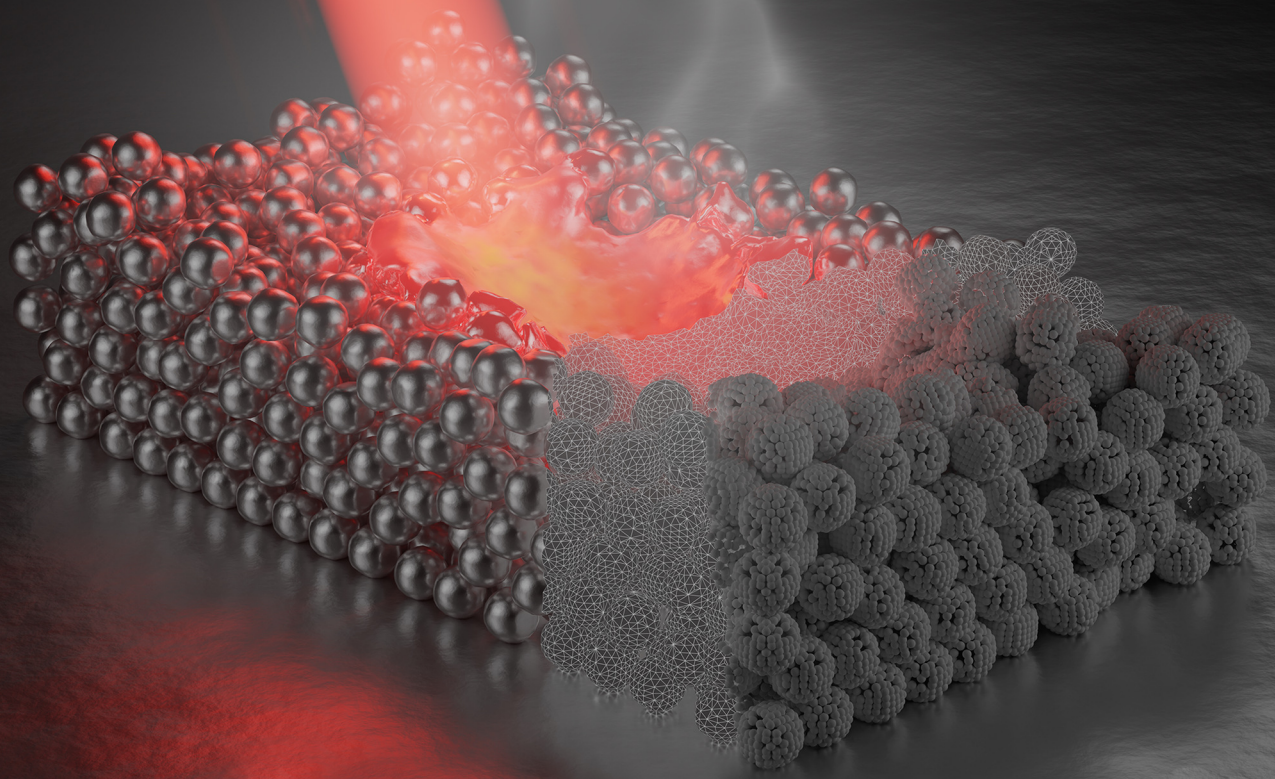
Institute for Multiscale Simulation

Prof. Thorsten Pöschel
Prof. Michael Engel

Friedrich-Alexander-Universität Erlangen-Nürnberg

2022
Annual Report

Powder Sintering in Additive Manufacturing



FAU
Friedrich-Alexander-Universität
Technische Fakultät

Institute for
Multiscale Simulation
MSS

Institute for Multiscale Simulation
https://www.mss.cbi.fau.de
Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)
Cauerstraße 3, 91058 Erlangen

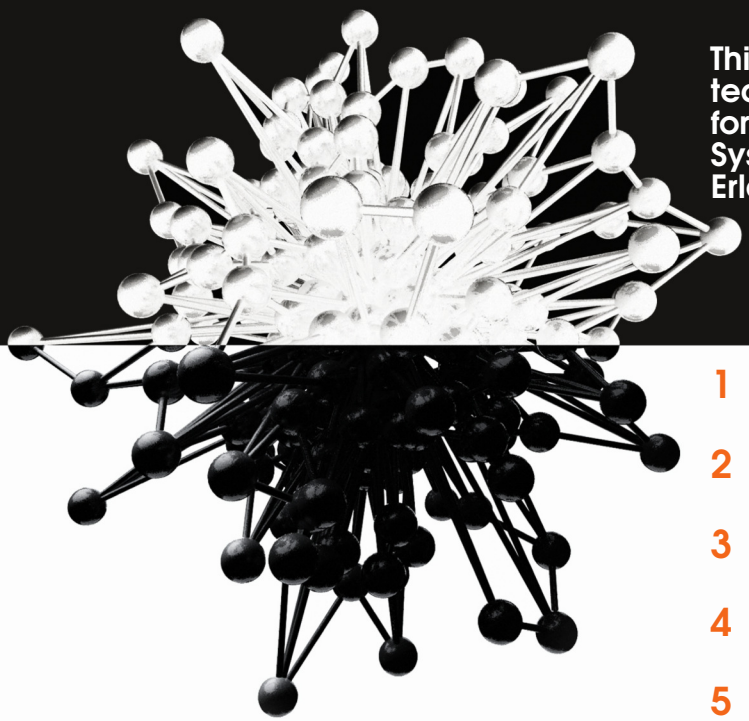
Editor: Meysam Bagheri

Titelpage: Simulation of the selective laser melting of titanium powder by Michael Blank, designed by Meysam Bagheri.
Back cover: Multi-sphere DEM simulation of a granular sediment by Ali Mauricio Velasco Sabogal.

Institute for Multiscale Simulation

Annual Report 2022

Preface



This annual report describes the scientific, teaching, and social activities at the Institute for Multiscale Simulation of Particulate Systems at Friedrich-Alexander-Universität Erlangen-Nürnberg in 2022.

Erlangen, December 2022
Thorsten Pöschel, Michael Engel

1. Staff Members

Professors

Prof. Dr.
Thorsten Pöschel

Prof. Dr.
Michael Engel

Visiting Professors

Prof. Dr.
Seyed Habib
Ebrahimnazhad Rahbari

Prof. Dr.
Leopoldo Gómez

Assistant Professor (Privatdozent) and Habilitation Candidates

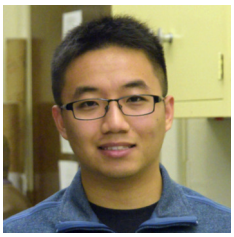
Priv.-Doz. Dr. habil.
Igor Goychuk

Dr. rer. nat.
Patric Müller

Dr.-Ing.
Sudeshna Roy

Postdoctoral Researchers

Dr. Artem Panchenko



Dr.-Ing. Hongyi Xiao

Dr.-Ing. Vasileios Angelidakis

Dr.-Ing. Carlos Lange Bassani

Dr.-Ing. Olfa D'Angelo

Dr. Aswathy Muttathukattil Narayanan

Dr. rer. nat. Achim Sack

PhD students

M. Sc. Huzaif Rahim

M. Sc. Utku Canbolat

M. Sc. Ayman Ameen

M. Sc. Meysam Bagheri

M. Sc. Michael Blank

M. Eng. Felix Buchele

M. Sc. Holger Götz

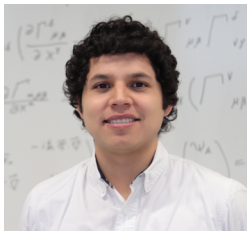
M. Sc. Sarthak Jadhav

M. Sc. Valentina Marzulli

M. Sc. Atharva Pandit

M. Sc. Angel Santarossa

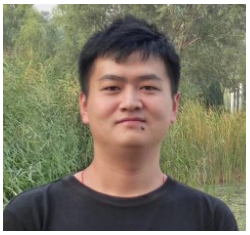
M. Sc. Federico Tomazic



M. Sc.
Luis Torres Cisneros

M. Sc.
Nydia Roxana
Varela-Rosales

M. Sc.
Ali Mauricio
Velasco Sabogal



M. Sc.
Song Zhiyu

Visiting students

M.Sc.
Laureano Ortellado
PhD student
Universidad Nacional
del Sur Argentina

Adriana Enriquez
Student at the
department of Physics
University of Havana

Master, Bachelor and Mini-project students

Chandrew Aseervatham
Master student

Deniz Fakioglu
Master student

Navid Panchi
Master student

Omar Zeair
Master student

Nicolas Pechler
Master student

Qing Yu
Master student

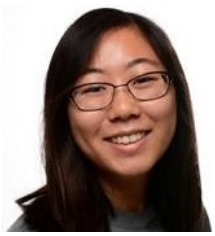
Yazan Alzaghah
Bachelor student

Frederik Keil
Bachelor student

Isabella Schneider
Bachelor student

Lan-Tien Hsu
Miniproject

Tengda Huang
Miniproject



Natalie Lam
Miniproject

Khaled Mansour
Miniproject

Jonathan Martín
Miniproject

Anirudh Suri
Miniproject

Aditya Pratap Singh
Miniproject

Technical and Administrative Staff

Dipl.-Pol.
Roland Haberkorn[redacted]
Technician

Ulrike Hansl
Team Assistant

Dr. Michael Heckel
Technician

Meister
Walter Pucheanu
Technician

[redacted]

2. MSS Seminar

145. **Dr. Olfa D'Angelo**[1] **and Dr. W. Till Kranz**[2]
[1] Institute for Multiscale Simulation, FAU Erlangen-Nürnberg [2] Institute of Materials Physics in Space, German Aerospace Center (DLR)
"Constitutive law for dense agitated granular flows: from theoretical description to rheology experiment"
January 26, 2022

146. **Dr. Thorben Könemann**
Center of Applied Space Technology and Microgravity (ZARM), University of Bremen
"ZARM's New Next-Generation Drop Tower System"
March 2, 2022

147. **Dr. Hongyi Xiao**
Institute for Multiscale Simulation, FAU Erlangen-Nürnberg
"Granular experiments and machine learning-informed modeling for the plastic deformation of amorphous solids"
June 8, 2022

148. **Dr. Adil Mughal**
Department of Mathematics, Aberystwyth University
"Dense packing of spheres in cylinders"
June 29, 2022

149. **Prof. Arno Formella**
Department of Computer Science, Univsersity of Vigo
"Quadrilaterals: ¿simple or complex?"
July 13, 2022

150. **Prof. Lou Kondic**
Department of Mathematical Sciences, New Jersey Institute of Technology
"Force networks in particulate systems"
July 13, 2022

151. **Prof. Habib Ebrahimnazhad Rahbari**
School of Chemical and Biological Engineering, Seoul National University
"Active microrheology of a bulk metallic glass"
August 10, 2022

152. **Dr. Jonathan Kollmer**
Faculty of Physics, University of Duesburg-Essen
"Impacts on and interaction with regolith covered surfaces in low gravity"
August 24, 2022
153. **Ph.D. Sakurako Tanida**
Research Center for Advanced Science and Technology, University of Tokyo
"Do elevators synchronize if not everyone boards an elevator that arrives early?"
September 22, 2022
154. **Prof. Anthony Thornton**
Department of Fluid and Thermal Engineering, University of Twente
"Multi-scale modelling of segregating granular flows: From particles in a laboratory heap to a vulcano"
September 26, 2022
155. **Prof. Habib Ebrahimnazhad Rahbari**
School of Chemical and Biological Engineering, Seoul National Universit
"Power fluctuations in sheared amorphous materials"
September 28, 2022
156. **Dr. Yu-Fan Lee**
Department of Chemical Engineering, Delft University of Technology
"Microstructure and Rheology of Concentrated Colloidal Suspensions with Varying Nanotribological Interactions"
October 5, 2022
157. **Laureano Ortellado**
Department of Physics, Universidad Nacional del Sur-IFISUR-CONICET
"Understanding Hydraulic Fracture through X-Ray Tomography"
October 26, 2022
158. **Michael Blank**
Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg
"Simulation of the laser melting process of titanium using Smoothed Particle Hydrodynamics"
December 19, 2022

145th MSS-Seminar
Wednesday, January 26th,
15:30 hrs, H3,
Egerlandstr. 3, Erlangen.

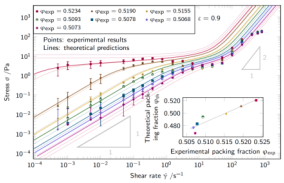
Constitutive law for dense agitated granular flows: from theoretical description to rheology experiment

Dr. Olfa D'Angelo[1] and Dr. W. Till Kranz[2]

[1]Institute for Multiscale Simulation, University of Erlangen-Nuremberg
[2]Institute of Materials Physics in Space, German Aerospace Center (DLR)

The variety in granular materials' behaviour makes them a fascinatingly counterintuitive material, but also one that is difficult to encompass into a globalised theory. Recently, Kranz et al. described granular fluids close to the glass transition using mode coupling theory (MCT), and extended this theory towards the non-linear rheology of such granular fluids submitted to shear at finite shear rates [1]. This approach allows to embrace in a single theoretical framework the variety of rheological responses observed in dense granular fluids, as it predicts and delineates rheological regimes comprising Newtonian, shear thinning, and shear thickening (Bagnoldian).

We provide the first experimental validation of this theory [2], through flow curves spanning six orders of magnitude in shear rate, and over a wide range of packing fractions. As we uncover the predicted rheological regimes in an air-fluidised granular bed of glass beads, we explore the areas of uncertainties in comparing our careful measurements to the theory. Experimental results and theory compare very favourably; besides the predicted regimes, experiments reveal an additional regime at high Peclet number where the Bagnold scaling is lost.



[1] W. T. Kranz, F. Frahsa, A. Zippelius, M. Fuchs, and M. Sperl, "Integration through transients for inelastic hard sphere fluids," Physical Review Fluids, vol. 5, p. 024305, 2020.

[2] O. D'Angelo, A. Shetty, M. Sperl, and W. T. Kranz, "Constitutive law for dense agitated granular flows: from theoretical description to rheology experiment," 2022, in preparation.

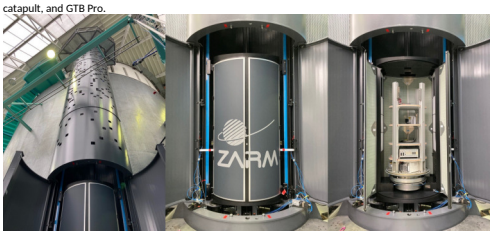
146th MSS-Seminar
Wednesday, March 2nd,
15:30 hrs, H3,
Egerlandstr. 3, Erlangen.

ZARM's New Next-Generation Drop Tower System

Dr. Thorben Könemann

Center of Applied Space Technology and Microgravity (ZARM), University of Bremen

With a height of 146 m, the Bremen Drop Tower is the predominant facility of ZARM, the Center of Applied Space Technology and Microgravity, and also the only drop tower of this kind in Europe. ZARM's ground-based laboratory offers the opportunity for daily short-term experiments under conditions of high-quality weightlessness at a level of 10(-6) g. Scientists may choose up to three times a day between a single drop experiment with 4.74 s in simple free fall and an experiment in ZARM's worldwide unique catapult system with 9.3 s in microgravity. Since the start of operation of the drop tower facility in 1990, over 9400 drops or catapult launches of more than 300 different experiment types from various research fields have been accomplished so far. In addition, more and more technology tests have been performed under microgravity conditions at the Bremen Drop Tower, in order to prepare single space instruments or appropriate space missions in advance.
The GraviTower Bremen Pro (GTB Pro) represents ZARM's new next-generation drop tower system, which makes use of a rail-guided rope drive being able to perform over 12 short-term microgravity experiments per hour. Its technology is based on a commercial hydraulic winch system with more than 4000 hp of engine power that moves a rail-guided drag shield in a 16 m high tower, upwards and downwards. With its Release-Caging-Mechanism (RCM), the actively driven GTB Pro located in the integration hall of the Bremen Drop Tower is capable to control heavy payloads in a very smooth and precise manner. Furthermore, its user-friendly software interface brings microgravity experimenting on a laboratory level. Due to the fact that the same standard capsule can be used, high synergy effects are given for ZARM's drop tower users. It means a simple change in all operation modes, between drop, catapult, and GTB Pro.



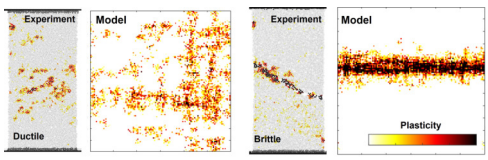
147th MSS-Seminar
Wednesday, June 8th, 15:30 hrs,
Seminar room (00.156),
Cauerstraße 3, Erlangen.

Granular experiments and machine learning-informed modeling for the plastic deformation of amorphous solids

Dr. Hongyi Xiao

Institute for Multiscale Simulation, University of Erlangen-Nuremberg

Understanding the interplay between local disordered structure and dynamics is important for modeling the deformation of soft amorphous materials. I will discuss how granular materials can be used as a highly tunable disordered solid to address this challenge and inform theoretical modeling. A granular raft was experimentally designed which consists of particles trapped at an air-oil interface that induces capillary attractions. Under tensile deformation, particle rearrangements gradually localize into an inclined shear band, upon which failure occurs, and the ductility of the raft can be controlled by tuning the capillary attraction. For the local structure-dynamic interactions, a machine learning method was used to develop a scalar field, softness, which is a structural descriptor that predicts the propensity of a particle to rearrange. Microscopic interactions between elasticity, local rearrangements and their nearby softness field were extracted and used to inform a structro-elasto-plastic model that can capture detailed statistics, shear band formation, and the brittle-to-ductile transition for the deformation of various soft disordered solids.



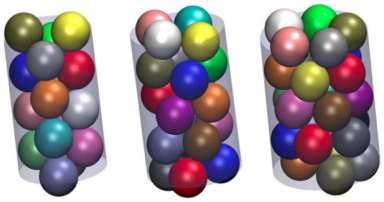
148th MSS-Seminar
Wednesday, June 29th, 15:30 hrs,
Seminar room (00.156),
Cauerstraße 3, Erlangen.

Dense packing of spheres in cylinders

Dr. Adil Mughal

Department of Mathematics, Aberystwyth University

That nature creates forms and structures of great diversity according to the requirements of simple physical laws is a subject of endless fascination. The possible ways in which atoms, spheres or cells fit together into alternative structures depends on both symmetry and the nature of the physical forces involved. While these physical interactions maybe simple, nevertheless the high pressures encountered in strongly confined systems can compel molecules to adopt complex yet ordered arrangements. In such systems there exists an intimate connection between morphology and the precise shape of the container. An example of this is the dense packing of idealised particles inside narrow channels. Extensive results from simulations and experiments have shown that in such systems the particles form extended helical or chiral structures - of the type usually associated with various biological microstructures (e.g. flagella, the morphology of the tobacco virus and microtubules). Such one-dimensional structures are the focus of considerable scientific attention because of their potential utilisation as functionalized devices. This presentation will give a broad historical overview of columnar crystals, the progress that has been made in rationalising them, review some relevant experiments and show that these results generalise to cylinders packed with soft (deformable) spheres



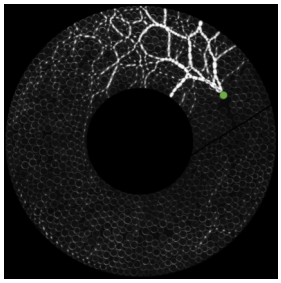
149th MSS-Seminar
Wednesday, July 13th, 15:30 hrs,
Seminar room (00.156),
Cauerstraße 3, Erlangen.

