\delta X/X$ is plotted as a function of the packing fraction ϕ, for the shear modulus as well as the bulk modulus, the potential, and the pressure. We clearly see that the shear modulus fluctuation grows as $\phi \to \phi_c^+$, which is fitted by a power law scaling. In our contribution, we will show that the characteristic length scale ξ_G, associated with the shear modulus fluctuation, diverges in a similar manner as the length ξ_T from the vibrational properties. We emphasize that the length ξ_G is a static quantity, which characterizes the static structural property (the spatial distribution of the shear modulus) in the jamming system.

Acknowledgments We acknowledge supports from DAAD (German Academic Exchange Service) and DFG within FOR1394.

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Poster 17 Matthias Möbius

The viscoelastic response of concentrated Graphene suspensions

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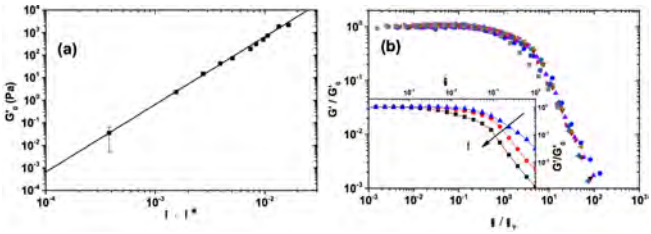
Nanoparticles such as rods and platelets are often used as filler materials to enhance the mechanical properties of composite materials[1]. At high concentrations beyond the rigidity percolation, the rheological response is dictated by the microstructure of the stress-bearing network that is formed by these non-spherical particles. The presence of the network gives rise to a yield stress and corresponding yield strain which depend critically on the reduced volume fraction $(\phi - \phi^*)$, where ϕ^* corresponds to the rigidity transition. In this work we study suspensions of Graphene flakes in NMP solvent that have been created through liquid exfoliation [2]. This process creates suspensions of stiff, few layer Graphene flakes with high aspect ratios of about ~ 1000. The typical thickness is $\sim$ 1nm and the typical size of the sheets is $\sim 1\mu$m.



The viscoelastic response of concentrated Graphene suspensions.(a) The plateau of G' in the linear response regime (f=1Hz), denoted as G'_0, as a function of the reduced volume fraction $(\phi - \phi^*)$. The line corresponds to a logarithmic slope of 3. (b) The normalized storage modulus G'/G'_0 versus the strain normalized by the yield strain for various $\phi > \phi^*$. Inset: G'/G'_0 versus strain at three different ϕ. More concentrated suspensions have a lower yield strain.

We probe the microstructure of these suspensions by measuring their viscoelastic properties at various concentrations beyond the rigidity percolation. We find that the viscoelastic properties exhibit robust scaling with $(\phi - \phi^*)$. The storage modulus plateau G'_0 scales with $(\phi - \phi^*)^3$ (see figure a). Furthermore we

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observe that the yield strain decreases with increasing ϕ. This allows us to scale the viscoelastic response onto a master curve (figure b). We propose a simple model based on affine deformations to relate the empirical scaling relation of the yield strain to the mesh size of the network, which decreases with ϕ. The yield stress measurements at different concentrations allow us to infer the typical bond energy between the flakes and the ϕ dependence of the bond number density.

Acknowledgments: This research has been supported by Science Foundation Ireland.

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Poster 18 **Mohammad Mohseni**

Dynamics Analysis of Moving Bed of Particles on a Vibrating Grate using XDEM

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The objective of the current study is to investigate numerically the packing density of particles subject to external forces. Therefore particle motion and their arrangement on a vibrating grate (Figure 1) is predicted by implementing eXtended Discrete Element Method (XDEM). The particulates are described as a packed bed of woody particles defined as non-spherical shapes with various sizes. In order to survey the effects of varied shapes on the packing density, two different shapes as cylindrical and elliptical are taken into account.

In this approach, the particles are resolved as the discrete phase so that the interaction between particles including external forces caused by particle impacts demonstrates motion of the particles. Moreover, in this method non-spherical shapes are defined as system of spheres describing cylindrical and elliptical shapes for instance. (Figures 2 and 3)

The external forces here acting on the particles are caused by the gravity and contact forces between particle–particle and particle–wall. The contact forces are dependent on the deformation between the two shapes, dynamics of the particles as well as material properties. Therefore this contact force because of collisions are modelled in this study by linear Spring-Dashpot, non-linear Hertz–Mindlin and Hysteretic Walton–Braun models. Thus different impact models are discussed and compared together.

In addition to the force calculations and subsequent accelerations based on the Newton's second law, the velocities and positions of particles are estimated by different numerical integration schemes. In this work Simplectic Euler, Velocity Verlet and Gear models are used and verified.

Keywords: XDEM, non-spherical particles, vibrating grate, moving bed.

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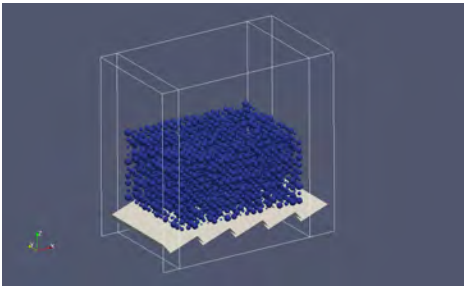

Fig. 1: Packed bed of particles on the Vibrating Grate

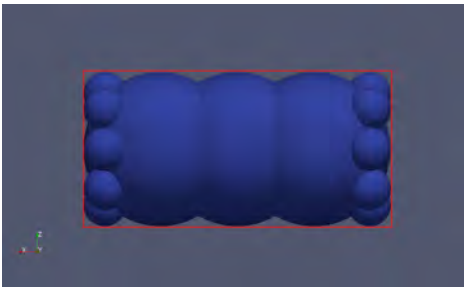

Fig. 2: Cylindrical particle 2D-view based on spherical subshapes

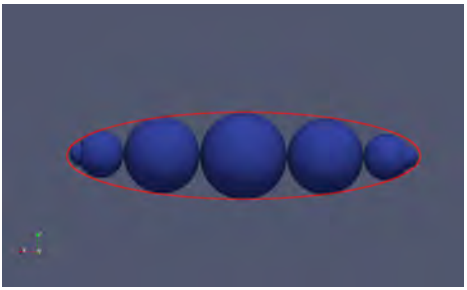

Fig. 3: Elliptical particle 2D-view based on spherical subshapes

Poster 19 **Osvaldo Munoz**

Weibull distribution applied to describe the density and entropy of granular ensembles

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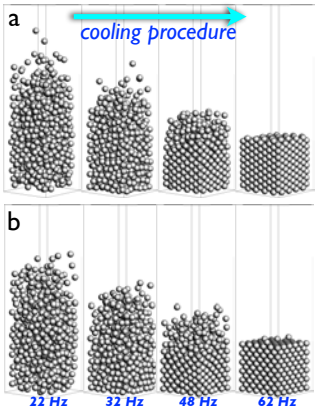

Fig. 1: A few snapshots of the isogamma cooling procedure from molecular dynamics. The ensemble consist of 666 beads, inside a box of lengths $L_x = L_y = 19.3$ mm and $L_z = 10$ cm. This box ensures that either a Body Centered Tetragonal dry structure ($L_x = L_y = 2r(1 + 4\sqrt{3})$) or a Faced Centered Cubic cohesive structure ($L_x = L_y = 2r(1 + 5\sqrt{2})$), where $r = 1.19$ mm, commensurately fit inside. (a) The final structure is a BCT. (b) The final structure is a FCC.

Powders and grains are present in the world as one of the most used materials. Despite the effort of researchers in the last three decades, their full description remains incomplete. Nevertheless, this athermal systems composed of grains can be described by means of an statistical mechanic formalism proposed in 1989

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by S. Edwards and R. Oakeshott [1]. Such formalism is based on a statement of equiprobability: all jammed available states of equal volume have the same probability, theoretically, by counting the number of available jammed states a configurational entropy would be calculated, where the entropy of the random close packing configurations is greater than the entropy of the ordered systems (granular crystals). Makse et al.,[2], based on information theory, used an alternatively approach to estimate de entropy of granulates. They measured the entropy of jammed matter, by calculating the volume occupied (Voronoi volume) by a particle through a Voronoi tessellation. This procedure is performed by considering the coordination number of the particle. The method, applied to 3D packed spheres, shows to be appropriate for estimating the entropy for either the random loose or the random close packing.