Force networks in particulate systems

Prof. Dr. Lou Kondic

Department of Mathematical Sciences, New Jersey Institute of Technology

Force networks spontaneously form in particulate-based systems. These networks, most commonly known as 'force chains' in granular systems, are weighted, dynamic structures, which are by now known to be of fundamental importance for the purpose of revealing the underlying physical causes of a number of physical phenomena. The presentation will focus on applications of persistent homology (PH) to analysis of such networks found in both simulations and experiments (the figure shows an experimental example). PH allows for a simplified representation of complex interaction field in both two and three spatial dimensions in terms of persistent diagrams (Pds) that are essentially point clouds. These point clouds could be compared in a meaningful manner, meaning that they allow for the analysis of both static and dynamic properties of the underlying systems. In the second part of the talk, we will focus on few case studies: interaction networks in suspensions, and in dry granular systems experiencing stick-slip, intermittent type of dynamics. In the case of suspensions, we will show that the interaction networks are closely related to the rheology, and in the context of stick-slip dynamics, we will discuss potential of the considered approach to explain and possibly even predict system's behavior. If time allows, we will also discuss an ongoing project focusing on computing persistence from experimental data.



150th MSS-Seminar
Wednesday, July 13th, 17:00 hrs,
Seminar room (00.156),
Cauerstraße 3, Erlangen.

Quadrilaterals: ¿simple or complex?

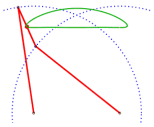
Prof. Dr. Arno Formella

Department of Computer Science, Univsersity of Vigo

Quadrilaterals are well known. All of you learnt their properties, or at least some of them, in school. Actually, they are often used to introduce importants concepts such as classification, subsets, and supersets in a geometric context. However, there are differences in different countries: are squares a special type of rectangles? are parallelograms a special type of trapezoids/trapeziums?

In physics, there are two classes of quadrilaterals you maybe heard of: the Hjelmslev quadrilaterals and the Watt linkages.

This talk presents a complete classification of the (convex) quadrilaterals according to 12 common properties and presents some curious findings and open questions. All done just to develop an application that helps young students in school to study the funny world of quadrilaterals.



151th MSS-Seminar
Wednesday, August 10th, 15:30 hrs,
Seminar room (00.156),
Cauerstraße 3, Erlangen.

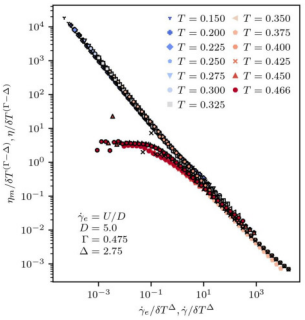
Active microrheology of a bulk metallic glass

Prof. Dr. Ebrahimnazhad Rahbari

School of Chemical and Biological Engineering, Seoul National University

Rheology is the science of response of a material to a deformation rate-- e.g. how much force will be generated by a system to resist the applied deformation. Any deformation will take a time to relax. How can mechanical properties of a material that will never relax, such as a metallic glass, be investigated? In this talk, I will discuss a remedy for this problem. We investigate dynamics of a singled-out probe particle driven into a bulk metallic glass-- akin to a nanoindentation test. We demonstrate that not only one can recover all properties of a metallic glass with microrheology, yet, we found many evidence that microrheology is superior to macrorheology-- the latter only provides an average response. We then use principles of critical phenomena to describe scaling of microrheologycal flow curves.

References:
[1] Yu et al., Science Advances 6, eaba8766 (2020)
[2] Madani et al., Soft Matter Advance Article 17, 5162 (2021)



152nd MSS-Seminar
Wednesday, August 24th, 15:30 hrs,
Seminar room (00.156),
Cauerstraße 3, Erlangen.

Impacts on and interaction with regolith covered surfaces in low gravity

Dr. Jonathan Kollmer

Faculty of Physics, University of Duesburg-Essen

The surfaces of many planetary bodies, including asteroids and small moons, are covered with dust to pebble-sized regolith held weakly to the surface by gravity and contact forces.
The granular mechanics of these surfaces, especially in a regime where gravity and contact forces are of the same magnitude, however are poorly understood so far.
Through a series of low gravity experiments I will show how such a surface reacts to external perturbations.
In a first set of experiments we conduct low velocity impacts and show that even for millimeter sized particles the interparticle cohesion has a major influence on the coefficient of restitution (COR). For rubble pile asteroids this has implications regarding their surface evolution and size sorting effects that have been observed to occur there.
In a second set of experiments we explore the stick-slip mechanics of a granular material in low gravity as is related to technological applications such as digging and anchoring. Both of which are important for future exploration missions to asteroids and the moon.

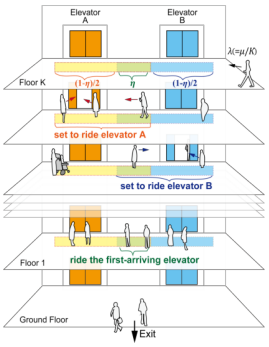
153rd MSS-Seminar
Thursday, September 22nd, 16:30 hrs,
Seminar room (01.021),
Cauerstraße 7, Erlangen.

Do elevators synchronize if not everyone boards an elevator that arrives early?

Ph.D. Sakurako Tanida

Research Center for Advanced Science and Technology, University of Tokyo

Elevators are a familiar transporting system exhibiting nontrivial out-of-equilibrium behaviors. In this study, the dynamic behaviors of elevators are investigated, mainly focusing on the interaction between elevators. I introduced a new control parameter that changes the proportion of passengers who can get in an earlier-arriving elevator and investigated the behaviors of elevators when the proportions of those passengers and the inflow of passengers were varied. When we increased the inflow of passengers, the synchronization was promoted and the round-trip time increased. On the other hand, when we increased the proportion of those passengers, the synchronization was promoted while the round-trip time decreased. To elucidate the relationship between the parameters and dynamics and clarify the mechanism, we established simple mathematical models.



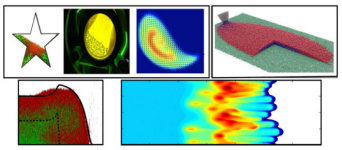
150th MSS-Seminar
Monday, September 26th, 15:30 hrs,
Room P3.88,
Egerlandstraße 3 Erlangen.

MZlti-suale modelling of segregating granular flows: From particles in a laboratory heap to a vulcano

Prof. Anthony Thornton

Department of Fluid and Thermal Engineering, University of Twente

Many granular flows in the natural environment or in industry are segregating, shallow and rapidly moving. Examples include snow avalanches, landslides, debris flows, pyroclastic flows to industrial flows in rotating drum mixers, kilns and crushers. It is important to be able to predict the degree of segregation in such flows, as it is vital for the accurate prediction of the dynamics.
Continuum methods are able to simulate the bulk behaviour of such flows, but have to make averaging approximations, reducing the degrees of freedom of a huge number of particles, to a handful of averaged parameters.
On the other hand, the discrete particle method is a very powerful computational tool that allows the simulation of individual particles, by solving Newton's laws of motion for each particle. With the recent increase in computational power it is now possible to simulate flows containing a few million particles; however, for 1mm particles this would represent a volume of approximately 1 litre, which is many orders of magnitude smaller than the flows found in industry or nature.
This talk will focus on a simplified example of bi-dispersed (by size and density) dry granular flows, on inclined planes, in rotating drums and in the natural environment. We will investigate these problems via both the continuum modelling approach, particle simulations and compare with experiments. Then we will show how the particle simulations can be used to calibrate the continuum model. Finally, we will discuss how to calibrate the particle simulations from simple laboratory unit tests, resulting in a fast multi-scale framework that can predict segregation in both industry and the natural environment.



Images showing work on segregation. Top left: Experiments (Optical, RIMS, PEPT). Top right: Particle simulations of dry segregation out of a hopper. Bottom left: Validation of analytical model with simulations. Bottom right: Continuum simulation of segregation-mobility feedback.

155th MSS-Seminar
Wednesday, September 28th, 15:30 hrs,
Seminarraum 00.156,
Cauerstraße 3 Erlangen.

Power fluctuations in sheared amorphous materials

Prof. S. H. Ebrahimnazhad Rahbari

School of Chemical and Biological Engineering, Seoul National University

We recently used a stochastic thermodynamics approach to describe power fluctuations in frictionless [1] and frictional [2] amorphous materials in first-principle simulations. In this approach, we treated the injected power as a stochastic thermodynamic quantity which equals stress multiplied flow rate. However, a quantitative comparison with mean-field elastoplastic models such as Soft Glassy Rheology was not possible because these models consider only stress fluctuations and the flow rate is an average quantity. Recently, a theory specifically developed to address our work [Phys. Rev. E 105, L052601 (2022)] which treats both stress and flow rate as stochastic processes. In this talk, we give an overview about our approach and where possible we make qualitative and quantitative comparisons with the above mentioned model.

References

[1] S. H. E. Rahbari et al, Nat. Comm. 8, 11 (2017).
[2] S. H. E. Rahbari, M. Otsuki, and Thorsten Poeschel, Nat. Comm. Phys. 4, 71 (2021).

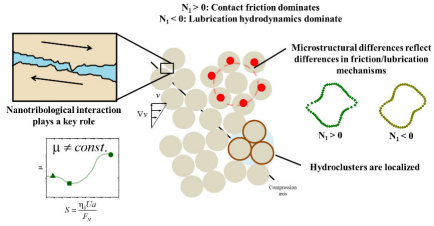
156th MSS-Seminar
Wednesday, October 5th, 15:30 hrs,
KS I,
Cauerstraße 4, Erlangen.

MiZrostruutcre anp Rheology of Concentrated Colloidal Suspensions with Varying Nanotribological Interactions

Dr. Yu-Fan Lee

Department of Chemical Engineering, Delft University of Technology

The shear thickening of dense colloidal suspensions is an active area of research to understand the non-linear flow response relevant to various processing conditions, such as high-speed coating, spraying, printing, pumping, and other industrial applications. Efforts in theoretical models and simulations seek to examine the underlying physical forces acting between particles in the suspension, including nanotribological forces such as lubrication hydrodynamics and frictional contact forces, to predict suspension shear rheology. However, few experimental investigations directly measure the nanotribological forces acting between particles or measure the associated suspension microstructure under flow, despite these being essential for connecting colloidal forces to the measured bulk rheology. Thus, there is a scientific need to perform direct nanotribological and microstructural measurements to resolve the origins of this complex rheological behavior. Such research has technological value for improving the processing of high solid dense suspensions, which is often limited by shear thickening, and commercial products that benefit from the shear thickening behavior, such as door stops and speed bumps and armor movement reactive fabrics. The overarching goal of this thesis is to systematically investigate how the nanotribological interactions affect the microstructure and rheology of concentrated colloidal suspensions.



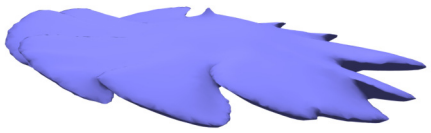
157th MSS-Seminar
Wednesday, October 26th, 15:30 hrs,
04.023,
Cauerstraße 7, Erlangen.

Understanding Hydraulic Fracture through X-Ray Tomography

Laureano Ortellado

Department of Physics, Universidad Nacional del Sur-IFISUR-CONICET

Hydraulic fracturing of solids is a rich and complex physical phenomenon. Currently, hydraulic fracturing is a process commonly used in the petroleum industry, in hydrocarbon production and well stimulation. Despite being widely used, hydraulic fracture is still poorly understood, in part because it depends on mechanisms that operate at multiple length scales. Even in homogeneous materials, hydraulic fracture subjected to mixed loading conditions (tension and shear stresses) becomes unstable and displays interesting fragmented fracture patterns. Here we study hydraulic fracture of gels through X-ray tomography (CT). This allows us to obtain the three-dimensional details of the crack-front under such mixed loading. By using the CT image of the crack, we perform finite element analysis to infer fracture mechanics parameters that otherwise will be inaccessible by experimental methods.



158th MSS-Seminar
Monday, December 19th, 18:30 hrs,
Seminarraum (00.156),
Cauerstraße 3, Erlangen.

Simulation of the laser melting process of titanium using Smoothed Particle Hydrodynamics

Michael Blank

Institute for Multiscale Simulation, University of Erlangen-Nuremberg

The high heating rates generated by focused laser beams are utilized in a range of industrial applications such as laser welding, Selective Laser Melting (SLM), or wire-based Laser Metal Deposition (LMD-w). Inappropriate processing parameters may lead to material defects that deteriorate the mechanical properties of the weld or the manufactured part. To some extent, this is caused by a lack of understanding of the influence of the process parameters on the governing physical effects arising in laser-metal processing (see Fig. 1).
This work presents a three-dimensional numerical model based on the Incompressible Smoothed Particle Hydrodynamics method capable of simulating liquid flow dynamics, heat transfer, and phase transitions of titanium simultaneously. In a series of simulations of single-line laser tracks on titanium metal sheets, the influence of the material's optical properties, laser process parameters, and the emerging vapor on the weld geometry is investigated. Moreover, the influence of the wetting forces on the melt geometry is studied. The fragmentation of the melt, also known as humping in laser welding, as shown in Fig. 2, is observed when large temperature gradients across the solid-liquid interface occur. Strategies to avoid humping are presented subsequently.
Finally, the LMD-w process of titanium is simulated both with and without gravitational forces. A more continuous deposition of titanium can be achieved when using LMD-w in zero-gravity environments.

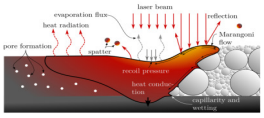


Fig. 1: Physical phenomenon arising in laser-metal processing.

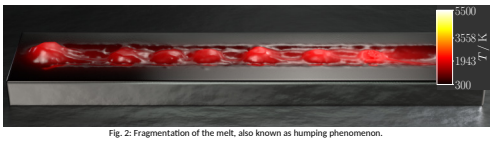
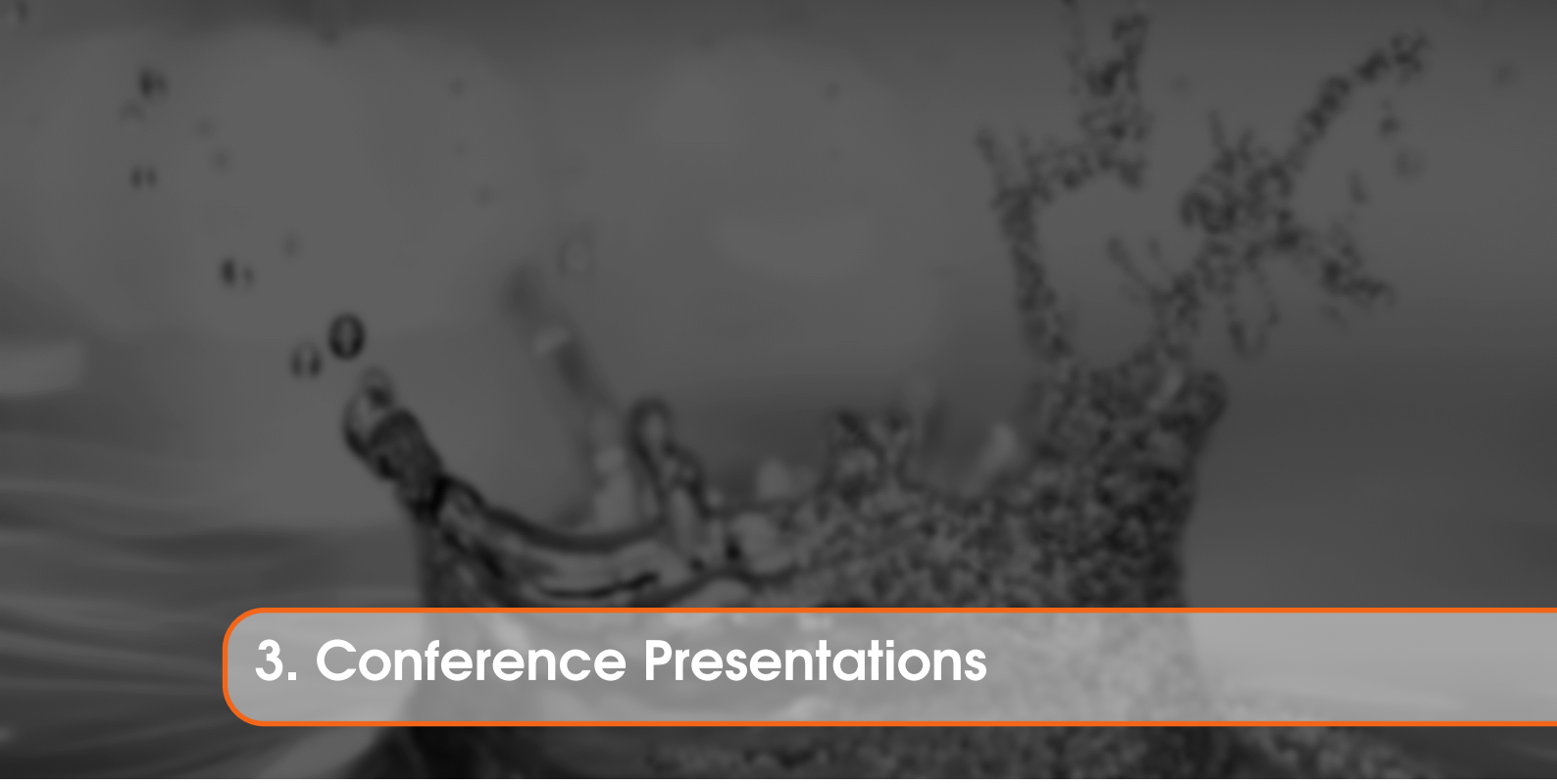


Fig. 2: Fragmentation of the melt, also known as humping phenomenon.