Entropy of information provides a simple and robust way to characterize the randomness of a granulate for a given configuration, nevertheless, the above approaches only are applicable to static systems. But what happens if by the influx of a given perturbation a granulate evolves from one state to another? In this work we introduce an extended powerful way to evaluate the entropy of a granular system that is mechanically brought from a very loose state (gas-like) to the maximum attainable compaction (crystal structure). The system, never in equilibrium but in local steady states that change with time, self-organizes into a perfect array. Our approach is based on a function of wide applicability called the Weibull probability distribution function (WPDF) [3]. Such distribution contains two parameters, c and k (positive), associated to the scale and shape of the distribution, respectively. We implement molecular dynamics to study an ensemble of beads confined inside a rigid box driven mechanically by an isogamma cooling procedure, where the vibration is applied by monotonically increasing the frequency (ω) and decreasing the amplitude (A) in such a way that $\Gamma = A\omega^2/g$ (where g is the gravity) remains constant. This procedure drives the system from a low density state to a condensed one if certain conditions are satisfied [4], see Fig. 1.

It is shown that using the WPDF we can accurately reproduce the density profiles obtained by molecular dynamics simulations, hence we can obtain the values of the parameteres c and k of the WPDF, see Fig. 2 (a). We prove also that the integral of the WPDF gives the configurational entropy of the system. The entropy is given by Eq. (1).

$$S = \gamma\left(1 + \frac{1}{k}\right) + \ln\left(\frac{c}{k}\right) + 1, \tag{1}$$

where γ is the Euler-Mascheroni constant (0.5772) [5]. Finally we are able to estimate the information content at each step of the cooling, see Fig. 2 (b). As far as we know, this is the first time an analytical expression is used to quantify information entropy changes of a granular system that self-assembles by cooling.

Acknowledgments: This work has been supported by Conacyt, Mexico, under

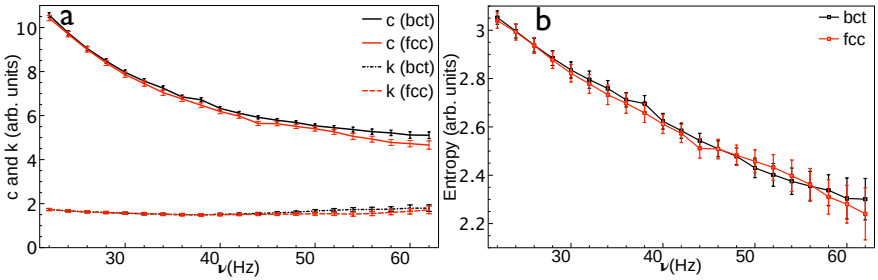

Fig. 2: (a) The values of parameters c and k at each step of the cooling process. Note that k is almost constant along the cooling (around $k = 1.8$). (b) Entropy S as a function of frequency, revealing that at the beginning of the annealing is large and as the number of configurational states reduces, it drops, black lines for the final body centred tetragonal crystal and red lines for the final face centred cubic crystal.

Grants 168281 and 101384.

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Poster 20 **Piotr Parafiniuk**

DEM examination of an influence of particle aspect ratio and sample width on uniaxial compression of assembly of spherocylinders

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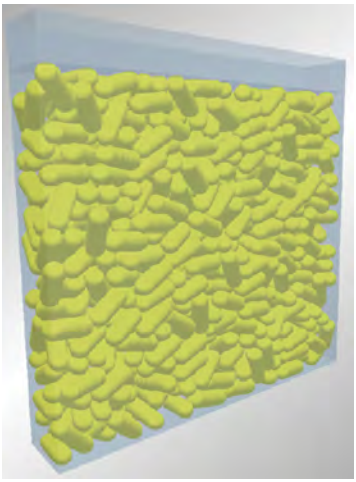
Random packings of non-spherical granular particles are in vivid interest both in science and industry. Modelling of such systems under load is important not only from theoretical point of view but also for process technology. In particular, the behavior of a granular material during compression plays an important role in the design of the storage tanks, packaging, and transporting devices. To this day models of mechanical phenomena in particulate materials during deformation are often incomplete and mainly phenomenological. Difficulties in analytical modelling of particulate systems are inherently associated with variety of shapes, sizes and material parameters of particles composing a granular system.



An example of examined system.

We study the effect of uniaxial compression on the mechanical properties of the assembly of spherocylinders. Cuboidal samples 1.025d to 10d thick (d - diameter of reference sphere) composed of spherocylinders of equal volume and aspect ratio from 1.0 to 2.5 were examined. DEM simulations have shown that the density of the deposits strongly depended on the aspect ratio of the particles and thickness of the deposits. In the case of the thinnest samples density achieved maximum for spherical particles and strongly monotonically decreased with increasing aspect ratio. For thicker samples the relationships between solid fraction and aspect ratio of particles were not monotonic and the maxima were observed at low values of aspect ratio. Pressure ratio, defined as normal stress on the side walls to the normal stress on the top cover increased with an increase in the thickness of the sample, as an effect of much less stress screening in thin systems.

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Poster 21 Jens Boberski

Anisotropy of force distributions in sheared soft particle systems

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In this numerical study, measurements of the contact forces inside a sheared system of soft frictional particles are reported. The distribution $P(f_n)$ of normalized normal forces exhibits a gradual broadening with increasing the shear deformation γ, leading to a slower decay for large forces. The process however slows down and $P(f_n)$ approaches an invariant shape at high γ. By introducing the joint probability distribution $P(f_n, \alpha)$ in sheared configurations, it is shown that for a fixed direction α, the force distribution decays faster than exponentially even in a sheared system and notably differs from $P(f_n)$ of an isotropic packing carrying the same average normal force.

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Poster 22 **Eric Parteli**

Attractive particle interaction forces and packing density of fine glass powders

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The packing behavior of powders can be strongly influenced by inter-particle attractive forces of different types, such as adhesion and non-bonded van der Waals forces. The relevance of the different types of attractive interactions for the packing density of powders of different materials and particle size distributions is, however, largely uncertain. That is, it is a challenging problem to *predict* the packing density of a certain granular system specified by the particle size distribution and the material properties of the particles. Numerical simulations by means of the Discrete Element Method (DEM) can offer a helpful tool in the investigation of the packing behavior of powders. Most previous studies of the density of dry powder packings using DEM simulations focused on monodisperse systems and included either van der Waals interactions or adhesive forces during contact. Indeed, typical powders are poorly sorted and may contain a broad interval of particle sizes. For fine powders, the attractive interactions between particles of different sizes should have an important effect on the dynamics, since cohesive forces become increasingly relevant compared to gravitational forces as the particle size decreases Consequently, the adequate description of attractive forces acting on particles of different size should be taken into account in DEM simulations in order to yield a predictive description of fine powders.

Here we study the packing of fine glass powders of mean particle diameter in the range $(4-52)\,\mu$m both experimentally and by numerical DEM simulations. We obtain quantitative agreement between the experimental and numerical results, if both types of attractive forces of particle interaction, adhesion and non-bonded van der Waals forces are taken into account. Our results suggest that considering only viscoelastic and adhesive forces in DEM simulations may lead to incorrect numerical predictions of the behavior of fine powders. Based on the results from simulations and experiments, we propose the following mathematical expression to estimate the packing fraction φ of fine polydisperse powders as a function of the average particle size, $\langle d \rangle$,

$$\varphi = \varphi_\infty - \frac{C}{\langle d \rangle^\alpha}, \tag{1}$$

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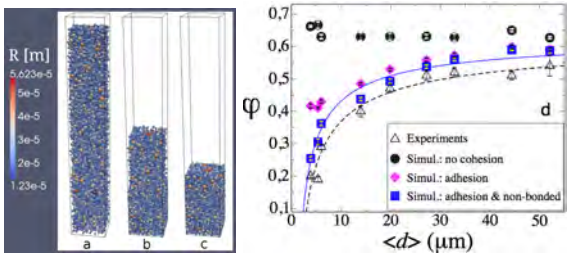
where $\varphi_\infty \approx 0.64$ is the packing density in the limit of large particles, where attractive forces are negligible. We believe that our results, obtained for the packing of fine glass powders will be of relevance also for other related systems that contain a significant fraction of small particles or a wide distribution of particle sizes.