3. Conference Presentations

- Olfa D'Angelo:
  Rheology of Lunar Regolith and its Simulants (poster presentation)
  Heraeus-Seminar: Mesoscopic Triboelectricity – from Patches to Particles to Planets
  17-20 January, 2022, Heraeus, Germany
- Olfa D'Angelo:
  From granular rheology to 3D printing in space – and back (oral presentation)
  ESA/ESTEC Netherlands - Meeting number 10 of the TEC-QEE Young Researchers' Forum
  23 February, 2022, Netherlands
- Thorsten Pöschel:
  Electro Impedance Tomography For Bubble Detection in Two-Phase Pipe Flow (oral presentation)
  ROBIN online meeting
  25 March, 2022, Dresden, Germany (online)
- Sudeshna Roy:
  Modelling granular materials: From particle simulations towards continuum (oral presentation)
  Institute of Fluid Mechanics and Environmental Physics in Civil Engineering, Leibniz Universität Hannover
  11 April, 2022, Hannover, Germany
- Thorsten Pöschel:
  Granular Packings due to Sequential Deposition: Structure and Relation to History and Dynamics (oral presentation)
  Statistical Mechanics
  3 May, 2022, Shanghai, China (online)
- Carlos L. Bassani:
  Hydrate Management: from theory to practice (oral presentation)
  SPE Brazil Flow Chat 11
  12 May, 2022, online
- Michael Blank:
  Computersimulationen - von Disney zur ISS (Computer Simulations - Frome Disney to ISS) (oral presentation)
  Die Lange Nacht der Wissenschaften (The Long night of Science)
  12 May, 2022, Erlangen, Germany

- Olfa D'Angelo:
  The Manifold Rheology of Granular Fluids (oral presentation)
  Dutch Soft Matter Meeting
  1 June, 2022, Delft, Netherlands
- Michael Engel:
  Kinetics and Anisotropy in Nanoparticle Assembly (oral presentation)
  Gordon Research Conference (GRC) on Noble Metal Nanoparticles
  12-17 June, 2022, South Hadley, USA
- Carlos L. Bassani:
  Hydrate Management by Pore-Sealing in Oil-Continuous Systems (oral presentation)
  ECGH 2022 – European Conference on Gas Hydrates
  13-16 June, 2022, Lyon, France
- Nydia Roxana Varela-Rosales:
  Effect of a Periodic Substrate on the Stability of a Dodecagonal Quasicrystal (oral presentation)
  PERIODIC 2022 – 10th International Conference on Aperiodic Crystals
  20-24 June, 2022, Sapporo, Japan (online)
- Olfa D'Angelo:
  The Manifold Rheology of Granular Fluids (oral presentation)
  Granular Matter Gordon Research Conference
  26 June, 2022, Easton, USA
- Olfa D'Angelo:
  Constitutive Laws for Dense Franular Fluids (oral presentation)
  Granular Matter Gordon Research Conference
  26 June, 2022, Easton, USA
- Michael Blank:
  Einfluss der Oberflächenqualität auf die Schmelzgeometrie beim Laserschmelzen von Titan (oral presentation)
  Industriebeirat des Sonderforschungsbereichs 814 - Additive Fertigung
  28 June, 2022, Erlangen, Germany
- Igor Goychuk:
  Nonlinear stochastic dynamics with memory in application to problems of biological physics (oral presentation)
  University of Augsburg
  5 July, 2022, Augsburg, Germany
- Thorsten Pöschel:
  3D-Druck im Weltall (keynote speaker)
  Förderkreis Ingenieurstudium - Schüler-Team-Wettbewerb
  6 July, 2022, Erlangen, Germany
- Nydia Roxana Varela-Rosales, Angel Santarossa, Michael Engel, Thorsten Pöschel:
  Effect of size Dispersity on the Efficiency of Granular Dampers (oral presentation)
  ESMC 2022 - 11th European Solid Mechanics Conference
  4-8 July, 2022, Galway, Ireland
- Patric Müller, Holger Götz, Angel Santarossa, Achim Sack, Thorsten Pöschel:
  Soft particles reinforce robotic grippers: robotic grippers based on granular jamming of soft particles (oral presentation)
  ESMC 2022 - 11th European Solid Mechanics Conference
  4-8 July, 2022, Galway, Ireland
- Michael Engel:
  Bifurcation of Colloidal Crystallization in a Sphere" (oral presentation)
  CECAM-Meeting - Complex colloidal crystals: Formation, inhomogeneities and defects
  11-14 July, 2022, Vienna, Austria

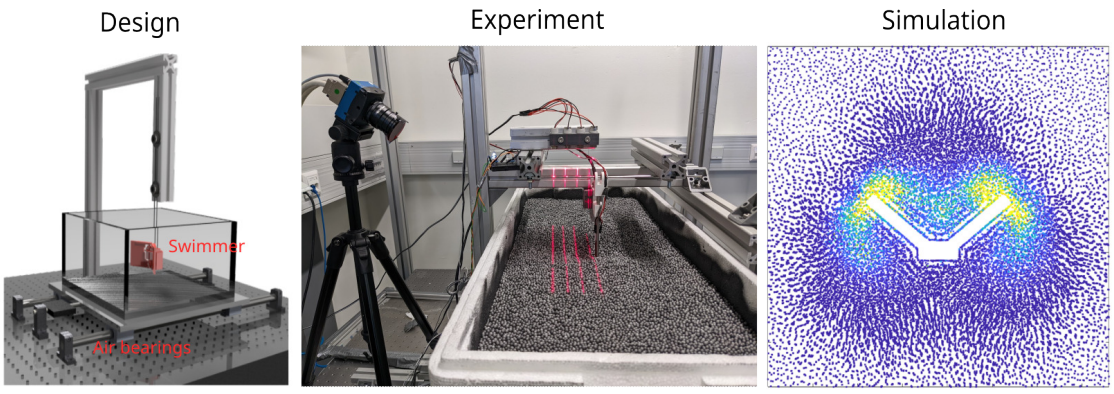
- Igor Goychuk:
  Quantum ergodicity breaking: Do ensemble theories suffice to describe statistics of single-electron transfer events in complex environments? (oral presentation)
  University of Stuttgart
  14 July, 2022, Stuttgart, Germany
- Vasileios Angelidakis:
  Towards Systematic Image-Informed Modelling of Granular Materials with Irregular Particles (invited keynote oral presentation)
  2022 International Conference on Green Intelligent Mining for Thick Coal Seam
  23-25 July, 2022, Beijing, China (online)
- Thorsten Pöschel:
  Fractal Dimension due to Sequential Deposition (oral presentation)
  Statistical Mechanics
  28 July, 2022, Berlin, Germany
- Ali Mauricio Velasco, José Daniel Muñoz, Thorsten Pöschel:
  Iterative Simulation of Fractures in Brittle Solids using Multisphere DEM (oral presentation)
  15th World Congress on Computational Mechanics (WCCM-XV)
  8th Asian Pacific Congress on Computational Mechanics (APCOM-VIII)
  31 July - 5 August, 2022, Yokohama, Japan (online)
- Holger Götz:
  DEM Simulation of Thin Elastic Membranes for Granular Jamming Applications (oral presentation)
  CMM-SolMech 2022 conference
  5-8 September, 2022, Świnoujście, Poland
- Atharva Pandit, Achim Sack, Thorsten Pöschel:
  Multi-Axial X-Ray Tomography (poster presentation)
  Image is Everything - Lorentz Centre, Leiden University
  12-16 September, 2022, Leiden, Netherlands
- Sudeshna Roy:
  Mechanisms across scales: A holistic modelling framework for reverse phase wet granulation (oral presentation)
  DFG Emmy Noether programme
  16 September, 2022, Erlangen, Germany (online)
- Federico Tomazic, Michael Engel:
  Modelling Anisotropic Interactions: Application to Tripods (poster presentation)
  Particle Based Material Symposium
  6 October, 2022, Erlangen, Germany
- Sudeshna Roy:
  Multiscale modelling of particulate systems (oral presentation)
  Stuttgarter Zentrum für Simulationswissenschaft, Universität Stuttgart
  7 November, 2022, Stuttgart, Germany
- Michael Blank:
  Temperature Gradients as a Source of Balling and Humping in Laser Processing of Titanium (oral presentation)
  Casablanca International conference on additive Manufacturing
  23-24 Novomber, 2022, Casablanca, Morocco
- Sudeshna Roy:
  Local Structural Anisotropy in Particle Simulations of Powder Spreading in Additive Manufacturing (oral presentation)
  Casablanca International conference on additive Manufacturing
  23-24 Novomber, 2022, Casablanca, Morocco

4. Selected Postdoc Projects

Dr. Hongyi Xiao, "Swimming with reciprocal motion in granular media"

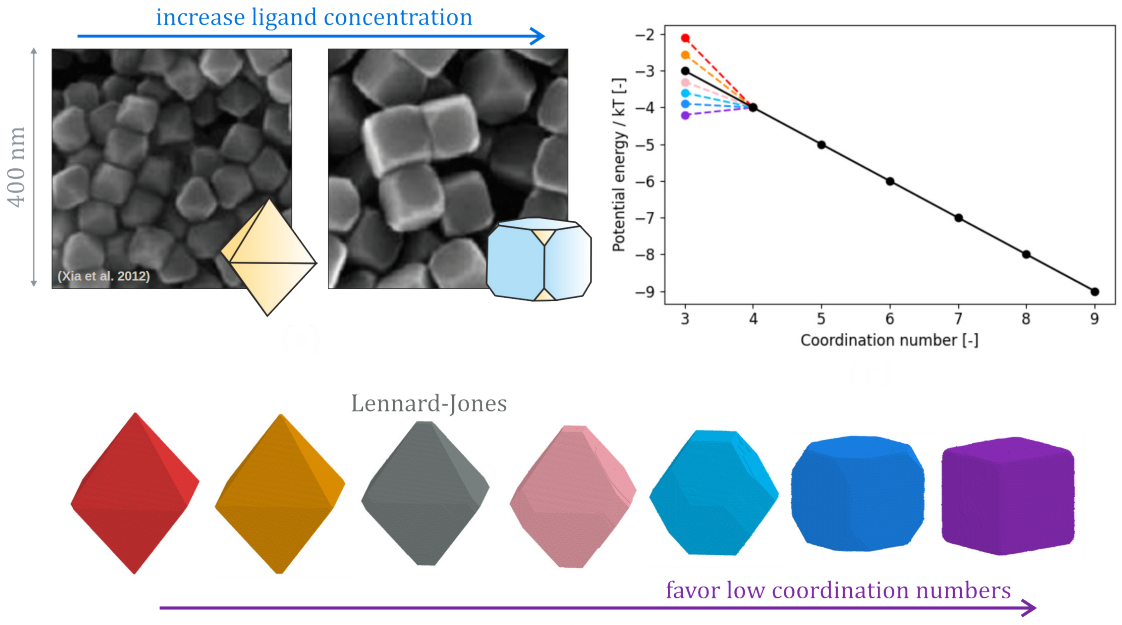
Locomotion in soft yielding media is difficult to model and design due to the complexity of their rheology, as these materials can show both liquid-like and solid-like behaviors. In this study, we demonstrate that a reciprocal swimmer is capable of generating propulsion in a granular medium, which is not possible for swimming at low Reynolds number in Newtonian liquid, i.e., the scallop theorem. Understanding this behavior can reveal important rheological properties of granular materials, and can help designing simple and robust mechanisms for traversing in soft disordered media.

To investigate, an experimental system is designed, which contains a scallop-like swimmer that opens and closes its wings in a perfectly reciprocal way inside a granular media. The resulting displacement and force can be measured, along with the surface deformation of the granular medium. Corresponding Discrete Element Method (DEM) simulations are performed, which well reproduce the experimental observations. Preliminary analysis indicates that the swimmer-induced transition of the granular materials between solid-like and liquid-like state could be responsible for the observed locomotion.



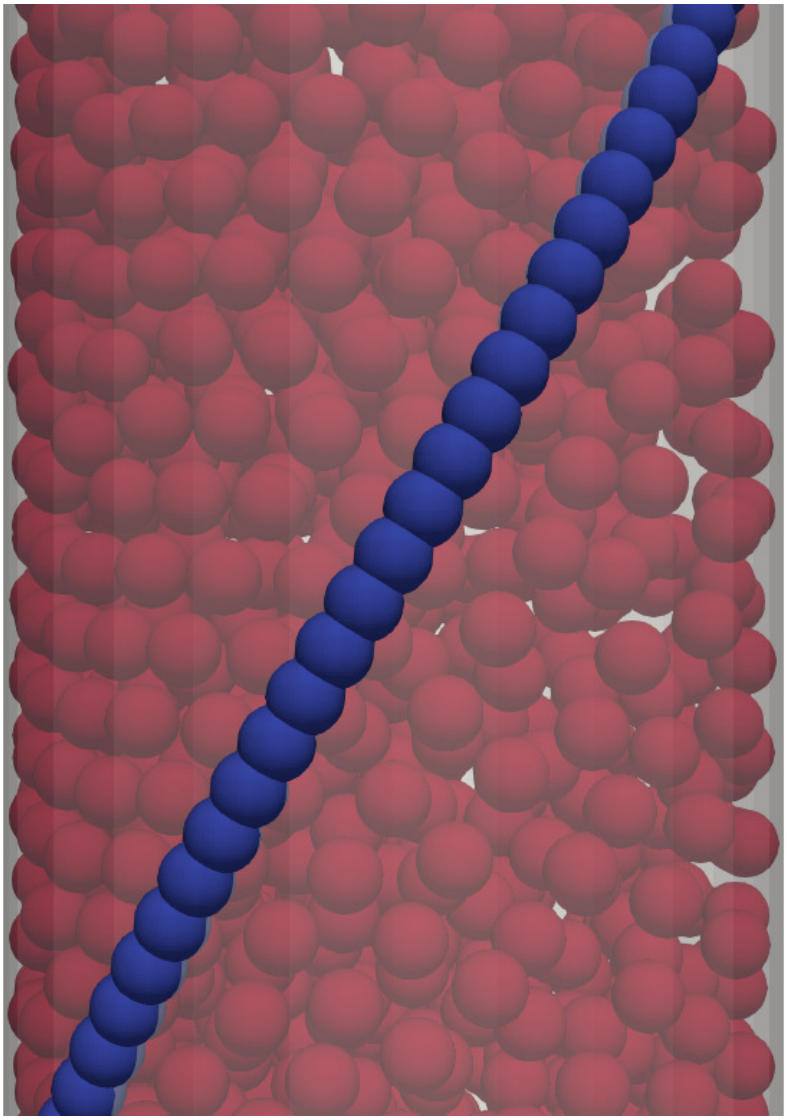
Dr. Carlos Lange Bassani, "Grand canonical Monte Carlo simulations of crystal growth based on surface energy sampling"

Crystals are ubiquitous materials in nature and science and are at the core of technology evolution along history. The same way science was able to tune material properties at the macroscale by mastering phase diagrams of metal alloys, tuning material properties at the nanoscale through nanoparticle synthesis and their self-assembly is expected to represent a similar cutting edge scientific revolution in the next decades. This project focus on enhancing the fundamental understanding and developing suitable simulation tools that capture such interchange in between scales in crystallization processes for better predicting nanoparticle shapes. The goals include understanding the role of ligands and temperature in the initial steps of faceting of nanoparticles and during facet transformations, thus enlightening the mesoscale events known as symmetry preservation, symmetry breaking, and twinning. The simulations are held in a new grand canonical ensemble, where the surface energy is sampled and new particles are added in a Monte Carlo approach. The specific system of study comprises gold and silver nanoparticles, being body-centered cubic and face-centered cubic crystal structures of importance. The effects of preferential adsorption of ligands in different crystal directions are indirectly modeled by a Lennard-Jones pair potential biased depending on the particle coordination numbers, in a similar fashion to the Embedded Atom Method (EAM), which shows able to capture different nanoparticle shapes as observed from experiments.



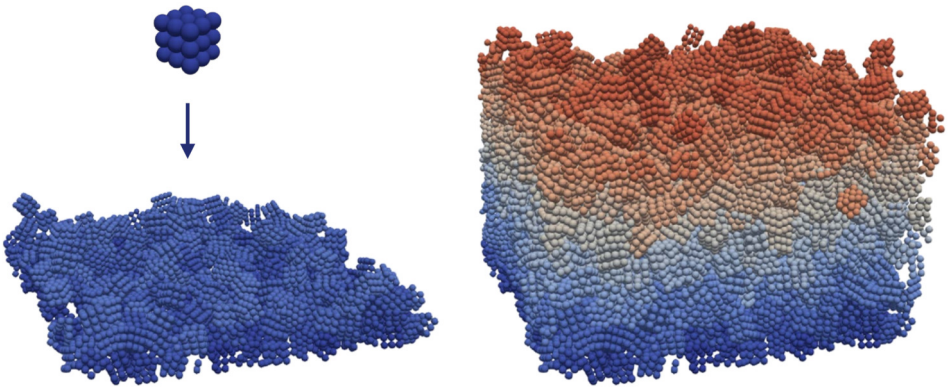
Dr. Artem Panchenko, “Homogenization of Granular Pipe Flow”

A granular pipe flow is intrinsically unstable and characterised by a variety of significant inhomogeneities (density waves). This behavior can lead to clogged or damaging pipes and/or equipment and to segregation of flow in the case of a mixture of different particles. It is necessary to re-prepare the segregated mixture after transportation for use. To produce a controlled, metric mass flux and homogeneous flow of granular material through a pipe is a challenging modern problem. By means of particle-based numerical simulations using the Discrete Element Method (DEM) we will investigate the influence of pipe texture on granular flow. We will determine the mechanism of formation of density waves and find optimal designs of texture of the inner tube-wall to control the various granular materials flow. First we focus on the segregation of gravity-driven mixtures in vertical pipes. Next, the horizontal flow of particles created by the flow of a gas or liquid will be investigated.