(a-c) Snapshots of a simulation of polydisperse powder packing. Time increases from left to right, and R denotes the particle radius; (d) packing fraction as a function of the average particle size. Empty symbols show experimental results, each corresponding to a different particle size distribution characterized by the average particle size $\langle d \rangle$. Simulation results are shown by filled symbols: Circles: no attractive forces; diamonds: with adhesion during contact; squares: with both adhesion and non-bonded van der Waals interactions. The best fit to the experimental data obtained using Eq. (1) gives $C \approx 1.05$ and $\alpha \approx 0.59$ (dashed line). The continuous line denotes the best fit to the simulation data obatined with the full model (including both adhesion and non-bonded van der Waals), which gives $C \approx 0.99$ and $\alpha \approx 0.68$.

Acknowledgments: We thank Nina Gunkelmann for discussion. The German Research Foundation (DFG) is acknowledged for funding through the Cluster of Excellence "Engineering of Advanced Materials" and the Collaborative Research Center SFB814 (Additive Manufacturing). The authors gratefully acknowledge the computing time granted by the John von Neumann Institute for Computing (NIC) and provided on the supercomputer JUROPA at Jülich Supercomputing Centre (JSC).

Poster 23 **Kuniyasu Saitoh**

Master equation for the probability distribution functions of forces in jammed soft particles

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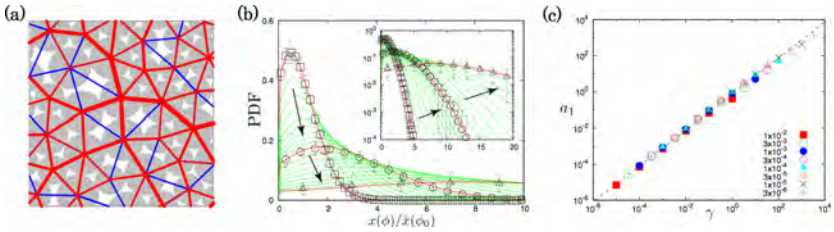
Mechanics of jammed soft particles (e.g. colloidal suspensions, emulsions, foams, and granular materials), have wide practical applications, where numerous studies have been devoted to continuum descriptions of them. However, there are many difficulties to predict their responses to global deformations, because a lot of undesirable events, due to randomness in the system, will be triggered by deformations. Most of such difficulties come from events in a particle scale, where *particle rearrangements* lead to a breakdown of affine approximations and *closing/opening contacts*, as well as *avalanches*, cause anomalous stress transmissions in the system. Therefore, it is necessary to connect these microscopic events to macroscopic, continuum approach to large scale problems.



(a) An extended force chain network, where the red and solid lines represent contacts and virtual contacts, respectively. (b) Non-affine evolution of PDFs of overlaps during isotropic compressions, where the open symbols are the results of MD simulations and the solid lines are the solutions of the Master equation. (d) A double-logarithmic plot of the non-affinity plotted against the ratio between the applied strain step and distance from jamming.

In this presentation, we try to understand such non-affine responses of jammed soft particles through *stochastic methods* [1], where all kinds of events in force chain networks are captured by conditional probability distributions (CPDs) (or transition rates) of overlaps and angles defined between particles. At first,

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we employ molecular dynamics (MD) simulations of two-dimensional soft particles, where we apply isotropic (de)compressions or quasi-static shear to static packings with different distances from jamming in order to measure microscopic changes of force chain networks. Here, we extend the force chain networks to the Delaunay graphs, where not only the particles in contact, but also the nearest neighbors without contacts are uniquely connected (Fig. a), so that closing and opening contacts can be properly taken into account. From our simulations, we find that the CPDs can be categorized into four types: contact-to-contact (CC), virtual-to-virtual (VV), virtual-to-contact (VC), and contact-to-virtual (CV), respectively, where the "virtual"means connections between the nearest neighbors without contacts. The CPDs in (CC) is given by a Gaussian distribution, indicating individual stochastic evolution of contacts, i.e. the Markov processes, while those in (VV) is found to be a stable distribution, implying multi-scale correlations between virtual contacts. The CPDs in (VC) and (CV) show exponential decays from zero-overlap, where the difference between characteristic length scales leads to discontinuous "jumps" in the probability distribution functions (PDFs) of overlaps. Then, we formulate a Master equation for the PDFs by using the CPDs (or transition rates), where a good agreement between the numerical solution and MD simulations is established as long as applied strain, i.e. (de)compression or simple shear, is kept much smaller than the distance from jamming (Fig. b). We also find several power law scalings for the quantities characterizing the non-affinity of the system, where all of them are linearly scaled by the ratio between distance from jamming and applied strain step, γ (Fig. c). We connect the Master equation with macroscopic constitutive equations through the microscopic expressions of stress tensor, where our stochastic model successfully describe the development of pressure under (de)compressions and *stress yielding* under simple shear.

Acknowledgments: This work was financially supported by the NWO-STW VICI grant 10828 and a part of numerical computation has been carried out at the Yukawa Institute Computer Facility, Kyoto, Japan.

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Poster 24 **Anna-Lena Hippler**

Mechanical properties of sheared wet granular piles

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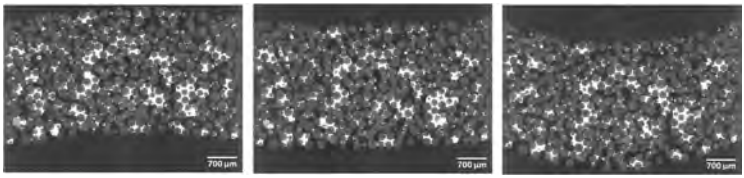
The mechanical properties of dry and wet granulates are explored when being sheared with a parabolic profile at constant shear volume using a custom made shear cell. The dissipated energy during shear is measured as function of liquid content and external pressure. Using a down sized version of the shear cell the reorganization of the granules and the liquid within the beads is imaged in real time using x-ray micro-tomography.



Slices of tomographic images of a shear cell over a whole shear cycle for $R = 250 - 300$ μm Glass beads with a liquid content of $W = 0.05$.

With the combined insight from mechanical behavior and internal granular geometry we find pronounced dilatation effects whenever the shear direction is inverted. For large external pressure the local jamming of the granules leads to a massive increase of the dissipated energy when inverting the shear direction. In the region of homogeneous shear, i.e. around zero crossing, and at low external pressure a dry granulate flows with only a minute energy dissipation. Adding some wetting liquid to the granulate, the dissipated energy at low external pressure is increased by virtue of the capillary forces exerted between the granules. Analyzing the trajectories of the granules during shear the dissipated energy by breaking capillary bridges can be calculated. This dissipated energy is found to be fairly insensitive to the exact liquid content. However, the dissipated energy increases linearly with increasing external pressure both for wet and

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dry granulates. This increase results from the increasing contact force between the granules and thus from the increase in friction between the granules. As the friction coefficient between dry granulates is larger than between wet granulates the dissipated energy for dry granulates increases faster with external pressure.

Poster 25 **Dan Serero**

Sedimentation and Collapse of a Granular Gas under Gravity

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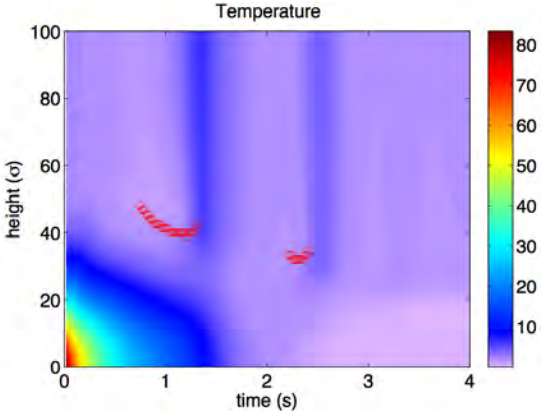
Due to its inherent dissipative nature, a granular gas needs external supply of energy in order to persist under gravity, otherwise it rapidly come to rest in the form of a dense granular packing. A hydrodynamic study of such a transition is presented: Employing a high-order, shock-capturing numerical scheme to solve the pertaining hydrodynamic equations, the gravity driven sedimentation of a system of inelastic hard disks initially heated from below, after energy supply is switched off, is analyzed. Our study reveals that the process exhibits a complex behavior, characterized by cycles of diffusive and inertial regimes. Self organized shocks appear, materialized by the propagation of fronts separating between subsonic and supersonic behavior accompanied by steep temperature profiles. The late stages of the collapse exhibit a scaling regime in accordance with recent experimental findings.