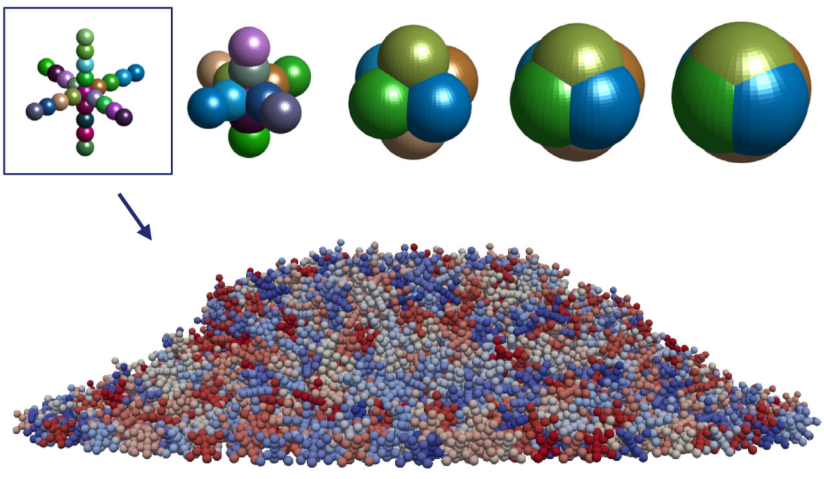


Dr. Vasileios Angelidakis, "Sequential Particle Deposition & Mechanical Properties of Granular Metamaterials"

The behavior of granular materials with irregular particles is widely unexplored. Particle shape plays a key role in the packing, mechanical and rheological properties of granular systems, and yet a straightforward link between particle shape and shear strength or flowability at the bulk scale has not been established. This is partly due to the fact that simulating irregular, highly concave particles is computationally challenging. A sequential particle deposition algorithm previously developed by the group allows for the packing of multi-million-particle assemblies within affordable time-runs. This algorithm is currently being equipped with a user-interface, and will be shared as an open-source software package. In addition, a new class of *granular metamaterials* exhibit extraordinary properties compared to conventional materials, such as the high capacity to interlock, due to their complex particle shapes. We use the Discrete Element Method to gain micro-mechanical insights into the behavior of systems made of these particles, seeking micro-to-macro links between particle-scale features and bulk-scale observed behavior.



sequential particle deposition

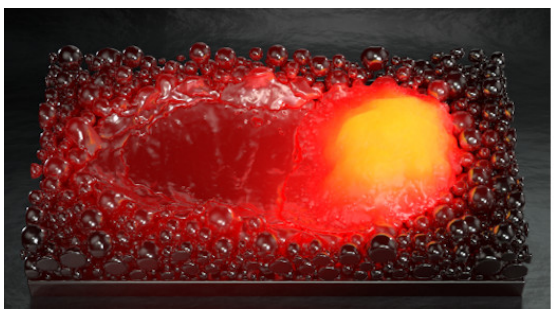


mechanical granular metamaterials

5. Ongoing PhD Projects

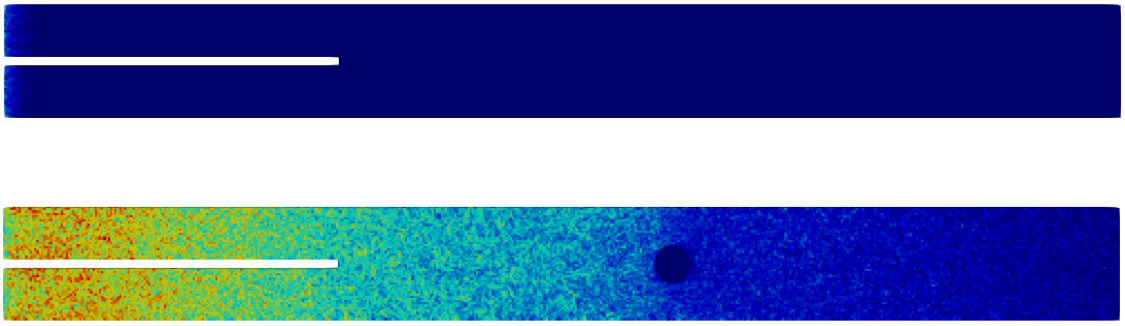
Michael Blank, "Simulation of the selective laser melting process"

The ability to generate high-energy radiation has made lasers an essential tool in metal processing. Inappropriate processing parameters may lead to material defects that deteriorate the mechanical properties of the weld or the manufactured part. This work presents a three-dimensional numerical model based on the Incompressible Smoothed Particle Hydrodynamics method which describes heat transfer, phase transitions, and liquid flow simultaneously. The interaction of laser radiation with an arbitrarily shaped material surface is modeled using a ray tracing approach. In a series of laser welding simulations, the influence of the material's optical properties and laser process parameters on the on the weld geometry is investigated and compared to experiments. In simulations of the wire-based Laser Metal Deposition (LMD-w) it is found that the absence of gravity has a positive effect on the stability of the formed liquid bridge and, therefore, improves the continuous deposition of molten metal, as shown in the right figure. Finally, the Selective Laser Melting (SLM) process of a polydisperse titanium powder bed is investigated. The coalescence of the melt and the formation of a depression of the melt pool behind the laser spot, as shown in the left figure may be attributed to the balling phenomenon which should be investigated in future work.



Felix Buchele, "Reactive Flow in Porous Media"

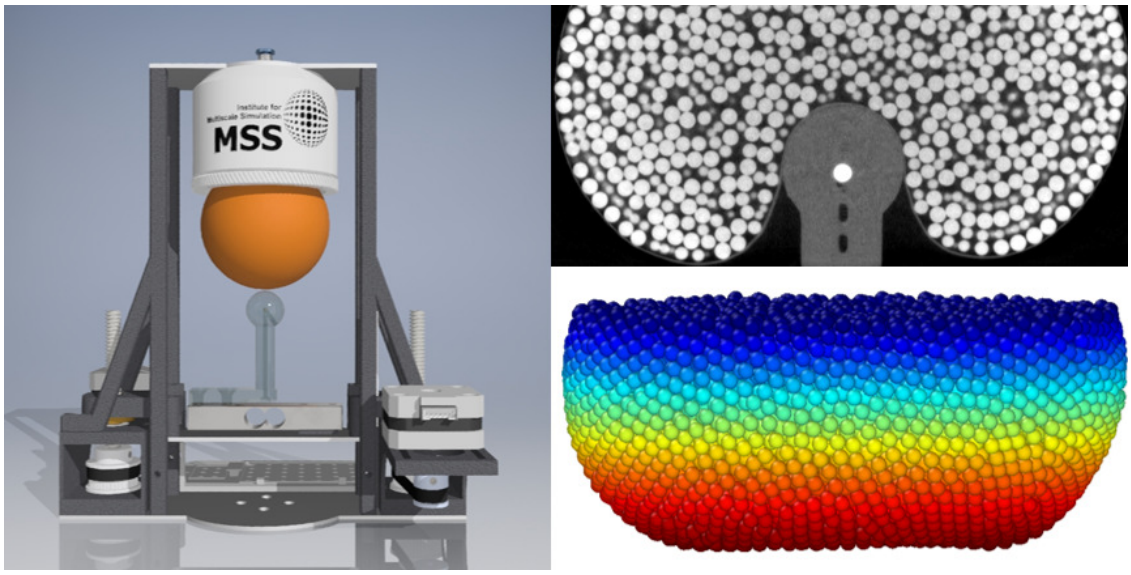
Porous catalysts are important materials in the chemical industry and may contribute to the future of our mobility by being key parts of electrolyzers and fuel cells. Understanding flow and reaction kinetics in porous catalysts however is limited to microscopic and macroscopic points of view. With tools like Density Functional Theory (DFT) one can investigate the properties of catalytic surfaces on a microscale. On the other hand, there are semi-empirical differential equations describing the properties of catalytic systems on a macroscopic, engineering scale. However, mesoscopic tools to investigate flow within porous catalysts and chemical reactions based on rate equations are virtually non-existent.
The aim of this thesis is therefore to develop suitable methodologies to simulate complex, catalytic reactions and flow in porous catalysts. The range of of adequate tools is however limited by the small characteristic length scales in porous catalysts. Flow in microchannels, is similarly to rarefied gas flow, governed by collisions with boundaries rather than intermolecular collisions. Continuum equations such as the Navier-Stokes equations are therefore not applicable anymore, since their continuum assumption does not hold true anymore. On the other hand, the length and time scales of flow within the porous structure of a catalyst are too large to efficiently perform molecular dynamics (MD) simulations. To bridge this gap, a Direct Simulation Monte Carlo (DSMC) code is chosen as a suitable tool.
The surface reactions will be modeled following mesoscopic rate equations for Langmuir-Hinshelwood kinetics with detailed adsorption and desorption computation. However, following the general idea of DSMC being a stochastic simulation method, adsorption, desorption and reaction will be modeled using efficient stochastic approaches.



Angel Santarossa, "Mechanics of granular grippers"

Robotic granular grippers are an emerging and promising technology whose main feature is their high adaptability to grasp a wide variety of objects of different shapes and sizes. They comprises a conglomeration of macroscopic particles contained within a flexible membrane. When pressed against an object, the granular assembly will deform around the object. Once the gripper has effectively taken the shape of the object, a vacuum pump may be used to evacuate the system, compressing the particles and causing them to become 'jammed', i.e. to form a static, rigid, solid-like body. Once the jamming state has been achieved, when the gripper is retracted, it will exert a lifting force on the object.

Despite its advantages, current-generation systems are far from being fully developed and optimized, by which their application to the industrial sector is still unsuccessful. In this sense, the interior dynamic of the granular material remains almost unresearched. My PhD. project is focused on the experimental study of granular gripping systems. The experimental branch of this work includes the design and construction of granular gripper prototypes, the generation of data to calibrate simulation models and the study of the internal granular structure of these grippers through x-ray computer tomography. An in-depth understanding of the particle-scale processes in these gripping systems let us enhance their grasping capacity and performance. For instance, we have significantly improved the granular gripper's performance through the use of soft particles as filling material and revealed the effect of particle's size on the suction mechanism of these systems. Within this project, I closely collaborate with Holger Götz for the simulation part and with Olfa D'angelo and Achim Sack in the experimental part.



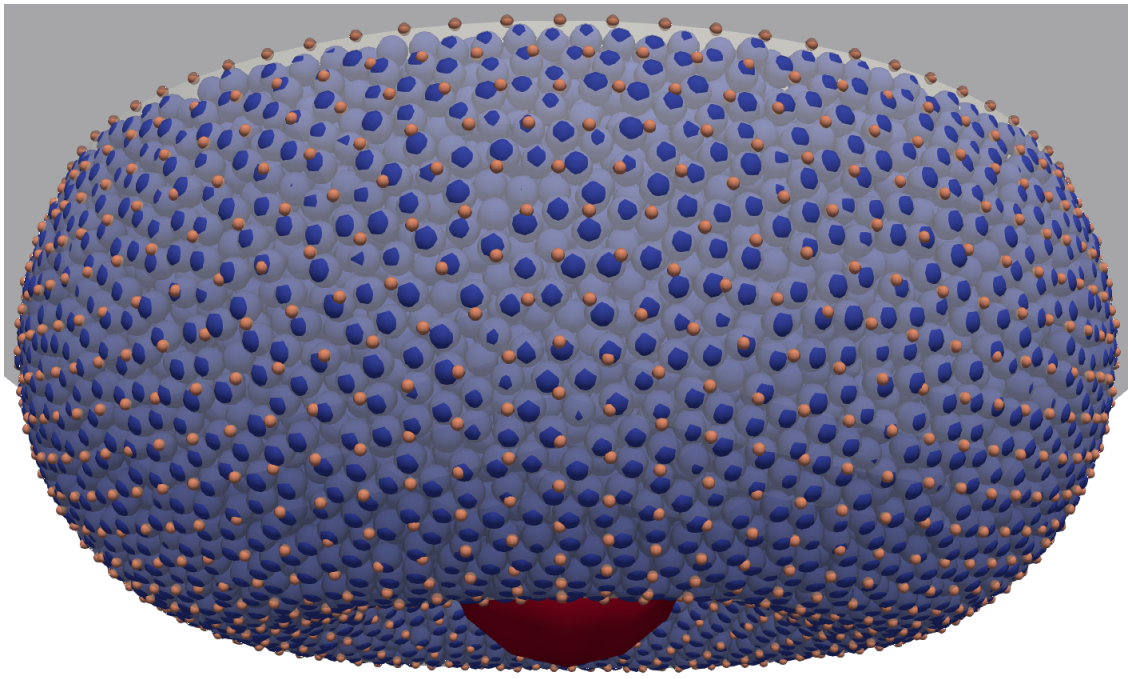
Mauricio Velasco, "Fragmentation in large scale DEM simulations"

Grain and bulk fragmentation is a very important phenomena in the dynamics of granular media. In the field of cominution, the study of fragment shape and size distribution is of great relevance for industrial applications like milling and soils transporting. The aim of this project is to build an accurate and fast extension to the Discrete Element Method in such a way that grains with a realistic irregular shape and their fragmentation processes can be simulated in large scale systems (ca. 10^7 grains). The irregular shape of the grains is represented by a clump of overlapping spheres, after a fracture occurs, the shape of the fragment is tracked and a new multisphere representation is computed. The fracture criteria of the grains is modeled by computing the stress strain energy field on the particles.

Holger Götz, "Optimization of a robotic granular gripper using simulations and machine learning"

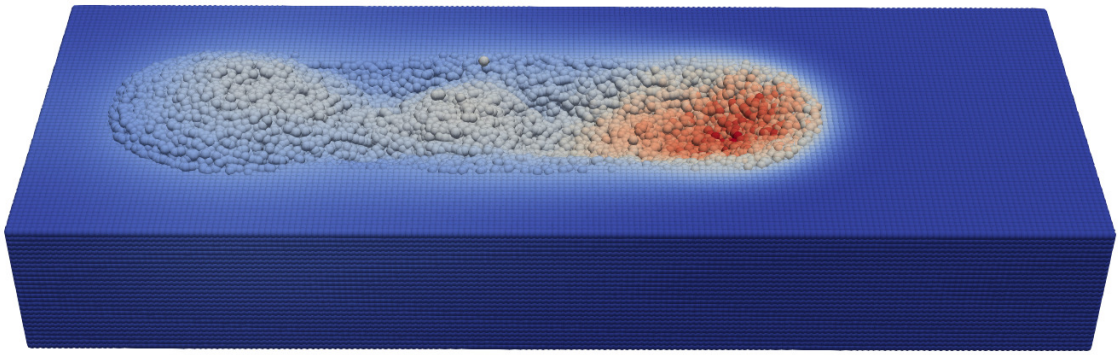
Within my PhD, I am focusing on the granular gripper. The granular gripper is a robotic end effector, that consists of particles enclosed by a flexible membrane. Such grippers exploit the process of granular jamming to manipulate a vast range of diverse objects and represent a hugely promising nascent technology with potential applicability spanning almost all industrial sectors. While these soft-robotic grippers carry the potential to prove transformative to the modern manufacturing process, current-generation systems remain unoptimised and unreliable, and their microscopic dynamics and structures almost entirely unresearched.

Within this PhD project I am developing a simulation model for the granular gripper. This model is used to get a better insight in the interior of the gripper, as this is hard to study using conventional experimental techniques. These insights are used to improve the gripper, potentially with automatized optimizations using machine learning techniques such as artificial evolution. Because my PhD focuses on a computational model of the gripper, I closely collaborate with Angel Santarossa for the experimental part.



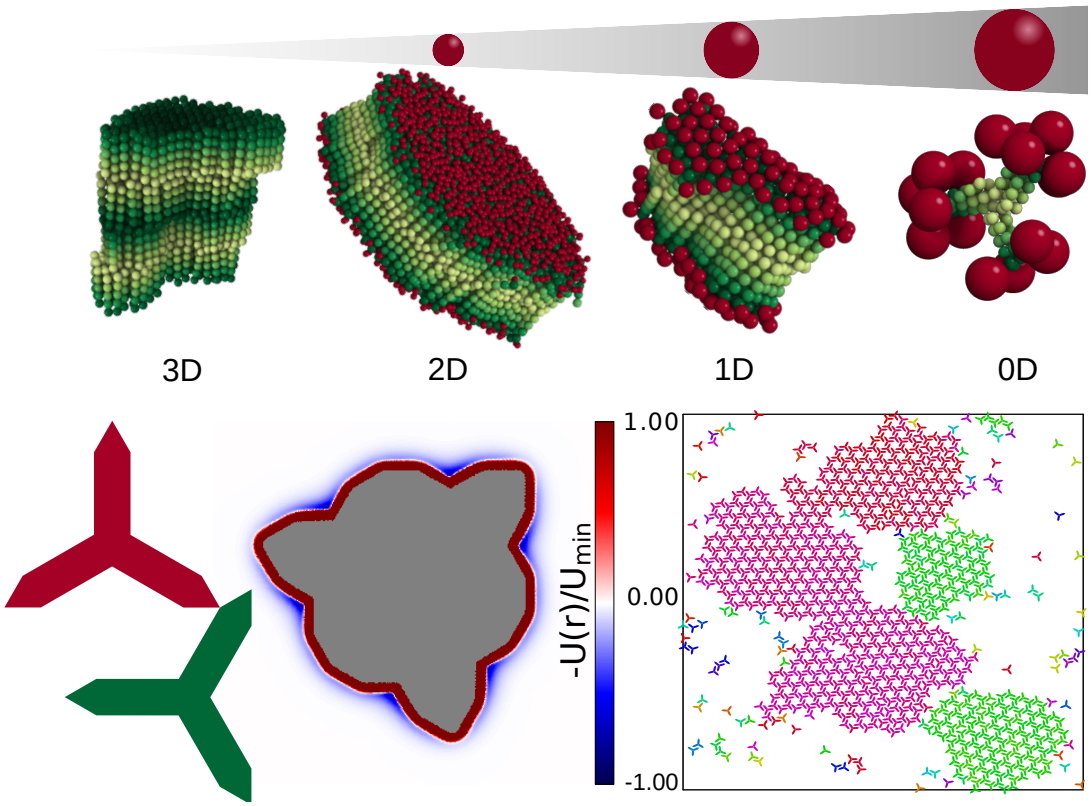
Sarthak Jadhav, "Optimizing energy distrbution for laser additive manufacturing"

The process of laser additive manufacturing is rather new and it comes with its advantages and disadvantages. One particular problem with selective laser melting is its low efficiency i.e. the rate of manufacturing is low while the energy used is high. This research deals with this problem by optimizing the energy distribution of the laser beam which can affect the heat and mass transfer of the melt pool. The current industrial standard for energy profile of laser in additive manufacturing is the Gaussian beam. Changing it to other profiles like doughnut shape (ring laser) may increase productivity. The simulation technique used for this research is smoothed particle hydrodynamics. It is a mesh-free Lagrangian where the domain is discretized by particles which are interpolation points and carry its own physical properties. The influence of particles on each other is determined by a kernel function. This code contains models for raytracing, heat transfer(radiation, conduction and convection), recoil pressure, surface tension, phase transitions(melting, resolidification, vapourization), etc. These models allow the code to efficiently deal with the problem statement mentioned above.