Evolution of the temperature of a sedimentating granular gas. Circles represent the front separating between subsonic and supersonic areas

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Poster 26 **Reza Shaebani**

Nonaffine Deformation and Mechanical Response of Dense Granular Materials

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The mechanical response of granular materials considerably differs from that of an ordinary elastic solid. Understanding the behavior, besides the scientific interest, has important practical applications. The emerging nonlinear relation between stress and strain can be attributed e.g. to the presence of disorder, nonlinearity of the contact force law, and Coulomb friction threshold. However, even in the absence of these elements in the nature of the interactions and the environment, the nonlinear elastic response may still exist because of the unilateral interactions in dry granular systems [1]. Opening of a contact terminates the local transmission of restoring or frictional forces, while formation of a contact provides new possibilities for it. We first show how taking the unilateral interparticle interactions into account would improve the analytical predictions for the mechanical response, and compare the results with simulations [2]. We attribute the remaining discrepancy to the contribution of nonaffine motions during the deformation process [3], and discuss the possible ways to include these motions in the stochastic modeling of stress transmission in granular media. We also clarify how the evolution of the probability distributions of contact forces deviate from the affine assumption during isotropic compression or shear deformation processes [4].

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Poster 27 **Vaclav Smilauer**

WooDEM: researcher's tool for DEM

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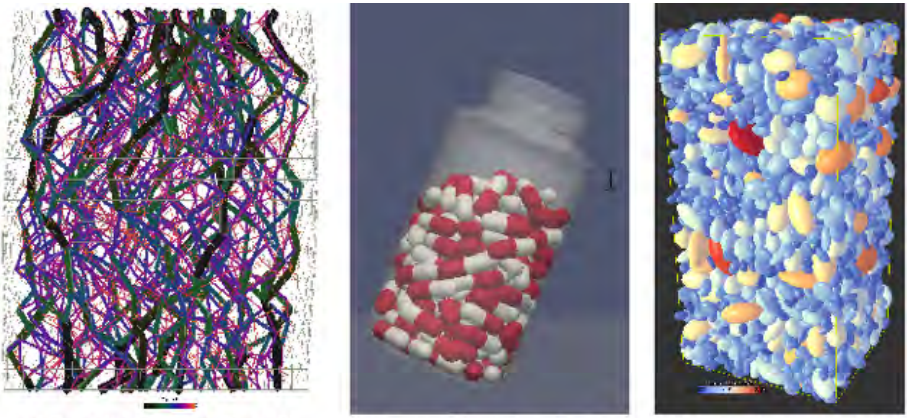
[2] *formerly CTU Prague, UJF Grenoble, UIBK Innsbruck*



(a) Force chains in triaxial test with elastic membrane (displacements scaled).

(b) Clumped 2-capsule packing in a bottle.

(c) Ellipsoids compressed via periodic boundaries; granulometry from PSD.

Examples of problems simulated in Woo.

WooDEM (`http://woodem.eu`) is open-source, portable, fully scriptable, extensible, well-documented code for discrete dynamic simulations, mainly the Discrete Element Method (DEM). Its history goes back to 2003 when the Yade project[4] started at UJF Grenoble, from which Woo forked off in 2011 by one of its main developers. Its development is funded from industrial contracts, from cooperation with the Academia and independent research projects. It is written in C++ with complete Python interface, runs under Linux and Windows; multiple processors are supported via OpenMP. Woo offers great flexibility in:

particle shapes: spheres, capsules, ellipsoids, facets, planes, clumps of any other shapes; potential particles[1], with arbitrary convex shape given by a potential function, are in development. New shapes and their collision routines are added via new classes, without modifying existing code.

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contact models: linear (Cundall), Hertz, DMT, JKR, Schwarz (interpolates between DMT and JKR; [3]); custom model for iron ore pellets; contact computation in local coordinates (normal, shear).

boundaries: triangle meshes, planes. Elastic deformable mesh (CST+DKT element). Periodic boundary with arbitrary scaling/skew/rotation and motion integration of the periodic cell deformation (∇v). Arbitrary motion constraints (e.g. 2d problems).

data analysis: access to all internal data from Python (interactive and non-interactive); live plotting; rich built-in 3d visualization capabilities, GUI inspection, averaged flow and segregation analysis, export to VTK, HDF5, XLS; batch system for parametric studies.

Woo was used in examination of critical states[2], friction influence, agglomeration, coating, sieving modeling, segregation and flow analysis.

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Poster 28 **Markus Spanner**

Universality of Anomalous Transport in Model Crowded Media

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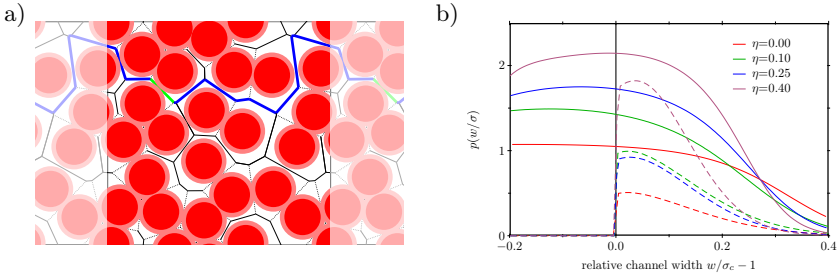

Fig. 1: 2d cherry-pit system with a narrow channel highlighted in green, b) channel size distribution in the cherry-pit Lorentz model for different hard spheres packing fractions η, obtained from a Voronoi tesselation. Solid lines: all channels, dashed lines: channels on the percolating cluster

The Lorentz model is a simple model for transport in porous materials, consisting of a point-like tracer moving through an array of random overlapping spheres. At a critical obstacle density, where the void space between the frozen-in obstacles undergoes a percolation transition, sub-diffusive transport $\delta r^2(t) \sim t^{2/d_w}, d_w = 4.81$ $(d = 3)$ can be observed. In this regime, transport is dominated by narrow channels in the host structure, i.e. gaps formed by three adjacent obstacles where the tracer can barely squeeze through.

With our simulations, we want to study the influence of these narrow channels on the critical tracer dynamics more closely, using two different approaches:

- By replacing the random overlapping obstacle matrix with equilibrated

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hard spheres systems of varied densities, we introduce correlations to the obstacle positions and thereby change the statistics of channel widths (see fig. 1). The percolations threshold σ_c is now reached by choosing the interactions distance σ (obstacle – tracer) larger than the hard sphere radius (cherry-pit model).

- By comparing ballistic and Brownian tracer dynamics, we change the way channels are probed by the tracer. While a ballistic tracer particle will always pass a channel as soon as it hits a suitable incident angle, a Brownian tracer can turn around inside the channel, giving relevance to the *length* of a channel.

In the first case, we find that the system is robust against introduction of obstacle correlations and d_{w} stays constant (fig. 2a). However, in the second case, when switching between ballistic and Brownian tracer dynamics, a splitting into two different universality classes $d_{\mathrm{w,bal.}} = 4.81$ vs. $d_{\mathrm{w,Br.}} = 4.23$ can by observed (fig. 2b).

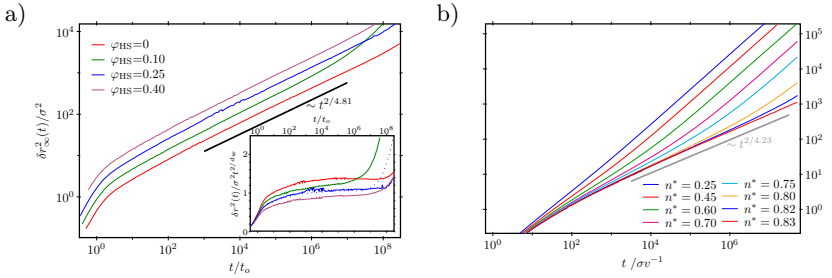

Fig. 2: a) Mean-square displacement in the cherry-pit Lorentz model for different hard spheres packing fractions η and ballistic tracer, $d_{\mathrm{w}} = 4.81$ is found to be independent of η. b) Mean-square displacement in the Lorentz model with Brownian tracer dynamics, $d_{\mathrm{w}} = 4.24$.