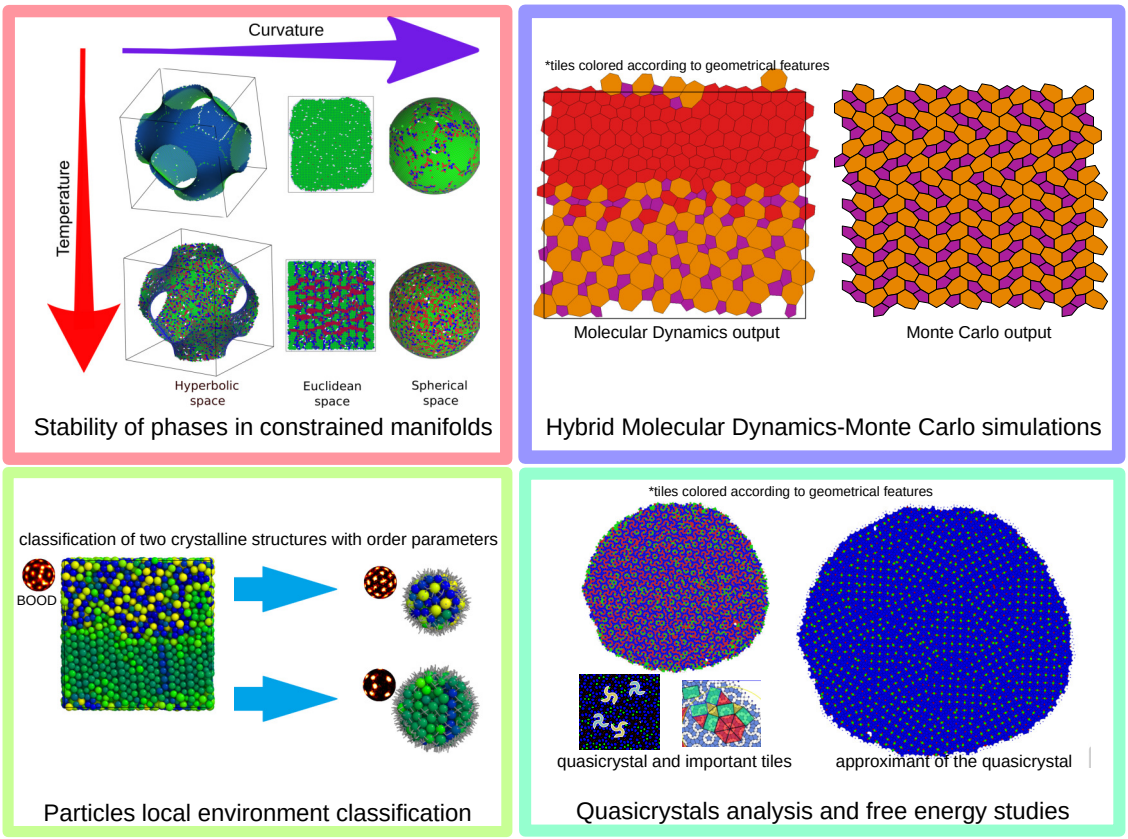
Federico Tomazic, “Modelling particle aggregation and assembly into optimal structures”

The self-assembly mechanisms of nanoparticles controls the formation of robust nanostructures, which have applications as structural color pigments and scaffolds for heterogeneous catalysis. In this project, new methods are developed to study not only the self-assembly process itself, but also the properties of the self-assembled structures, in the frame of the Collaborative Research Centre Design of Particulate Products. We are particularly interested in complex building blocks, because of the plethora of structures they can form and the difficulty of modelling the interaction between them. Complexity can be achieved by shape or by interactions. An example of complexity by shape is provided by the crystallization of polymeric ligands in rigid bundles. By coarse-grained molecular dynamics simulations, we find that by tuning the dimension of the ligand bundles we can control the shape of the self-assembled structures and obtain 0, 1, 2 and 3 dimensional clusters. To model the interaction between non spherical nanoparticles, we have to take into account that the potential is not only a function of the distance between the particles, but also of their orientation. Therefore, we develop a method that uses Derjaguin integration to calculate the potential between any two differently oriented nanoparticle faces. We apply this method to tripods, two-dimensional non-convex nanoparticles. We tabulate the potential between two tripods at different orientations. We then perform coarse-grained molecular dynamics simulations to observe how different potentials affect the self-assembly.



Nydia Roxana Varela-Rosales, "Thermodynamics and stability of aperiodic structures"

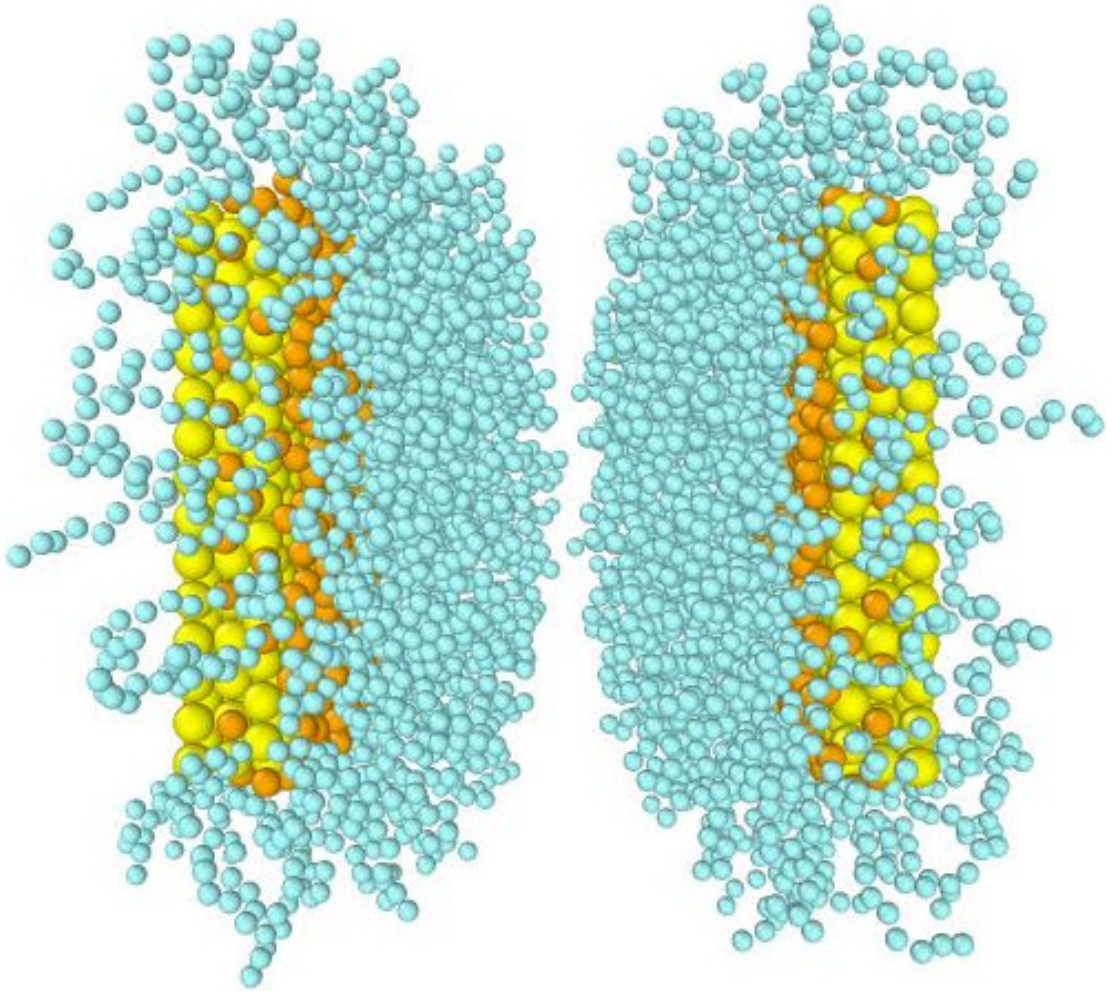
Quasicrystals are crystalline structures that lack periodicity (aperiodic structures). These structures revolutionized the field of crystallography just a few years back. These materials are found in all classes of substances, from mono/multi-component elements to one of the building blocks of life, proteins. Despite progress in understanding these structures, the answer to how their aperiodic order affects physical properties is still unclear. My thesis aims to develop a comprehensive understanding of the thermodynamics and stability of these aperiodic long-range order structures under circumstances where external constraints such as external forces and manifold constraints are taking place. With this, we use and develop particle local environments classification algorithms to characterize the different symmetries found in computational simulations of particles. As well we employ advanced free energy methods to analyze the stability of these structures. We also use hybrid sampling of the space to investigate quasicrystal approximants formation to facilitate descriptions that were only possible using quantum mechanical simulation approaches.



Zhiyu Song, "Atomistic molecular dynamics simulation of the interaction between self-assembled ligand monolayers"

Nanocrystals covered with alkane ligands possess a great potential for applications due to the high tunability of the interaction between the monolayers. An understanding of the interaction is still lacking with open questions remaining from past computational and experimental studies. Further developing and testing methodologies to better model monolayers at atomistic resolution and predict the interactions strength and specificity is essential.

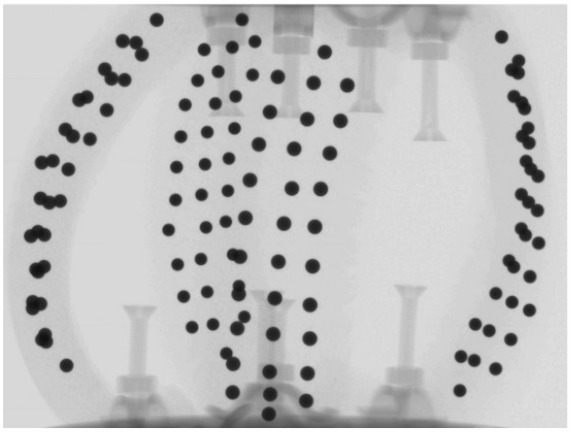
The purpose of this PhD research is to investigate the key factors that control the interaction between self-assembled monolayers, including temperature, pressure, ligand coverage, solvent effects, and the geometry of the surface. All research work is performed via molecular dynamics simulations in the HOOMD-blue computer simulation package. Specifically, we consider the case of decanethiol ligands on gold facets in the presence of explicit solvent. By changing thermodynamic and chemical conditions, we observe the states of ligands and measure the potential of mean force, which provides a detailed description of the interaction between monolayers.

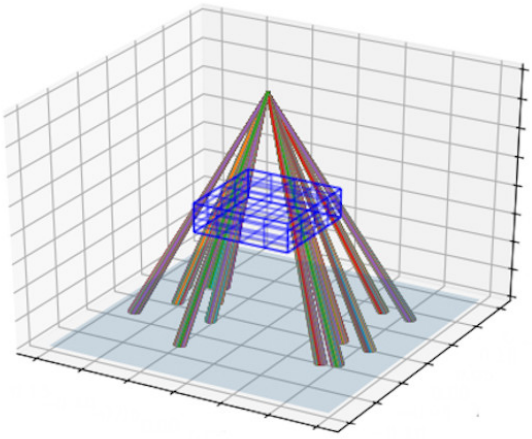


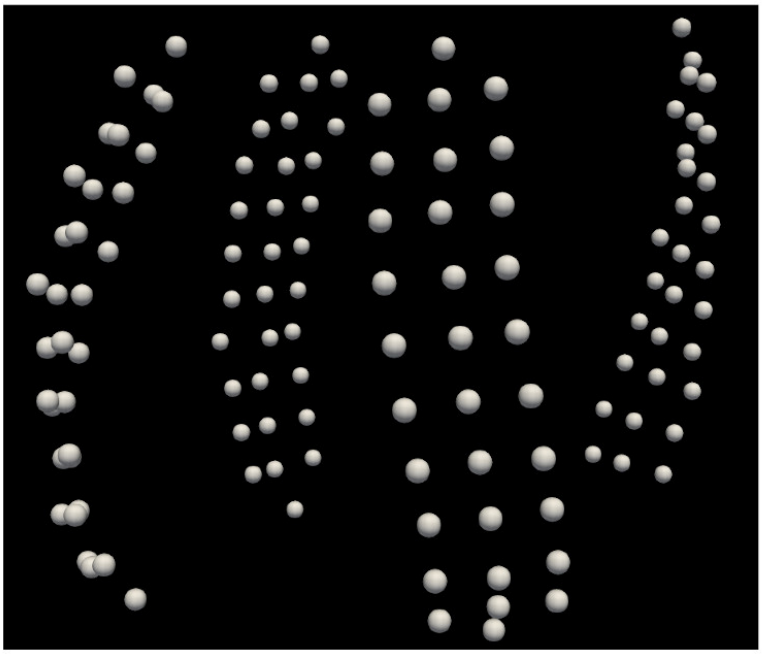
Atharva Pandit, "Multi-Axial X-Ray Computed Tomography"

X-Ray Computed Tomography (CT) devices are widely used in order to study systems in a non-invasive manner. In general, acquiring data for a full CT scan requires a lot of time and the rotation of the sample may introduce centripetal forces into the system being studied. Development of a Multi-Axial X-Ray CT device will be essential in studying rapidly changing dynamic systems of short timescales and fluid systems which cannot be rapidly rotated. The device would use multiple X-Ray sources and detectors to record radiograms of a system from different perspectives simultaneously. Using Radon transformations or similar techniques, a full time-resolved (4D) reconstruction can be achieved on timescales significantly smaller than what is currently possible.

A calibration procedure has been developed for determining the exact location and orientation of the sources and detectors. Codes are being developed for reconstruction using the following techniques: (i) Simple Back-projection (ii) Algebraic Reconstruction Technique (ART) (iii) Multiplicative Algebraic Reconstruciton Technique (MART). A comparison of the three methods across different systems will be done in order to determine an optimal combination.







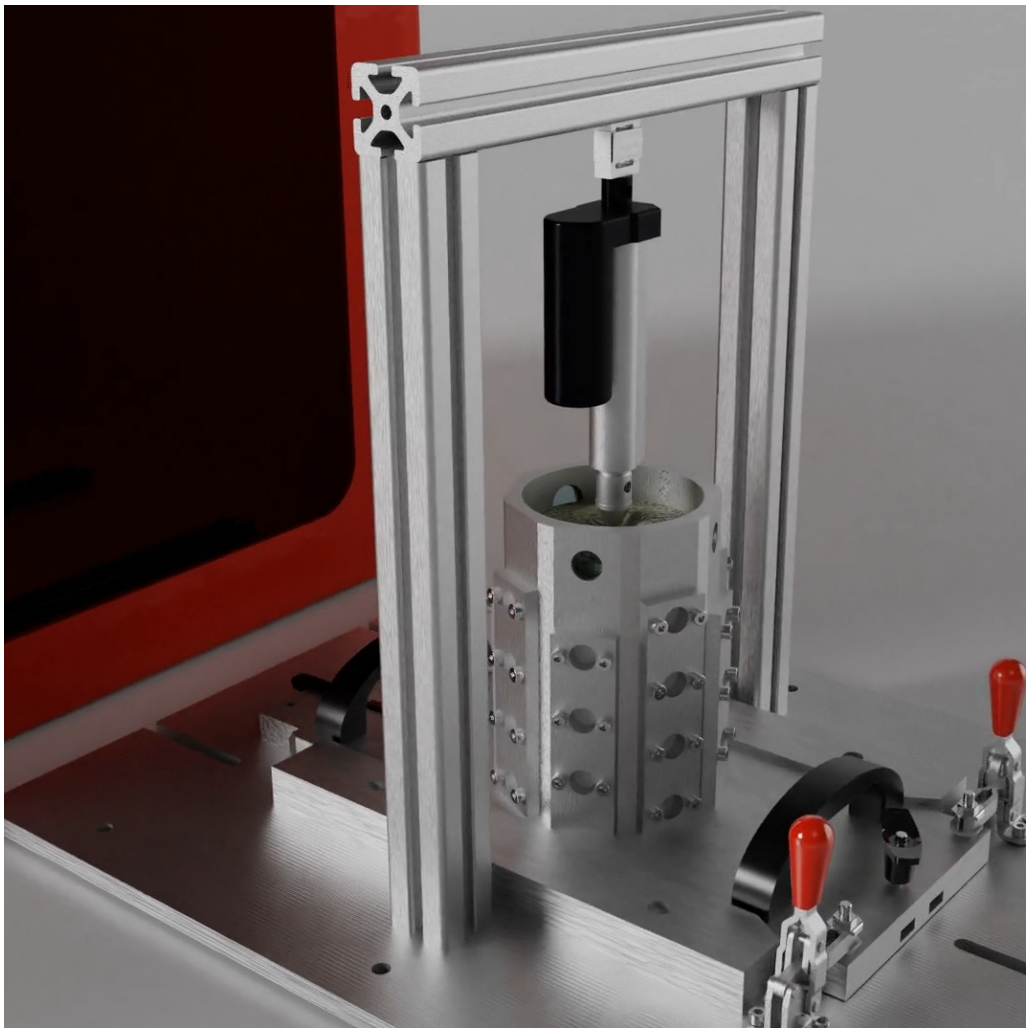
Valentina Marzulli, "Stress regimes within a layer of granular material during quasi-static penetration at different levels of gravity"

We measure the stress at the boundaries of a container filled by granular matter while quasi-statically inserting a metal cylinder into the packing. This process will be repeated at different values of gravity, $g > g_{\text{Earth}}$. Conditions of hyper-gravity can be obtained in the Large Diameter Centrifuge of ESA and to this end, the experiments shall take place within the ground-based facilities programme of ESA-CORA-GBF. A corresponding proposal to ESA has been submitted and granted.

There are two main objectives of this research: (a) understanding the physics of quasi-static deformation processes in granular materials, and (b) develop a reliable mechanical model for processes that will take place on the Moon, such as building lunar structures, in-situ tests, wheel-soil interaction for rovers operating on the lunar surface, and others. Since there is no simple and reliable access to conditions $g < g_{\text{Earth}}$ (except $g \approx 0$ which is not relevant here), we follow a different plan: We try to obtain results with g as a parameter, in the region $g \in [g_{\text{Earth}}, 20 \times g_{\text{Earth}}]$ and then extrapolate these results for $g < g_{\text{Earth}}$, e.g. $g = g_{\text{Moon}}$.

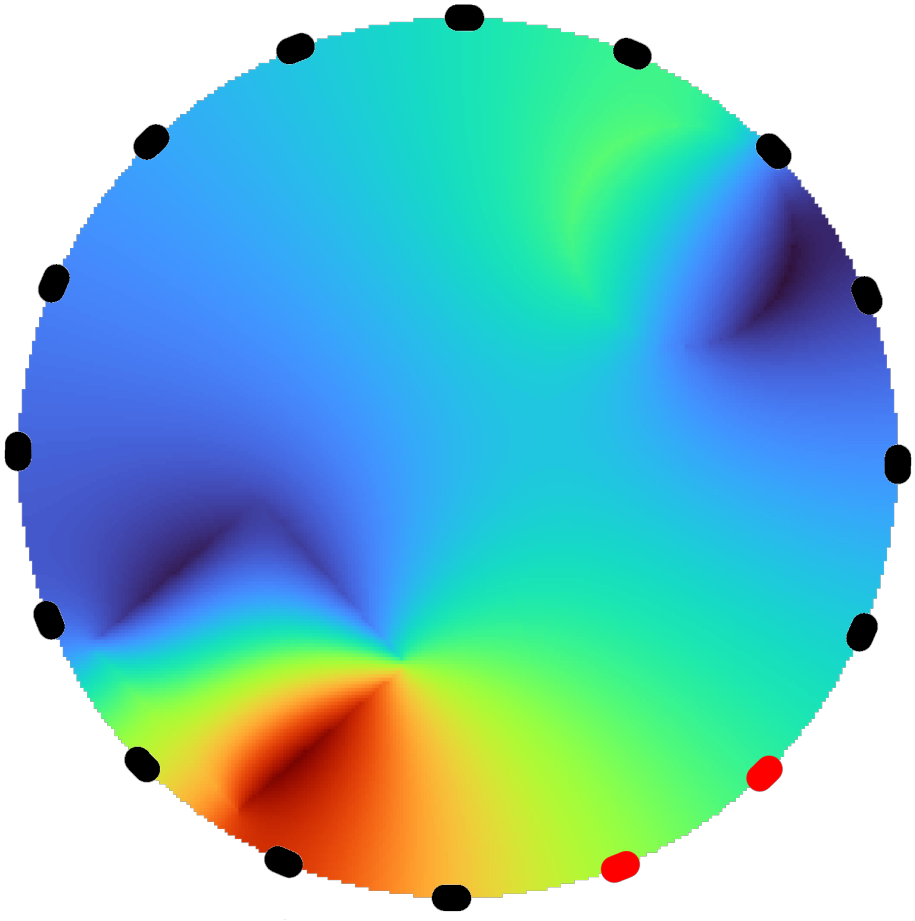
To gain further confidence to these results, complementary we will perform DEM simulations of the penetration process at $g < g_{\text{Earth}}$.

The image shows a computer model of the experimental setup. Pressure sensors, cameras, and electronic wiring are not shown.