Poster 29 **Masaharu Tanemura**

On the Areal Random Packing

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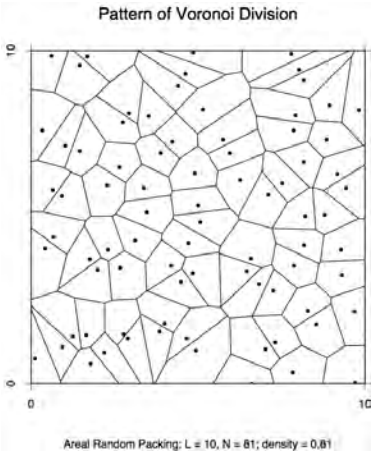
Random packing of non-overlapping objects is often seen in our daily life. Car parking problem in the street is a typical example of such random packings in one-dimensional space. In two-dimensional space, the random packing problem by identical disks will be a natural extension of the car parking problem into two-dimensions. These problems have many applications to material science, to biological science, and so on (e.g., [2]). In this paper, however, we present a new class of random packing problem. We suppose the critical size of area, instead of the non-overlapping object, which is the least accepted size of area for each generating point.



Sample pattern of an areal random packing

Example of the new packing process is given in the figure. We call this packing an 'areal random packing'. Let the whole region of the packing be a square $A = L \times L$, where L is the edge length of A, and let N be the number of points. We assume the critical value of the area allocated to each point be a_c.

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A rough sketch of the procedure of our random packing is as follows: **1**. Put $N \leftarrow 3$, and generate N points uniformly at random inside A; **2**. Compute Voronoi division of the point pattern. If the size of any Voronoi cell is below a_c, go to Step **1**, else go to Step **3**; **3**. Generate a test particle $\mathbf{x}_t$ uniformly at random in A, and compute the Voronoi cell $V(\mathbf{x}_t)$ of the point $\mathbf{x}_t$. If the areas of all cells are bigger than a_c, then go to Step **4**, else go to Step **3**; **4**. $N \leftarrow N + 1$. If a specified **Stopping Rule** is satisfied, then **Stop**, else go to Step **3**.

In the above procedure, a convenient **Stopping Rule** will be to specify the total number of test particles n_t: if a bigger n_t is used, the final value of N will become larger. It is obvious, however, how big a value is specified to n_t, the final N is limited below the value A/a_c. Then a suitable big value of n_t is needed to avoid the waste of computational effort. In our case presented in the figure ($A = 10 \times 10; L = 10 : a_c = 1.0$), $n_t = 10000$ is specified and the final value of N was 81.

It is interesting to estimate to what extent the whole area will be packed by the random packing process. The usual quantity for this estimate is to compute "packing density". In our case, the packing density ρA is defined as $\rho A = N \times a_c/A$ (see figure, $\rho A = 0.81$ was obtained). People are often interested in the mean value of ρ_∞, $E(\rho_\infty)$, the mean packing density in the limit $A \to \infty$. We performed computer simulations for several values of L and obtained the estimate $\bar{\rho}_\infty = 0.8274$ by a linear regression analysis. We point out that this packing density is rather high compared with the packing density of the random packing by disks (we have obtained the value 0.5473 for the case of disks [1]).

As an application of the areal random packing, we can consider the habitat of plants. It is natural to assume that an individual of plant occupies the area which is necessary for its existence through the competition for sun light and for water or nutrition. Then, as a result of competitions among individuals, the final pattern of the plant 'territory' might look like those of the areal random packing for the asynchronous (sequential) settlement of plants.

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Poster 30 **Nikola Topic**

Effect of surface profile on the distribution of coordination numbers in granular sediments

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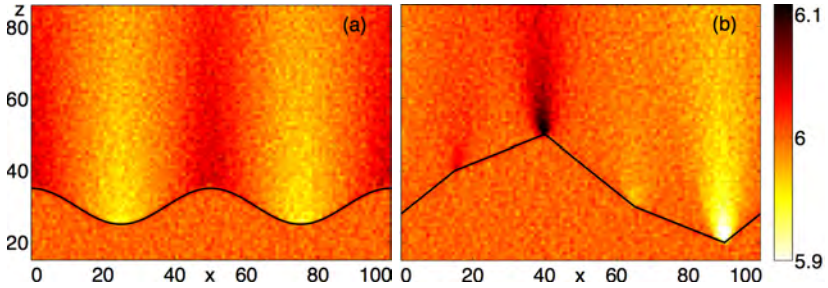
We study the packing properties of inhomogeneously grown three-dimensional sediments. In particular, we focus on the distribution of contact numbers. Inhomogeneous packings were created by dropping particles onto an initially wavy surface or by dropping them with inhomogeneous flux onto a flat surface, with particles behaving according to well-known Visscher-Bolsterli model, [1]. The resulting packings have spatially varying contact numbers determined by the historical surface profile, with higher than average contact numbers corresponding to convex surface and lower than average contact numbers corresponding to concave surface. Such effect has been observed in related systems, [2–5], though detailed analysis has not been performed. Here, we perform an in-depth analysis of how surface history is related to contact numbers and find a quantitative relation between them.



Contact numbers in three-dimensional inhomogeneous sediments. From an initial homogeneous packing all particles above the wavy surface, shown schematically as black line, are removed. Onto this exposed surface, particles are dropped with constant flux, resulting in inhomogeneous packing. Spatial variations in contact numbers induced by the surface profile are visible: convex surface increases contact numbers while concave decreases. a) Sinusoidal initial surface b) Piece-wise planar initial surface.

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Poster 31 **Lutz Torbahn**

Compaction behavior of fine and cohesive borosilicate glass spheres

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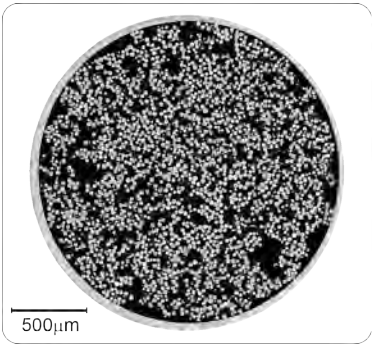
It is widely accepted that the microstructure and particularly the packing of bulk solids significantly influences the overall material behavior. This also applies to cohesive materials where the influence of packing caused by cohesional forces is manifold and plays a major role. Especially, for very fine granular materials with particle diameters of only a few micrometers the formation of the microstructure is of great scientific and industrial interest.



Cross section of the sample with the surrounding glass capillary (grey outer circle) and the borosilicate glass particles which form a microstructure that is typical for fine cohesive granular matter. Between the particle assemblages large pore spaces have been formed (dark areas).

This is why this study deals with a cohesive particle packing and investigated the packing features in more detail during the compaction process. Therefore, borosilicate glass spheres with a range of $27\,\mu$m $- 32\,\mu$m in particle diameter and a particle density of 2.2 g/cm^3 were used to observe changes regarding the packing behavior. For this purpose the borosilicate particles are filled into a very fine cylindrical glass capillary of only a few μl sample volume [1]. Additional to the standard glass spheres the surface properties of the same particles were

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modified, and hence, functionalized with silicon oil to artifically increase and highlight the cohesive features. On one of the two pistons that confined the glass capillary a compressional uniaxial force was applied and allowed for a defined lateral movement of single micrometers.
According to the microstructural analysis a high-resolution computertomograph was used to obtain single particle positions and the appropriate pore spaces which are distributed within the entire sample (see figure). This approach offer a non-destructive possibility to investigate the microstructure simultanenously to the compaction process. In this way the experiment showed how the internal particle structure behaves for very fine cohesive particles during the compaction process and provided important information on how pore spaces generally evolves and collapses in time while applying an external load. Finally, this study gives an indication how significant the influence of surface functionalization is, and thus, what effect a modification of the cohesional forces causes between the granular particles.

Acknowledgments: This work was funded by the Deutsche Forschungs Gemeinschaft within the priority programm SPP 1486.

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Poster 32 **Martin Tupy**

Desiccation effects in collidal films

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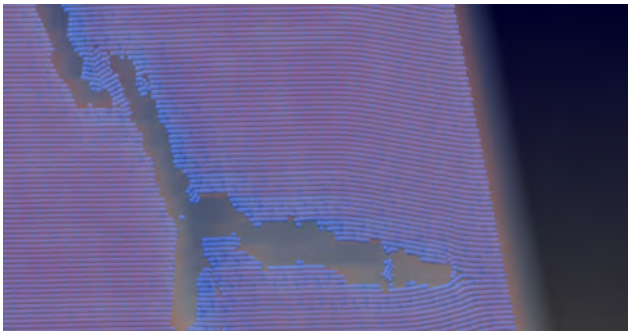

crack formation in a drying particulate monolayer

Different techniques are available to deposit colloidal suspensions on substrates, such as dip-coating or convective particle assembly [1, 2]. It has been observed that different processing setups can introduce the formation of pores or cracks. Both, in experiment and simulation, is has been found that the initial configuration of the colloidal film regarding the particle positions as well as the distribution of the fluid in the film has great influence on the final dry structure. Therefore, a deeper understanding of the dynamics of particulate suspensions during the transition from a fluid-like to a solid-like behavior is of great importance.

A multiphase model has been developed capable of simulating the dynamics of drying colloidal films. The particle dynamics are described by a force-based molecular dynamics algorithm. The liquid phase is modeled by capillary bridges between the colloids [3] acting as additional forces on top of the particle-particle interaction. These methods are combined with a finite difference framework handling the vapor phase by solving the diffusion equation with respect to different boundary conditions and distributing system variables needed for the evaporation process.

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In this contribution the model is described and structure formation in colloidal films, as shown in the figure, is studied with varying initial conditions depending on the distribution of particles and liquid in the film.

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Poster 33 **Simon Weis**

Changing friction in ellipsoid packings

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Friction is an important parameter for the stability of granular packings. We examine packings with different friction coefficients. Our particles of interest are ellipsoids with two types of apsect ratios as well as spheres as a reference system, see figure.

(Left) spherical particles in the cylindrical container that show surface crystallisation. (Right) close images of different particles, including spheres (white) and ellipsoids with two types of aspect ratios (orange and green & purple)

Interparticle friction is changed by grinding the particles with different abrasives like corundum and ottawa sand. The friction coefficient is measured using an inclined plane and correlated to surface roughness, measured by X-ray, profilometry and white light interferometry.

Various packings with different friction coefficients are prepared into a cylindrical container using different preparation methods to obtain different packing fractions. Boundary effects which would cause surface crystallisation are reduced by applying an amorphous structure to the container's surface.

The packings are recorded by X-ray tomography and the particles are detected[1]. A set Voronoi Diagram [2] is created from which the shape of the cells is characterized by isotropy indices based on Minkowski tensors. Other structural properties of interest are mean and local contact numbers and packing fractions as well as angle distributions and correlations.

The experimental results are compared to various simulations[3]. The data for

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spheres will be compared to various molecular dynamics simulations[4].

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Poster 34 **Alexander Weuster**

Simulation of Sheared, Caking Powder

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The flow behavior of some bulk solids changes with increasing storage time. Microscopically, solid bridges between particles are formed which consist of the material itself. But also crystallizing solute material from surrounding solutions, biological, or chemical processes can increase the cohesion force in bulk powder with time.

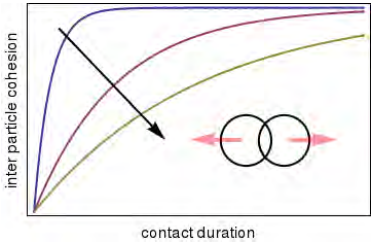

Fig. 1: Cohesive force between two particles as a function of contact duration for different characteristic times (t_c)

Starting from the assumption that within a characteristic time (t_c) a certain cohesive force builds up between two particles, we distinguish two regimes (see fig. 1). For small t_c, i.e. the full cohesive force has already been reached after a short contact time, the bulk behavior is governed by completely cohesive contacts. In the case of large t_c crystallization bridges between particles form on timescales larger than the contact time for a binary collision. Heterogeneous cohesion forces are the consequence. We study the impact of these time dependent contact properties on the bulk behavior. Focus is set on the structural changes induced by mechanical loading (see fig. 2). Results for compaction and shear simulations are presented and differences of the two regimes will be discussed.

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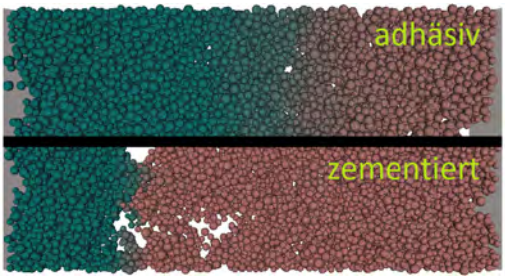

Fig. 2: Shear banding for different characteristic times (t_c): adhesive limit (top) vs. cementation limit (bottom). Colorcoding represents velocity in shear direction.

Poster 35 **Pascal Wieland**

Mechanical stability of random packings of rods

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We investigate the mechanical stability of random packings of rods for a range of different aspect ratios α. The study is a combination of experimental and numerical work.

In the experiments we use packings of uncooked spaghettis and gather data using X-ray microtomography. Image analysis is done with algorithms implemented in MATLAB. For the numerical simulation we model the rods as spherocylinders and use an energy-minimization technique to generate packings in the vicinity of the jamming point. In particular, we investigate the average number of inter-particle contacts z and its scaling with the packing fraction ϕ which follows the asymptotic relation $\phi\alpha = z$ [1]. We also quantify deviations from the Philipse-law and determine the origin of the deviation. By carrying out a nearest-neighbour transformation, Voronoi cells for each particle were obtained. These measurements allow to elucidate the relation between contacts and packing fraction on the local level of individual particles.

A random packing of spherocylinders ($\alpha = 40$) at the jamming point.

Acknowledgments: Funded by the Emmy Noether-Programm

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Poster 36 **Rene Wittmann**

Fundamental measure approaches to liquid crystals

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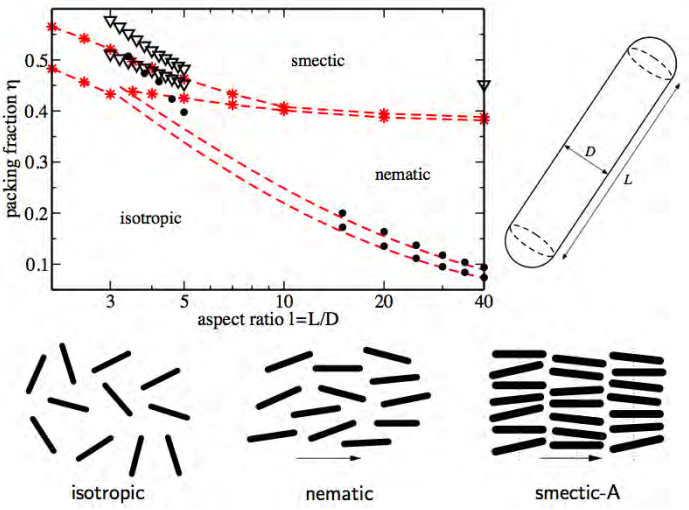
Fluids of hard spherocylinders exhibit a rich phase behavior including isotropic, nematic and smectic-A phases. A density functional for anisotropic hard bodies can be constructed in terms of tensorial weighted densities (FMT) which depend on geometry and position of only one single oriented particle [1]. We introduce a mixed measure of two bodies which can be expanded to the original tensor series within a new geometric method to derive the exact low-density functional. We compare this fundamental mixed measure theory (FMMT) to approximated results and Monte-Carlo simulations [2].

Closed formulas for the Frank elastic coefficients and the restriction to parallel spherocylinders verify the consistency of FMMT analytically. The isotropic–nematic interfacial tension remarkably improves on earlier, only qualitatively correct predictions [3]. For the first time, we obtain a phase diagram of hard



Phase diagram of hard spherocylinders from fundamental mixed measure theory. The dots and triangles denote simulation results [2].

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spherocylinders which can be quantitatively compared to simulations. We find a first order nematic–smectic-A transition up to an aspect ratio of at least 40. The computational effort and the relevance of other components of the functional is discussed.