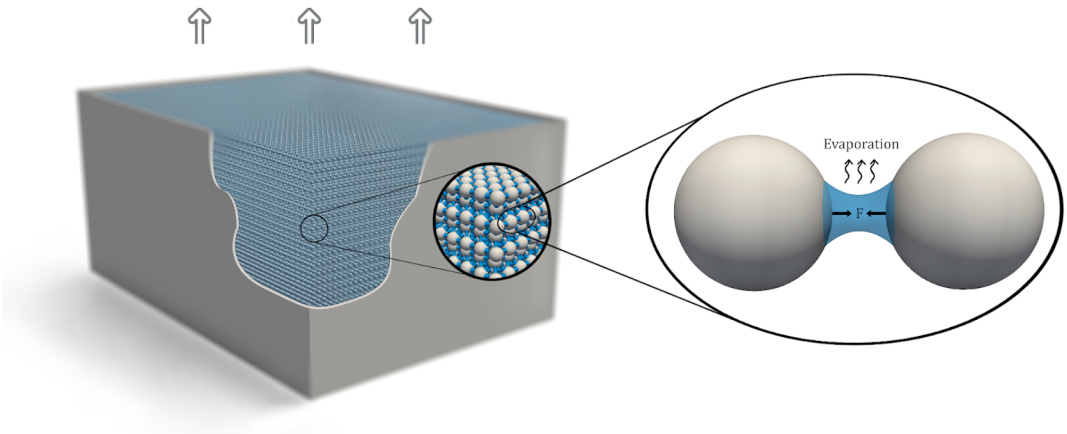
Ayman Ameen, "Image reconstruction for Electrical Impedance Tomography using AI approaches"

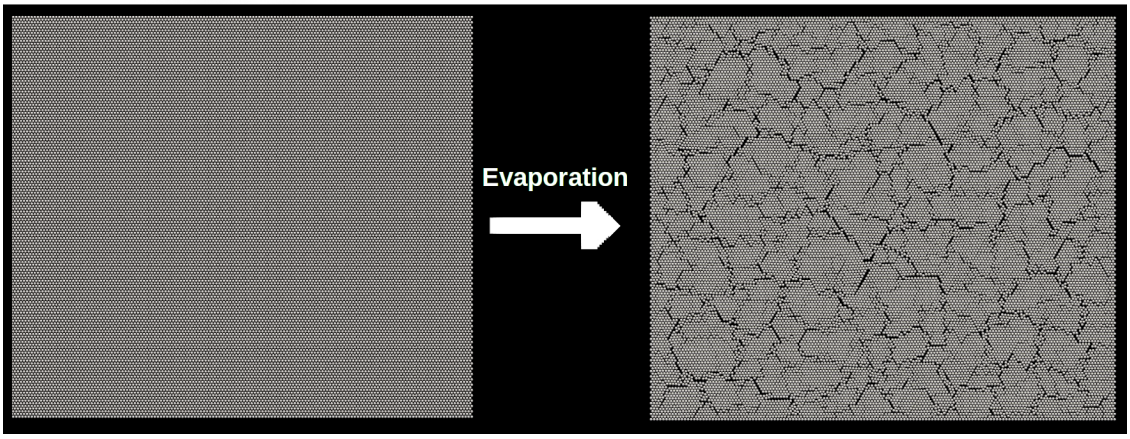
Electrical impedance tomography (EIT) is a noninvasive visual technique that aims to detect the conductivity distribution inside a certain domain using electrical measurements from the boundary of that domain. It has found numerous applications in many fields, such as medical imaging and different industrial applications. The main challenge with EIT is image reconstruction of conductivity distribution as the problem of image reconstruction is ill-posed, ill-conditioned, and highly sensitive to noise measurement. Through the past decades, a lot of image reconstruction techniques has been devolved, such as Tikhonov regularization, Newton–Raphson, Landweber, and linear back projection. These traditional methods depend on the Jacobian matrix with regularization terms in iterative or non-iterative steps. Traditional methods suffer from low spatial resolution. Recently, a new paradigm shift in image reconstruction has happened using artificial intelligence. This project aims to produce state-of-the-art artificial intelligence models for EIT image reconstruction. The project employs autoencoders and convolutional neural networks for accurate image reconstruction.



Meysam Bagheri, "Physics of drying suspensions"

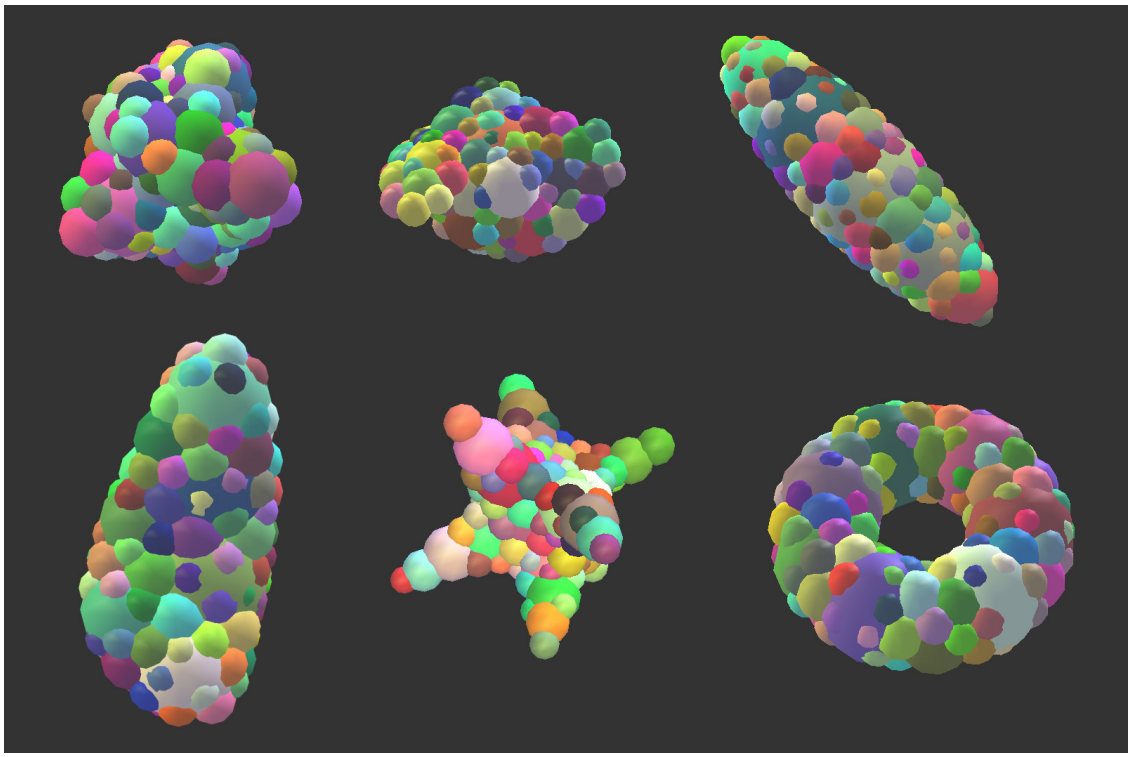
Drying suspensions display a fascinating network of cracks on drying. The cracks result from a number of complex interactions: The particles are concentrated into a close packed array due to the evaporation of the fluid. Further drying results in a network of particles which are interconnected by liquid menisci. These menisci exert compressive capillary forces on the particle network which eventually lead to the formation of cracks. The aim of the project is to understand the cracking dynamics of drying suspensions by means of multiscale simulations. Applications include the development of novel process strategies for printing electronic circuits.
A multiphase model has been developed capable of representing the dynamics of near drying suspensions. The particle dynamics are described by a force-based molecular dynamics algorithm. The liquid phase is modelled as capillary bridges between the particles, thus, acting as forces in addition to the particle-particle interaction. The closed-formed equations for force and area of capillary bridges has been developed to avoid solving the differential equation describing the profile of the menisci. This system will be embedded in a proper framework handling the vapor phase and temperature field by solving the diffusion equation on a coarse lattice with respect to different boundary conditions and distributed system variables needed for the evaporation process. For efficient simulation of large scale systems, the solver will be parallelized.





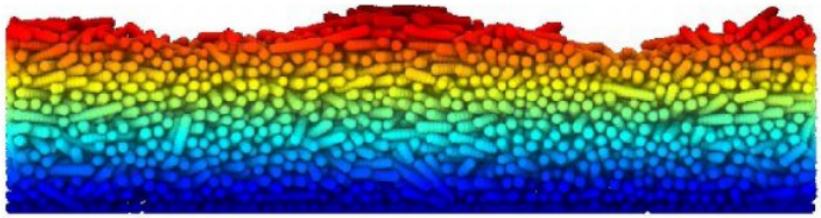
Ahmet Utku Canbolat, "Fractures in Granular Matter – Theory and large-scale simulations"

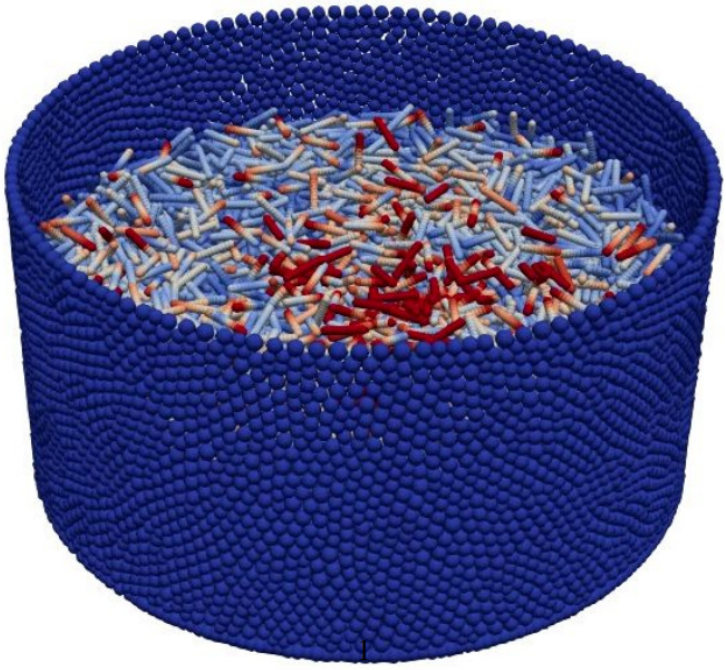
This Ph.D. thesis belongs to the second stage of the ongoing research project P04 in the research training group FRASCAL. The aim of FRASCAL is to understand fracture phenomena in different scales. Our work sits on the mesoscopic scale and particularly considers granular material fragmentation. The project consists of three parts focusing on modeling fragmentation and its applications in large-scale Discrete Element Method (DEM) simulations. It is essential to model realistic grains for granular material simulations to capture more accurate dynamics of the granular systems. In this manner, the multi-sphere particle generation method was developed for creating realistic grains at the beginning of the project. Then, DEM was extended to take into account the granular fragmentation in the first stage of the project. The second stage relates to implementing plastic deformation, heat transfer, and wear effect for the large-scale DEM simulations. Collisions between particles cause plastic deformation and heat up the particles. Since the fracture criterion depends on the temperature of the particles, it is crucial to consider the heat transfer between particles due to collisions. I am currently focusing on implementing this part in DEM simulations. In the next step, I will implement the wear effect. Wear is the loss of material surface as a result of the relative motion of particles. Wear of granular materials has great importance in many fields such as geotechnical engineering, mining, pharmaceutical, and chemical industries. To model wear, we will treat wear as small scale fractures on grains.



Huzaif Rahim, “Granular Weissenberg Effect”

Granular materials unveil fascinating and complex behavior due to the diversity of particle properties, such as density, size, shape, surface morphology, and interparticle interactions. More specifically, particle shape plays a remarkable role as it influences the bulk packing and flow behaviors. Granular materials made of non-spherical particles are common in a wide range of applications, such as agriculture, the pharmaceutical, the food industries, and in geology. Shearing, shaking, or pouring of such granulates can lead to the formation of local or global orientational orders, which extensively influence their macroscopic dynamic properties. Though it is acknowledged that shear in such materials is restricted to localized shear bands, resulting from the primary flows, a large-scale rearrangement of the material, that is a secondary flow, is observed. The aim of this project is the characterization of a "granular Weissenberg effect" using theory and numerical simulation, a newly discovered and not yet fully understood phenomenon observed when a system of non-spherical particles is sheared. The reported effect is only observed in the granular matter of pronounced anisotropic particles, while it is not detected for spherical or nearly spherical particles. The DEM (discrete element method) is an attractive numerical modeling technique for particle scale simulations. We study the "granular Weissenberg effect" in a three-dimensional split-bottom geometry with particles of varying shapes using DEM simulations.



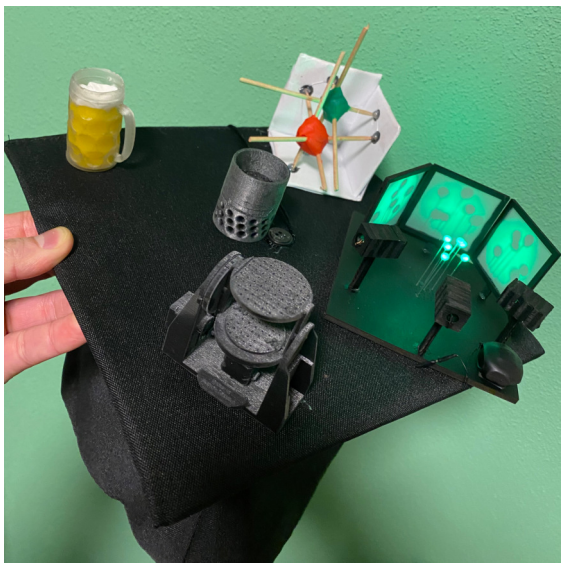


6. PhD Graduations

Luis A. Torres Cisneros, "X-Ray Multiaxes Reconstruction of Granular Flows"

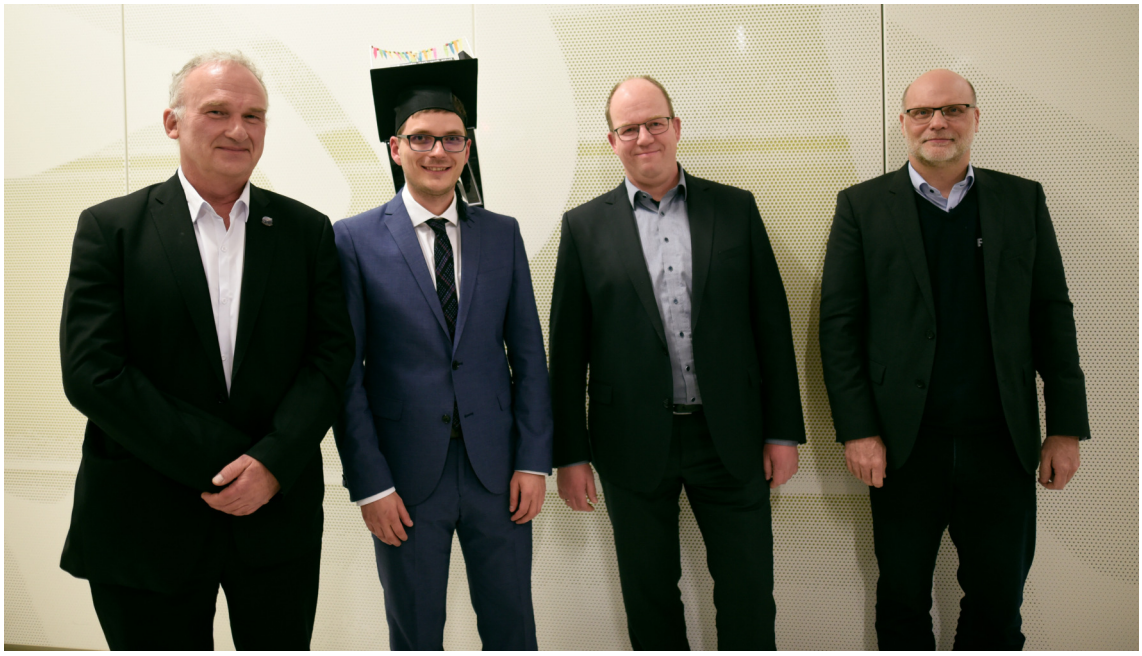
Faculty: Chemical Engineering / Dr. Ing.
Date: 24.03.2022
Chairman of the examination committee: Prof. Michael Engel
Members of the examination committee: Prof. Thorsten Pöschel, Prof. Ralf Stannarius, Prof. Andreas Maier

Luis at the FAU graduation ceremony


Luis's PhD hat

Michael Blank, "Simulation of the laser melting process of titanium using Smoothed Particle Hydrodynamics"

Faculty: Chemical Engineering / Dr. Ing.
Date: 19.12.2022
Chairman of the examination committee: Prof. Michael Wensing
Members of the examination committee: Prof. Thorsten Pöschel, Prof. José Daniel Muñoz Castaño, Prof. Jens Harting, Prof. Paul Steinmann



Michael with the committee members left to right: Prof. Thorsten Pöschel, Michael Blank, Prof. Jens Harting and Prof. Michael Wensing. Photos by Meysam Bagheri

After PhD defense

Michael's PhD hat

7. Teaching Activities

image: fau.de

Main Courses

- **Simulation granularer und molekularer Systeme (SIMSYS)**
  Lecture (Prof. Thorsten Pöschel, Prof. Michael Engel)
  Exercise (Prof. Thorsten Pöschel, Prof. Michael Engel)
  Laboratory (Michael Blank, Holger Götz)
- **Basics in Computational Materials Science and Process Simulation (B_Compu_1)**
  Lecture (Prof. Michael Engel, Prof. Andreas Bück)
- **Selbstorganisationsprozesse (SOP)**
  Lecture (Prof. Michael Engel, Prof. Nicolas Vogel, Prof. Robin N. Klupp Taylor)
  Exercise (Prof. Michael Engel, Prof. Nicolas Vogel, Prof. Robin N. Klupp Taylor)
- **Computeranwendungen in der Verfahrenstechnik 1 (CIV-1)**
  Lecture (Prof. Thorsten Pöschel)
  Exercise (Felix Buchele)
- **Scannen und Drucken in 3D (3DSD)**
  Lecture (Dr. Patric Müller)
  Exercise (Felix Buchele)
- **Messtechnik 2 - Messmethoden und Analytik (MT2)**
  Lecture (Dr. Achim Sack)
  Lab Course (Dr. Achim Sack)
  Exercise (Angel Santarossa)
  Laboratory (Angel Santarossa)
- **Digitale Bildverarbeitung (DBV)**
  Lecture (Dr. Achim Sack, Angel Santarossa)
  Lab Course (Dr. Achim Sack)
- **Particle-based Fluid Mechanics**
  Lecture (Michael Blank)
  Exercise (Michael Blank)

- **Machine Learning and Artificial Intelligence in Engineering (KI-ING)**
  Lecture (Dr. Patric Müller)
  Exercise (Dr. Patric Müller)
  Laboratory (Dr. Patric Müller)
- **Scannen und Drucken in 3D (3DSD)**
  Lecture (Dr. Olfa D'Angelo)
  Exercise (Dr. Olfa D'Angelo)
  Laboratory (Dr. Olfa D'Angelo, Felix Buchele)