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Poster 37 **Michael Klatt**

Characterization of Maximally Random Jammed Sphere Packings using Voronoi Correlation Functions

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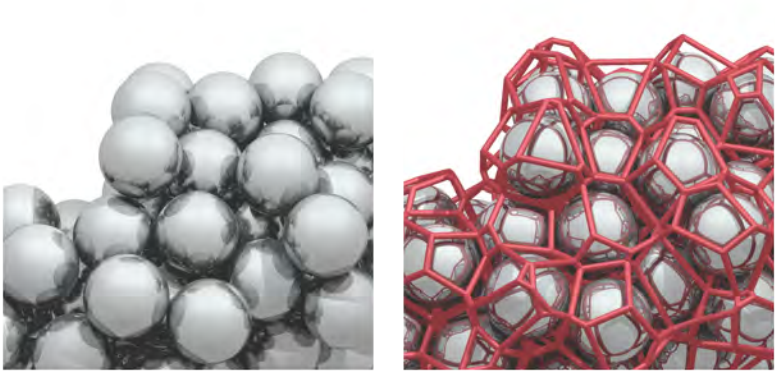
We characterize the structure of maximally random jammed (MRJ) sphere packings [1–4] by computing the Minkowski functionals (volume, surface area, and integrated mean curvature) [5, 6] of their associated Voronoi cells. However, they incorporate only local information and are insensitive to global structural information. Therefore, we extend this by evaluating descriptors that incorporate non-local information like correlation functions of the Minkowski functionals. We ascertain these higher-order functions on our MRJ packings as well as hard spheres in equilibrium and the Poisson point process.



Maximally random jammed sphere packing (left) and its Voronoi diagram (right).

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Poster 38 **Francois Ludewig**

Packing properties and compaction dynamics of ellipsoids

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The first step in the understanding of granular media where made by analyzing the static properties of a packing. Scientists intensely studied spherical packing [1] for a large number of configuration as 3D jamming with periodic limits without gravity or cylindrical container with gravity. The description of the state called "Random Packingïs a difficult challenge. Since it is used in opposition to lattice organization and has no proper definition. Nevertheless, the packing exists under precise mechanical conditions. In consequence, it can not be completely random.

Moreover, the static properties of granular packing are strongly linked to quasi-static dynamics as jamming in silo [2, 3] and compaction [4–7]. The compaction process consists in a succession of weak shocks which induce re-organization of the particles in the packing. The evolution of the packing should be completely described by the kind of shock and the initial properties of the packing.

Recently, the interest in the impact of the particle shape increased with the capacity of computers and the apparition of 3D printers. In our work, we investigate ellipsoidal particles that are built by agglomeration of spheres [8]. The positions and radius of the spheres are computed in order to obtain equality between surface of the ellipsoid and the convex hull of the spheres. Only prolates are studied through molecular dynamics simulations [9]. The packing properties are analyzed by creating packing with different friction coefficients. Voronoi neighbors are obtain by the minimizing a function described in [10]. Moreover, the size of the cylindrical container are tuned in order to obtain the theoretical random close packing [11]. In parallel, the compaction dynamics are realized for each size of particles and described in the diagram of the volume fraction and the coordinance.

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Poster 39 **Abhinendra Singh**

Three dimensional local rheology of dense, frictional granular material

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Using DEM simulations in the split-bottom ring shear cell, various continuum quantities like density, velocity, stress and structure can be calculated. In previous studies, several volume or pressure conserving experiments had to be performed to study the critical state rheology [1]. Here, we extract a wide range in strain rate, shear and normal stresses and volume fraction from a single simulation. The dilatancy and friction laws when plotted against the inertial number (ratio of microscopic and macroscopic time scales) are in good agreement with previous studies In the steady state [2]. The system is found to be heterogeneous, and local rheology shows a transition from a quasistatic regime at low shear rate to an inertial regime, where shear stress increases with shear rate. The evolution of the microstructure of the material is well characterized with a suitable parametrization of the fabric tensor and the coordination number.

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Poster 40 **Mohammad Saadatfar**

The topology of dense granular packings: a micro-tomography investigation

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The structural organisation of dense materials such as granular matter, glass, colloids, and some metals is naturally built upon local patterns that cannot tile the space, a phenomenon known as *geometrical frustration* [1]. Dense packings of identical spheres are commonly utilised to model complex frustrated structures as well as global ordering transitions. The densest local arrangement, the icosahedron, is often used to explain the existence of disordered structures [1]. Yet, recent computer models of frictionless packings emphasise that polytetrahedral aggregates are naturally composed of linear branches connecting ring structures which contain five tetrahedra (five-rings).

We employ a combination of novel experiments, x-ray computed tomography and topological analysis to investigate the structure of frictional packings (see Figure. 1a) before the Random Close Packing (RCP) limit and far beyond into the crystalline region. An extension of the bond order parameter method [2] is used to quantify these crystalisation regimes. Fig. 1b shows the variation of w_6^{hh} with packing fraction ϕ. There are two clear structural transitions: an abrupt increase at $\phi_{bernal} \simeq 0.64$ corresponding to the crystallisation onset, and a plateau starting at $\phi_c \simeq 0.68$.

At $\phi \approx 64\%$, crystalline clusters inevitably appear in the highly monodisperse packings, and this emerging order enforces a sharp transition in the packing of the underlying polytetrahedral structure [3]. Our analysis of the polytetrahedral clusters shows that branches of tetrahedra and five-ring structures are key topological features whose evolution is directly related to successive crystallisation regimes revealed by the local volume fluctuations (see Fig. 2, left).

Beyond $\phi \approx 64\%$, the increasing fraction of bipyramids discloses the growth of HCP crystalline structures. The presence of bipyramids below the RCP density may play a role in the slow compaction dynamics of amorphous packings, as reported for colloidal glass [4]. Below the RCP limit, $\approx 2/3$ of the polytetrahedral clusters are made of branched tetrahedra. This fraction decreases continuously with the increase in the packing density. However, these motifs are resilient

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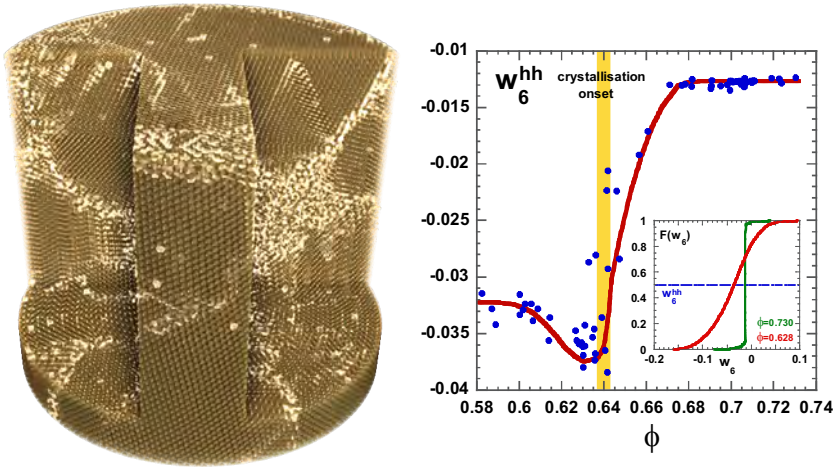

Fig. 1: (a) 3D visualisation of a partially crystallised packing containing 200,000 spherical acrylic beads. (b) Local order parameter w_6^{hh} versus ϕ. Inset: Calculation of w_6^{hh} from the cumulative distribution $F(w_6) = \int_{-\infty}^{w_6} P(w)dw$ for two volume fractions ($P(w)$ is the PDF of w_6).

features which survive for $\phi >= 68\%$ when the rings have almost disappeared. In this regime, a large amount of beads ($\approx 40\%$) are still connected via these linear patterns. These branched tetrahedra eventually vanish for $\phi >= 72\% - 73\%$ [5].

The propensity of tetrahedra to coalesce via their faces might be interpreted as the existence of a directional entropic force [6]. This may lead to the elaboration of a statistical framework for granular crystallisation and the related transitions observed in complex materials.

Further, we extend the characterisation tools discussed above to decipher the complex compaction process in natural systems such as packings of unconsolidated sands (see Fig. 2b).

[1] J. -F. Sadoc and R. Mosseri, *Geometrical Frustration*, Cambridge University Press, Cambridge, England, 1999).

[2] B. A. Klumov, S. A. Khrapak, and G. E. Morfill, *Structural properties of dense hard sphere packings*, Phys. Rev. B 83, 184105 (2011).

[3] A. V. Anikeenko and N. N. Medvedev, *Polytetrahedral Nature of the Dense Disordered Packings of Hard Spheres*, Phys. Rev. Lett. 98, 235504 (2007).

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[5] N. Francois, M. Saadatfar, R. Cruikshank, and A. Sheppard. *Geometrical Frustration in Amorphous and Partially Crystallized Packings of Spheres*, Phys. Rev. Lett. 111, 14, 148001 (2013).

[6] P. F. Damasceno, M. Engel, and Sharon C. Glotzer. *Predictive self-assembly of polyhedra into complex structures*, Science 337, 6093, 453-457, (2012).

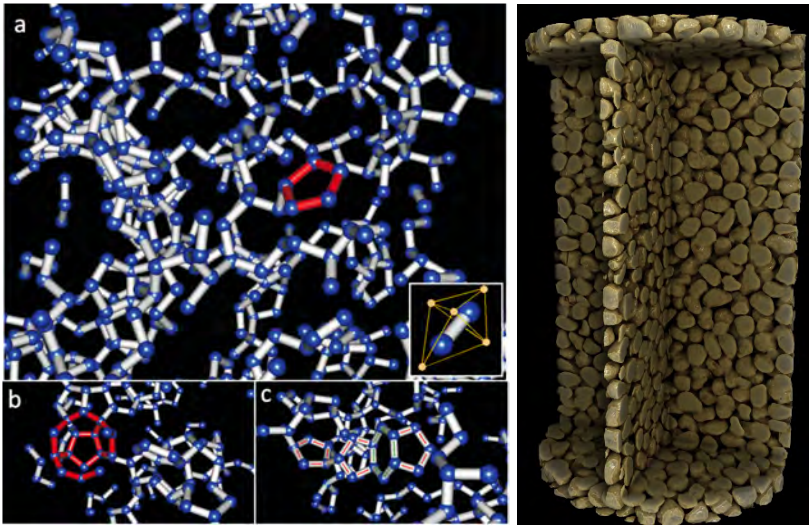

Fig. 2: Visualisations of the topology of polytetrahedral aggregates. Polytetrahedral clusters are represented as networks in which each vertex (blue sphere) is a dense tetrahedron and each bond (white tube) represents two tetrahedra sharing a face. The inset of (a) shows the centres of beads forming a pair of face-adjacent dense tetrahedra and their topological representation. (a) Polytetrahedral clusters in a packing at $\phi \approx 0.64$. A loop composed of five face-adjacent tetrahedra (five-ring) is highlighted in red. (b) Close-up on an "incomplete" icosahedral configuration. A cluster of 12 five-rings would form an icosahedron; here, this structure contains two five-rings adjacent to an eight-ring. (c) Close-up on a "chain" of rings composed of five-rings (red lines) and a six-ring (green lines). (d) 3D Visualisation of a packings of sands, a snapshot from a 3D time series.

Poster 41 **Frank Rietz**

Experiments with spheres around Random Close Packing

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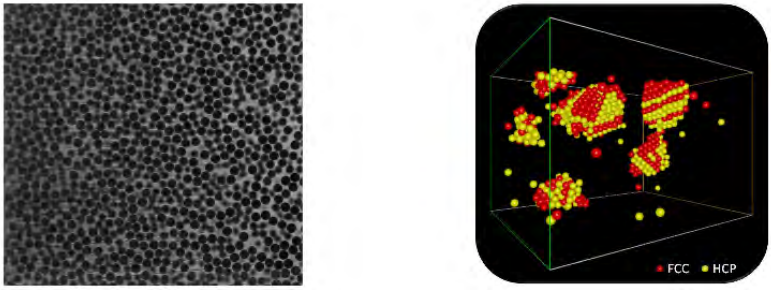
Sphere packings serve as a model for the microscopic structure of matter. Similar to atoms, spheres arrange in disordered and ordered phases. The densest disordered packing that is achievable for many experimental protocols is known as Random Close Packing. Frustration inhibits further increase of the density by crys- tallization. The theoretical picture of this barrier is still unclear. In our experiment the sphere packing is driven by periodical tilting of the container side walls. Three-dimensional information is obtained by an index matching technique [1]. The initial disordered packing compacts and above the Random Close Packing density we observe homogenous nucleation of the interior spheres. We characterize this first order phase transition by measurement of local volumes, crystal growth rates and critical nucleus size. Investigation of local structural changes allows us to better understand the jamming at the Random Close Packing density.



Slice through a three-dimensional disordered sphere packing visualized by index matching [1]. The sphere diameter is 3 mm.

[1] Dijksman et al.; Rev. Sci. Instrum. 83, 011301 (2012).

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Poster 42 **Robin Klupp-Taylor**

Crystal growth on curved substrates: A turning point in the synthesis of patchy particles based on noble metals?

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Fabrizio-Zagros Sadafi,[1,2] and Thomas Meincke[1,2]

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[2] *Cluster of Excellence "Engineering of Advanced Materials", FAU Erlangen-Nürnberg*

In this poster we present the scalable and tunable synthesis of patchy particles developed in the Nanostructured Particles Research Group at FAU Erlangen-Nürnberg. Such particles are prime candidates for the future fundamental studies and development of functional materials based on complex packings and assemblies. A key milestone in our activities has been the identification of the general conditions for the heterogeneous nucleation and surface conformal growth of crystalline patches on amorphous core particles. The motivation for this comes from our earlier finding that silver patches could be easily fabricated on non-functionalized colloidal silica particles using a modified Tollens reaction [Adv. Mater. 2011, 23, 2644]. The number, size and morphology of the patches, and thus their optical properties could be tuned by simple process parameters like temperature, reagent concentration and addition rate. In this contribution we will offer an overview as to how adaptable this process may be by considering how the heterogeneous nucleation and surface conformal growth of different metals on various colloidal particles can be promoted.

Firstly we considered the general requirements for the heterogeneous nucleation of noble metals onto core particles. While silver patches could be synthesized on silica and anionic polystyrene cores, no heterogeneous nucleation was observed on cationic polystyrene cores. This suggested that a Coulombic attraction between core particle and metal ion may drive surface supersaturation with respect to the bulk solution. We confirmed this by reducing the negatively charged chloroauric ion in the presence of cationic polystyrene spheres, resulting in dendritic gold patches being formed. Unlike with silver patches on negatively charged cores we found that the morphology of the gold patches could not be easily tuned. This suggested that while surface conformal growth occurs in both cases, the surface diffusion necessary for this process limits the growth considerably more in the case of gold patch formation. Via systematic experimentation and Monte Carlo simulations we show that ascorbic acid is responsible for both promoting and hindering surface diffusion in the case of gold patch synthesis. Furthermore,

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we investigated whether there are factors which influence the patch morphology beyond normal crystal growth kinetics e.g. core curvature effects. In the final part of the contribution we will show recent developments regarding the establishment of control over the locations where patches grow, a critical problem to be solved if the approach is to be used for the fabrication of identical patchy particles e.g. for self-assembly. Using non-spherical core particles we demonstrated that patch nucleation tends to follow a non-classical model, with regions of higher curvature being preferred as nucleation sites over planar surfaces.

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09:00-09:45	Hernan Makse	Michael Engel	Sidney Nagel	Tobias Kraus
09:45-10:05	Alvaro Marin	Jason Gallas	Gustavo Düring	Claus Heussinger
10:05-10:25	Dietrich Wolf	Ana-Suncana Smith	Andy Kraynik	Jeffrey Aguilar
	coffee break			
	chair: Sidney Nagel		chair: Stefan Luding	chair: Gary Delaney
11:00-11:20	Matthias Schröter	poster session	Jonathan Kollmer	Corey O'Hern
11:20-11:45			Richard Gerum	
11:45-12:05	Edan Lerner		Balazs Szabo	Yujie Wang
12:05-12:25	Mario Liu		Gary Delaney	Takenobu Nakamura
	lunch break			
	chair: Michael Engel	chair: Hernan Makse	chair: Tobias Kraus	chair: Yujie Wang
14:30-15:15	Stefan Hutzler	Brian Tighe	Matthias Sperl	Hans Herrmann
15:15-15:35	Ralf Stannarius	Günter Last	Denis Weaire	Nick Rivier
15:35-15:55	Massimo P. Ciamarra	Fabian Schaller	Kai Huang	Jens Boberski
				closing remarks
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	chair: Denis Weaire	chair: Matthias Sperl	chair: Matthias Schröter	
16:30-16:50	Stefan Luding	Patric Müller	Tomaso Aste	
16:50-17:15		John Amend		
			poster award presentation	
	conference soccer & bbq (6-8pm)	conference dinner (6-10pm)		

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