Smaller Courses

- **Soft Matter Journal Club**
  Seminar (Prof. Michael Engel, Prof. Michael Schmiedeberg, Prof. Vasily Zaburdaev)
- **Granular Matter - MSS Seminar (MSS-GM)**
  Seminar (Prof. Thorsten Pöschel)
- **Multiphase Flows - MSS Seminar (MSS-MF)**
  Seminar (Prof. Thorsten Pöschel)

Multiscale Simulation - MSS Seminar (MSS-MS)
Seminar (Prof. Thorsten Pöschel, Prof. Michael Engel)

14.01.2022	Alberto Leonardi	*Disorder in nanostructured materials*
28.01.2022	Dr. Olfa D'Angelo	*From granular rheology to 3D printing in space — and back*
04.02.2022	Dr. Achim Sack	*Introduction to RIT and Robin projects*
11.02.2022	Dr. Carlos Lange Bassani	*A Multiscale Approach for Gas Hydrates Considering StructureAgglomeration, and Transportability under Multiphase Flow Conditions*
18.02.2022	Dr. Patric Müller	*Thermal conductivity of thermal foams*
25.02.2022	Niklas Tobie	*Can you hear the temperature of water?*
04.03.2022	Holger Götz	*Core-Shell Particles under Jamming*
11.03.2022	Michael Blank	*Simulation of the laser welding process of Titanium*
18.03.2022	Dr. Sudeshna Roy	*Modeling of granular materials: From particles simulation to continum*
25.03.2022	Angel Santarossa	*Combined suction and granular jamming for a strengthened, more versatile gripper*
08.04.2022	Zhiyu Song	*Interaction between self-assembled Monolayers: The role of coverage density*
22.04.2022	Dr. Olfa D'Angelo	*Constitutive law for dense agitated granular flows From theoretical description to rheology experiment*
29.04.2022	Dr. Carlos Lange Bassani	*Gas-Liquid-solid flows: Linking turbulent scales with macroscopic slug flow structures of dilute suspensions*
06.05.2022	Dr. Vasileios Angelidakis	*Image-informed modeling of granular materials with realistic particles of controlled simulation fidelity*
13.05.2022	Dr. Sudeshna Roy	*Effect of cohesion on powder layers spreading in additive manufacturing*
20.05.2022	Dr. Patric Müller	*Thermal conductivity of thermal foams*
03.06.2022	Prof. Igor Goychuk	*Resonance-like enhancement of driven diffusion in nonlinear viscoelastic media as nonequilibrium phase transition*

01.07.2022	Utko Ahmet Canbolat	*Electrical control of the indirect exchange interaction in two-dimensional materials*
08.07.2022	Jonathan Martin Gonzalez Federico Tomazic	*Numerical methods for structural color representation*
15.07.2022	Holger Götz	*DEM simulations of membranes interacting with a granulate*
22.07.2022	Dr. Hongyi Xiao	*Direct experimental evidence of Gardner physics beyond isotropic interactions*
29.07.2022	Husaif Rahim	*Theoretical analysis of turing pattern in a three components reaction-diffusion system*
05.08.2022	Meysam Bagheri	*Closed-form equations for the area of a capillary bridge*
12.08.2022	Dr. Hongyi Xiao	*Modeling Stratified Segregation in Periodically Driven Granular Heap Flow*
19.08.2022	Atharva Pandit	*Multi-Axial X-ray Tomography*
26.08.2022	Sarthak Jadhav	*Releasing droplet in micro gravity*
02.09.2022	Holger Götz	*Granular Jamming Beam: Influence of Particle Stiffness*
09.09.2022	Dr. Sudeshna Roy	*Mechanism across scale: A holistic modeling framework for reverse phase wet granulation*
16.09.2022	Laureano Ortellado	*Shock melting of lamellae-forming block copolymers*
23.09.2022	Dr. Patric Müller	*Thermal conductivity of thermal foams*
07.10.2022	Dr. Hongyi Xiao	*Dragging Plate(s) Through Granular Materials: What is Important for Locomation?*
14.10.2022	Dr. Vasileios Angelidakis	*Acquisition and Characterization of Particle Morphology: 2D – 3D – 4D?*
21.10.2022	Prof. Thorsten Pöschel	*Collisions and Forces and all that*
21.10.2022	Felix Buchele	*Chemical Reactions in DSMC simulations*

8. Students Projects

Master theses

- **Bijohn Chandrew Aseervatham, "Dzhanibekov Effect"**

  In this work, the so called Dzhanibekov-effect will be observed in both analytical and practical way. The effect was firstly observed by the russian astronaut Wladimir Dzanibekov, in space. Apparently he spinned a wing nut around one of its axis and regarded a mind blowing phenomena. The wing-nut periodically changed its orientation around the axis which the astronaut initially charged. In fact this only occures, when a rigid body is turned around its intermediate axis. This is based on Euler's equations to model the motion of rigid bodys in the three main axes. Goal of this work will be to find a simulative way to intuitively explain the "intermediate axis theorem" in such way it can be used in teaching devices at the FAU-Erlangen. Also a experimental setup is used to justify the theoretical approach and to validate the simulative considerations.

- **Deniz Fakioglu, "Automation of an electrical impedance tomograph"**

  The master thesis is part of a research project that is dealing with the electrical impedance tomography. It represents a noninvasive type of imaging. In the electrical impedance tomography electrodes, placed circumferentially around a body, are used to determine its electrical impedance distribution. This is followed by a reconstruction step to generate a cross sectional image of the body. Since the reconstruction step is to be performed by a neural network, a lot of training- and test data must be generated. Therefore, it is necessary to automate the measurement procedure. The tasks of my thesis include the automation of the full measurement procedure by using a robotic arm and a webcam (to take the desired images), testing the automation and generating measurement data for a neural network. In the final step, the trained neural network is integrated into the evaluation of the measurements.

- **Omar Zeair, "Modeling Acid Gas Capture Using Eva Amines"**

  Chemical absorption by amines is an established and mature technology for both post combustion carbon capture and acid gas (H_2S and CO_2) removal from natural gas. Eva amines are polyamines that offer increased capacity and better performance than state of the art amine solvents. For the widespread adoption of Eva amines, thermodynamic models that describe the solubility of acid gas in aqueous solutions of Eva amines need to be established. Using

the Pitzer activity coefficient model, the solubility of both H_2S and CO_2 was described and compared to solubility predictions using the Electrolyte NRTL (ENRTL) activitcoefficient model. In addition, an attempt to describe the chemical speciation behavior of both gases in aqueous Eva solutions was made. Two sets of chemical reaction equilibrium constants were used to model the speciation and solubility of Eva amines. The equilibrium constants were unable to give a full description of the absorption of both CO_2 and H_2S. Using modified equilibrium constants, a solubility model was implemented and the interaction parameters of the Pitzer model obtained. The model was found to give comparable results to the ENRTL model. The predictions of the Pitzer model were better for both gases at the highest temperature and concentration studied. At the cases when the predictions of the Pitzer model were of less quality than the ENRTL model, interaction parameters that will improve the performance were identified.

- **Navid Panchi, "Bayesian Optimization for Diffraction Profile Modeling"**

  X-ray diffraction profiles contain incredible insights into the crystalline structure of materials. To extract this information, the observed diffraction profiles must be modeled using suitable mathematical models. These models rely on a set of optimizable parameters to effectively capture the diffraction profile. The optimization process requires repeated evaluations of the modeling function to find the best parameters for approximating the observed profile. Depending on the model used, this process can become computationally expensive and time-consuming. This is similar to the problem faced in deep learning model selection. To solve this problem, Bayesian optimization is actively used in deep learning research to find the correct hyperparameters with high sample efficiency. We can harness this sample efficiency in our diffraction modeling task to reduce the model evaluation cost during parameter optimization. We use the Heteroscedastic Evolutionary Bayesian Optimization (HEBO) algorithm proposed in NeurIPS black box optimization challenge 2020 to optimize parameters for the Rietveld method. Although this method is remarkable at reducing the number of model evaluations, the time taken for the optimization process leaves room for improvement. We also explore a learnable optimization method to design a suitable optimizer for diffraction profile modeling.

- **Qing Yu, "Granular jamming density versus gravitational acceleration"**

  We are studying the connection between gravitational level and the critical packing fraction of jamming transition.

Bachelor theses

- **Isabella Schneider, "Development of a transient framework to predict pore shrinkage of gas hydrates"**

  Gas hydrates are crystals formed of light molecules $(CO_2, N_2, CH_4, C_2H_6)$ that get entrapped into cages formed of hydrogen-bonded water molecules. Gas hydrates present a gamma of applications, from their high-capacity of storing gases with application to carbon dioxide sequestration in the global warming scenario, to the intelligent oil and gas production in deep offshore fields without flow line plugging due to uncontrolled formation of natural gas hydrates. In the latter context, recent advances showed that the state of pores (open or sealed to the) is very important to understand transportability of gas hydrate crystals, a key knowledge to insure safe production (both to personnel and structure), without production stop, and yet to minimize the injection of chemicals. The pore shrinkage is solved by the concomitant gas diffusion through water entrapped in the pores, and its crystallization in the

pore walls, using Finite Volumes in a pseudo 2d (radial terms are modeled as source terms) formulation that hold for low Biot numbers of mass transfer. The set of differential equations is discretized using 1st order Central Differencing Scheme in space, and a Crank-Nicholson Scheme in time, and implemented in an in-house code in Python. Regarding the current analytical solutions for gas hydrate pore shrinkage for steady-state conditions, the transient terms of the simulation show able to capture a mass transfer mechanisms due to necking of the pores, which relates to a reduction of approximately 30% of gas consumption per capillary.

- **Frederik Keil,"Random packings of Meissner Tetrahedra"**

  Meissner Tetrahedra are solids of constant width like spheres. The packing density of random packings of Meissner Tetrahedra shall be measured by evaluating tomographic images and shall be related to sphere packings. The packings shall also be investigated with respect to their spatial order structure. If order phenomena occur, they shall be quantified.

- **Yazan Alzaghah, "Electrical Impedance Tomography (EIT) - Experimental Setup and Measurement"**

  The main task of this thesis is to operate the EIT-Setup and measure the complex impedances between the electrodes to generate as much data as possible to train an AI model with it for the reconstruction. However, after a set of measurements, a modification of the setup was essential to gain more accuracy and to try to match the experimental results with the simulation. For that we replaced the electrodes by a set of 32 electrodes designed as a flexible PCB and the results were promising. Moreover, we're working on automating the whole measurements-taking process, and to automate the liquid leveling step to keep it constant during the process.

Miniprojects

- **Adriana Enriquez, "Vibrots propelled by acoustic resonance"**

  Self-propelled particles are of great interest in the study of collective behavior. A new type of self-spinning particles, called Vibrot, was proposed by Altshuler 2013. With a mass and tilted elastic legs, the system transforms vibrations in rotational motion. Earlier studies developed an analytic model, addressed the lack of collective behavior and its manufacture using rapid prototyping.We propose a different driving mechanism for the Vibrots based on the acoustic resonance of a deformable thin plate. When being excited at its natural frequency, the plate oscillates, inducing the vibration of the Vibrot's body, hence bending its legs and producing rotation. This new mechanism to transform acoustic energy into motion could allow significant miniaturization of the Vibrots. We want to implement the acoustic waves propelled Vibrots in experimental studies of colective motion of active particle systems.

- **Jonathan Martín González, "Optimizing Monte Carlo Ray-Tracing for Structural Color Prediction of Photonic Crystal Balls"**

  Structural color is a phenomenon originated by the nanostructure properties of a system. Due to this connection between nanostructure and structural color, this structural color produced can also be used for the characterization of nanostructures. In this work, a Monte Carlo ray-tracing approach is proposed for the prediction of the structural color. The advantage that provides this approach with respect to other methods like the Transfer Matrix Method is that ray-tracing approaches can directly deal with 3D systems. The nanostructure object of the study are photonic balls, where a 3D method is required for its proper characterization. The simulation approach has been successfully validated by analysing the effects of the

different characteristics that define the structural color of a system, and a Pearson Correlation Matrix analysis of the different design variables has shown the most relevant parameter in the accuracy of the results, which also does not have a large impact over the simulation time. This parameter, the maximum number of allowed reflections that are allowed for each ray, has been identified as the perfect candidate for simulation time optimization. Finally, a visual guide has been developed for the optimal selection of the number of allowed reflections to reach the maximum accuracy reached by the algorithm, obtaining a considerable reduction of the simulation time just with the smart selection of simulation variables.

- **Khaled Mansour, "The Search for Tetrahedra Crystals"**

  Recent advances in nanotechnology allow precise control over the size and shape of nanoparticles. Specifically polyhedral nanoparticles can now be produced and interactions between them can be introduce through surface ligands. In this miniproject we were interested in studying the packings of such tetrahedral nanoparticles in the presence of interactions between their faces through polymer ligands. Our study focused on five possible crystal structures, which are the Scottish, Irish, Welsh, Erlangen and Approximant crystals. We investigated the stability of each of these crystals using Monte Carlo simulations with HOOMD-Blue package and an inhouse Molecular Dynamics code. For hard tetrahedral particles we show the spontaneous formation of the quasicrystal and redemonstrate that the Approximant is our most stable structure for tetrahedral packings. The Approximant followed by the Irish crystal were the most stable for interacting tetrahedra. The structure stability for the interacting particles showed a dependence on the potential energy per particle at low simulation temperature. Additionally our study of hard tetrahedra resulted in the discovery of a new crystal structure which we called the Erlangen crystal.

- **Tengda Huang, "Simulation of composite crystals"**

  Study on the distribution of particles of colloidal composite crystals in five columns and particle diffusion in channels. The project focus on using Monte Carlo method to simulate the AB7 phase-based structure of colloidal crystals and their diffusion behaviors. By tuning size ratio and number of particles as well as changing the density, we try to find the most stable structure of the five-fold columns. As density is considered to be a function of particle diffusion, we try to develop computational method to investigate the motion of crystal particles with varied density.

- **Lan-Tien Hsu, "Coarse-Grained Molecular Dynamics Simulation of Ligated Tripod Nanocrystals"**

  Branched ligated nanocrystals are of interest for their complex self-assembled structures. However, exploration of complete phase diagram by merely experiments is challenging, as there are too many factors available for tuning. In this work of simulation, the Morse potential with a set of potential parameters determined based on the experimental data is used to describe the interaction between tripods. 2D coarse-grained molecular dynamics in NVT ensemble is performed to study the self-assembly. Reference energy of each phase is shown to be a good indicator for the experimentally observed self-assembled structures. To study the influence of kinetic trapping and initial configuration, longer simulations are run and collected in phase diagrams. From the longer simulations, it's clear that the systems suffer from kinetic trapping caused by too strong interaction, and thus fail to reproduce the experimental data. This work serves as a good starting point for potential parameters tunning, and it shows that it is possible to predict the experimentally observed self-assembled structures from this simulation setup.

- **Omar Zeair, "Simulating disorder order transformation in Cu Pd alloy nanoparticles"**

  We investigate disorder to order transformations of copper palladium alloy nanoparticles using a hybrid molecular dynamics Monte Carlo scheme. The scheme involves blocks of molecular dynamics steps followed by Monte Carlo swaps. We used the swaps in their standard form as provided by the LAMMPS package and adapted them to only allow swaps between neighbour atoms. The simulations were performed on 30/70% and 50% mole ratio Cu/Pd particles at temperatures of 300 K and 800 K with both the Embedded Atom Method and the Finnis Sinclair potentials. We first show using energy comparisons and melting point verification that the ordered state is more favourable. Simulations performed on systems with half A1 and B2 structures glued together and performed close to the melting point failed to show transformation to the ordered state. The transformations to the B2 state were captured by simulations at 300 K for both 30/70% and 50% mole ratio Cu/Pd particles using the Embedded Atom Method and the Finnis Sinclair potentials and performed using the standard swaps. We simulated XRD patterns for one of the transformed configurations to examine the transformation and measure its extent. The patterns showed the presence of two different sets of crystalline sub-domains with different degrees of phase transformation.

- **Aditya Pratap Singh, "Characterization of shear zones for mixture of hard and soft granular materials"**

  This work involves developing a numerical setup of split-bottom shear cell and study the geometry of shear zones for soft, low-frictional and hard, frictional granular materials and their mixtures. We take the properties of hydrogel as soft, low-frictional material component and mustard seeds represent rigid, frictional grains. We shear the materials mixture in a split-bottom sear cell and determine the shear profile from the velocity gradient. We find that the shear zone geometry differs considerably between the different mixture ratio of soft and hard particles.

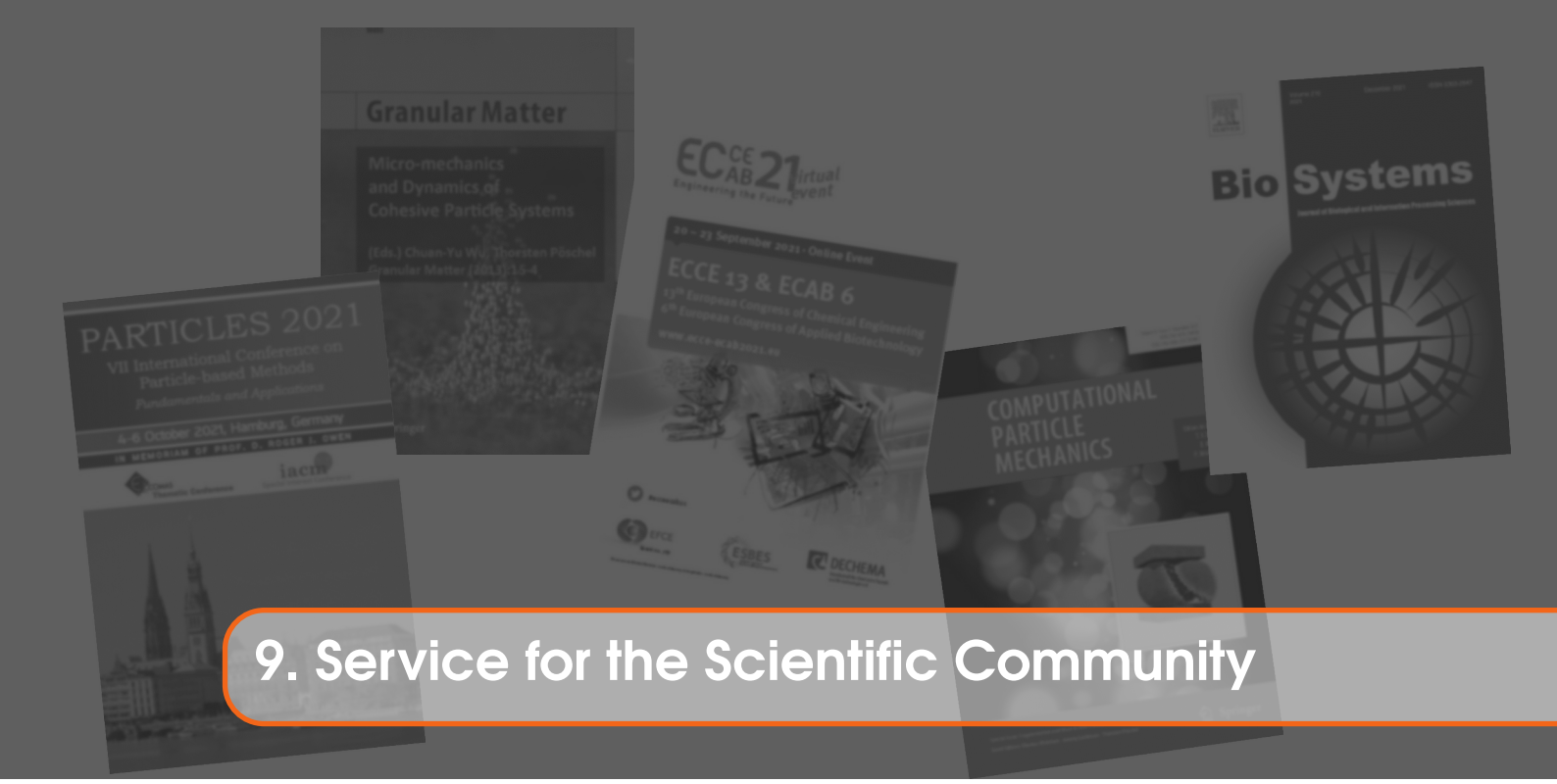
Programming Projects

- **Navid Panchi, "Hybrid network simulation"**

  The project focuses on the programming part of a hybrid (MD + MC) network simulation. The main aims include: 1) Implementation of an efficient data structure for storage and manipulation of the network structure. 2) Implementation of different phase transformations in Ba-Ti-O perovskite structure. 3) Optimization of Code, this includes implementation of the Monte Carlo simulation in C++ with HOOMD Blue like python scripting interface.

- **Anirudh Suri, "Dynamics of discrete Objects (DynamO)"**

  My project is consists of three parts: 1) Modifying in-house developed particle dynamics package called DynamO. 2) Simulating Granular Flows using event-driven particle dynamics approach. 3) Implementing a new boundary condition in C++ event-driven DEM code to optimize the number of particles present in a granular flow.



9. Service for the Scientific Community

Editorial Boards

Physchem
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Physchem is an international, peer-reviewed, open access journal of science and technology in physical chemistry published quarterly online by MDPI.

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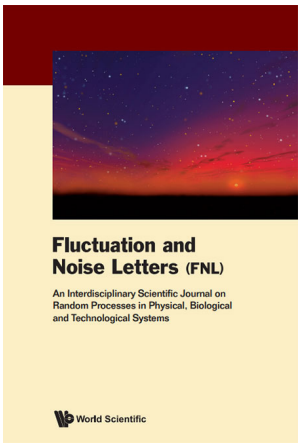

Dr. Igor Goychuk
Editor since 2001 (founding member)

Revista Cubana de Física
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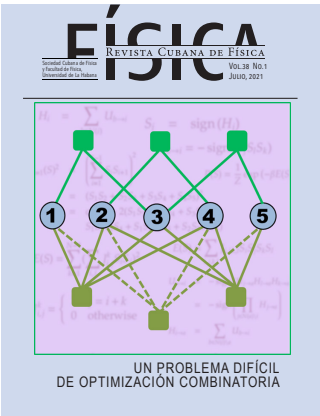


Prof. Thorsten Pöschel
Senior Editor since 2014

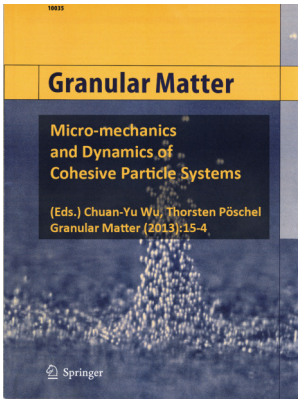
Computational Particle Mechanics
Springer/Nature

`www.springer.com/journal/40571/`

Prof. Thorsten Pöschel
Editorial Board Member since 2014
(founding member)

Granular Matter
Springer/Nature

`www.springer.com/journal/10035`



Prof. Thorsten Pöschel
Editor since 2006

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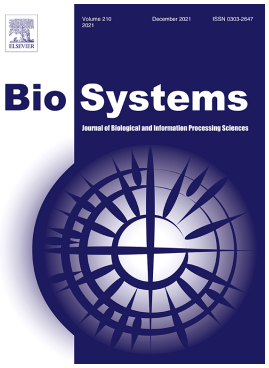


Prof. Thorsten Pöschel
Associate Editor since 2003

INJAVIS – INteractive JAva VISualization

Public release March 26, 2021
`https://engellab.de/injavis`
The software package Injavis (acronym for INteractive JAva VISualization) displays, analyzes, and manipulates particle simulation data. An emphasis lies on geometry and structural analysis as well as interactivity. The main input and output file format is .pos, which is a format developed specifically for Injavis and designed to be easily human readable and editable. The software is written in the Java programming language, which makes it transferable among operating systems without recompilation.

Injavis has been developed since 2007 by **Prof. Michael Engel** with some additions and bug fixes by members of the Glotzer Group at the University of Michigan.

Examples of application:

- analyze (many) simulation trajectories
- identify crystal structures of a self-assembly simulation
- perform interactive simulation by coupling Injavis to external MD or MC code
- generate high-quality images for publication

The Injavis software is provided free of charge and without warranty of any kind, express or implied, including but not limited to the warranties of merchantability, fitness for a particular purpose and noninfringement. The full license information is included in the software.

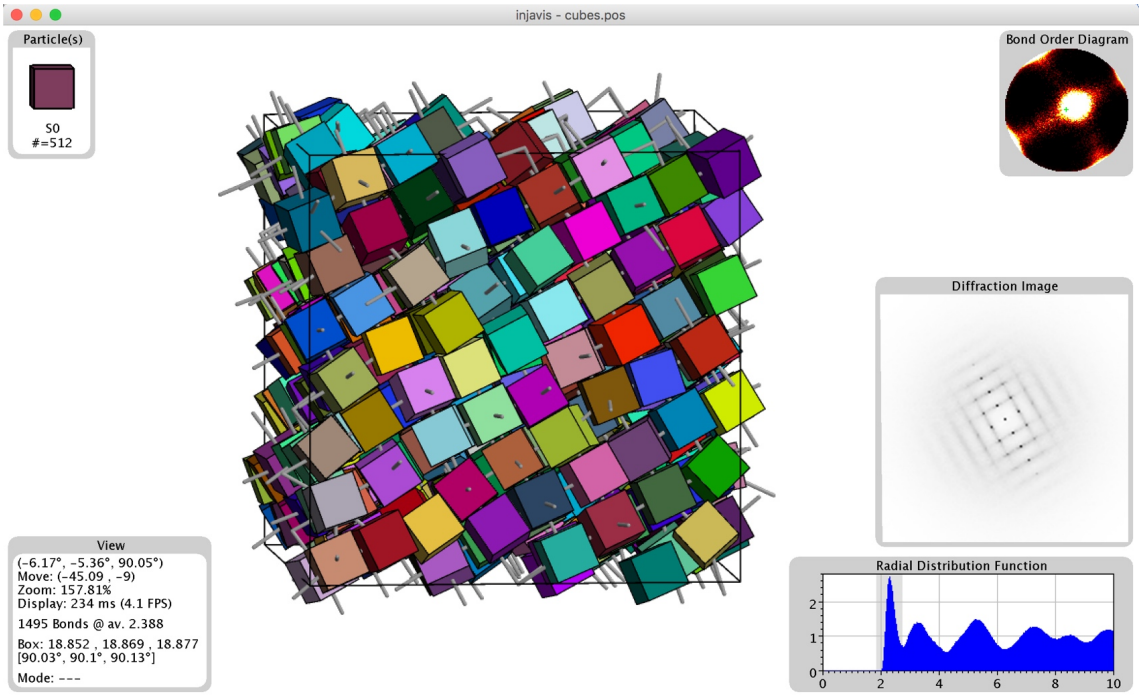


Figure: Screenshot of injavis showing a snapshot of a simulation of hard cubes. (top left) particle module; (top right) bonds module; (middle right) diffraction module; (bottom left) view module; (bottom right) RDF module

Yade - Yet Another Dynamic Engine

`https://yade-dem.org`

Yade is an extensible open-source framework for numerical models based on the Discrete Element Method. The computational parts are written in C++ using a flexible object model which allows independent implementation of new algorithms and interfaces. Python3 is used for rapid and concise scene construction, simulation control, postprocessing and debugging. Stable releases of the software are distributed yearly, alongside with daily packages. Launchpad and Gitlab are used to host the source code, bug tracking, source downloads and more. Yade is written and maintained by an active international and multidisciplinary group of developers, including **Dr. Vasileios Angelidakis**, whose contributions are focused on non-spherical particles and contact laws.

Yade comprises a wide range of contact laws, for dry and wet granular materials, along with various classes for non-spherical particles, including polyhedra, potential particles, flexible spheropolyhedra and flexible surface elements, concave non-spherical particles using the LS-DEM, just to name a few. High-precision calculations are supported. The interactive Python interface allows for live plotting, modifications and post-processing in real time. Couplings with other methods, such as the FEM and CFD allow for the modelling of multiphase and multiscale problems. The performance of calculations is enhanced utilising both shared memory (OpenMP) and distributed memory (MPI) parallelisation schemes, as well as hybrids of the two, which allow efficient deployment of the software in both personal computers and HPC clusters.

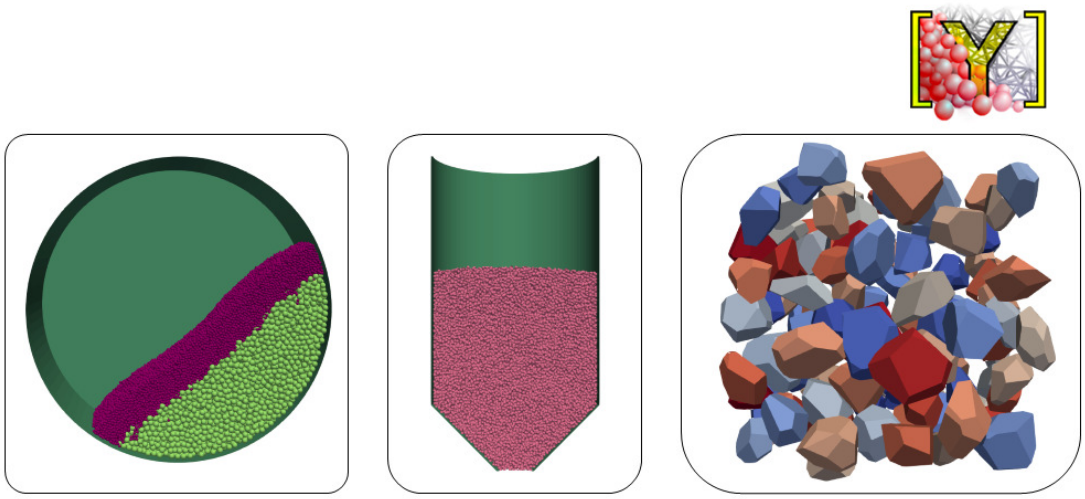


Figure: DEM applications in YADE; rotating drum, silo flow and sample of polyhedral particles.

Yade Hackathon

Dr. Vasileios Angelidakis participated in the YADE Hackathon held at TU Bergakademie in Freiberg, Saxony during **23-24 June 2022**. The event aimed to further the development of YADE (Yet Another Dynamic Engine), one of the largest open-source codes using the Discrete Element Method at the time of writing.

Figure: Dr. Vasileios Angelidakis during his talk at the Yade Hackathon.

Figure: From left to right: Vasileios Angelidakis, Anton Gladky, Katia Boschi, Jerome Duriez, Robert Caulk, Bruno Chareyre, Janek Kozicki and Vaclav Smilauer.

Robin - Second Project Meeting

Within the framework of ROBIN, new robust imaging measurement techniques are being developed, with which it will be possible in the future to instrument large-scale test facilities in reactor safety research in such a way that thermal-hydraulic data can be acquired in CFD quality, i.e. with very high spatial and temporal resolution.
The second regular project meeting took place on 03-04 November 2022. together with the cooperation partners of TU Dresden (TUD-PBM, TUD-WKET, TUD-IAVT) and the project management of KIT in Erlangen. In four presentations of the project partners, the current status of the research work was discussed and the strategy for the coming six months was discussed. A guided tour through the large-scale test facility "PKL" of FRAMATOME, in which the primary cooling cycle of a power plant can be simulated, concluded the event.

Figure: The guided tour through the large-scale test facility "PKL" of FRAMATOME, on November 4, 2022.

Visiting Researcher at Newcastle University

Dr. Vasileios Angelidakis has been appointed as a Visiting Researcher for a period of two years **04/2022-03/2024** at the School of Engineering, Newcastle University.

`www.ncl.ac.uk/engineering/staff/profile/vasileiosangelidakis.html`

Developer in MercuryDPM team

Holger Götz joined the MercuryDPM team. He added the mass spring system to the kernel, which has been available in version 1.0 since **May 2022**.

`https://www.mercurydpm.org/about/team#h.4xjfxeowlicv`

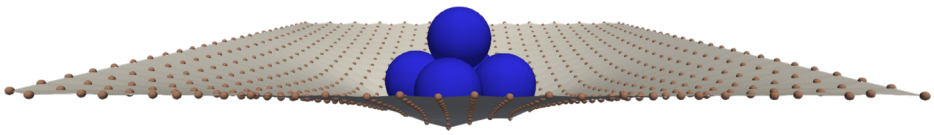


Figure: Snapshot of a simulated membrane with the spring system by MercuryDPM.

Elected chair for Gordon Research Seminar

Dr. Olfa D'Angelo was elected as chair of the next Gordon Research Seminar. She will be responsible for organising the seminar in 2024 at Stonehill College, with the help of her co-chair, Navid Hooshanginejad from Brown University.

10. University Self-Administration

image: fau.de

Activities within the University Self-Administration

Library Commission of the University, Representative of the Faculty of Engineering	Prof. Thorsten Pöschel
Competence Unit for Scientific Computing (CSC), founding member, head of “Application Lab Particles”	Prof. Thorsten Pöschel
[redacted]	
[redacted]	
Council of the Faculty of of Engineering (Fakultätrat)	Prof. Michael Engel
Habilitation Committee of the Faculty of Engineering (Kommission für Habilitationen und wissenschaftlichen Nachwuchs)	Prof. Thorsten Pöschel
Council of the Department for Chemical and Biological Engineering	Prof. Thorsten Pöschel Dr. Patric Müller
Study Grants Committee (Studienzuschüsse kommission)	Prof. Michael Engel

[redacted]

Study Commission, Study program manager CEN (Studienkommission)	Prof. Michael Engel
Spokesman of the early-stage researchers (habilitands) of the Department for Chemical and Biological Engineering	Dr. Patric Müller
PR-Team of the Department for Chemical and Biological Engineering	Ulrike Hansl
Interdisciplinary Center for Nanostructured Films, cooperative head	Prof. Thorsten Pöschel
Chairman of the Election Committee for the Implementation of the General Staff Council Election (Vorsitzender des Wahlvorstandes zur Durchführung der Gesamtpersonalratswahl)	Dr. Michael Heckel
Executive Board Member and Focal Subject Head for Computational Materials Science and Process Simulation, Advanced Materials and Processes (MAP)	Prof. Michael Engel

11. Awards

MSS postdoctoral researcher won best oral presentation award for young researchers at European Conference on Gas Hydrates

Dr. Carlos L. Bassani received the Prize of Best Oral Presentation for young researchers (up to 5y after completion of PhD thesis) at the European Conference of Gas Hydrates, held 13 to 16 of June 2022 in Lyon, France. The work entittled "Hydrate Management by Pore-Sealing in Oil-Continuous Systems" was developed during his PhD thesis in the collaboration between UTFPR/Brazil, Mines Saint-Etienne/France, and Colorados School of Mines/USA. Carlos is currently a postdoctoral fellow at the Institute for Multiscale Simulation.

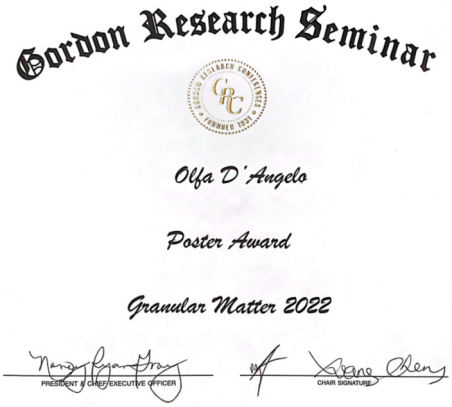
PRICE OF THE BEST ORAL

SPONSORS

MSS postdoctoral researcher won two Gordon Research Conference and Gordon Research Seminar poster awards.

Dr. Olfa D'Angelo received two separate prizes for the following two poster titles:

- "The manifold rheology of granular fluids" at the Granular Matter Gordon Research Conference.
- "Constitutive laws for dense granular fluids" at the Granular Matter Gordon Research Seminar.



MSS paper selected for Best Paper Award at Casablanca International Conference on Additive Manufacturing

Michael Blank and **Prof. Thorsten Pöschel** won the Best Paper Award for their paper titled "Temperature Gradients as a Source of Balling and Humping in Laser Processing of Titanium" at the Casablanca International Conference on Additive Manufacturing, held November 23-24, 2022.

MSS postdoctoral researcher won CBI's best teacher award

Dr. Achim Sack won the Best Teacher Prize of Chemical and Bioengineering Department for his contribution to the 2022 teaching courses. The award was presented to him during the CBI Christmas celebration.

Photo by Meysam Bagheri

12. Funding

- “Enhanced Robotic Gripper Optimisation: Simulation utilising Machine-Learning”
  German Science Foundation (DFG)
  SPP 2100 “Soft Material Robotic Systems”
  Applicant: **Prof. Thorsten Pöschel**

- “Modeling Fragmentation in Large Scale DEM Simulations”
  German Science Foundation (DFG)
  Research Training Group GRK 2423: “FRASCAL – Fracture across Scales”
  Applicant: **Prof. Thorsten Pöschel**

- “DEM Simulationen des Pulverauftrags unter Berücksichtigung der thermischen und mechanischen Eigenschaften bereits geschmolzener Bereiche”
  (“DEM simulations of powder application taking into account the thermal and mechanical properties of already molten areas”)
  German Science Foundation (DFG)
  Collaborative Research Centre SFB 814: “Additive Manufacturing”
  Applicant: **Prof. Thorsten Pöschel**

- “Aperiodische Kristalle: Struktur, Dynamik und elektronische Eigenschaften”
  German Science Foundation (DFG)
  Applicant: **Prof. Michael Engel**

- “Homogenization of Granular Pipe Flow”
  German Science Foundation (DFG)
  Applicant: **Dr. Patric Müller**

- “Granular Weissenberg Effect”
  German Science Foundation (DFG)
  Applicants: **Prof. Thorsten Pöschel** and Prof. Ralf Stannarius (Otto-von-Guericke-Universität Magdeburg)

- "Anomale Diffusions- und Transportprozesse in Anwesenheit von räumlicher und energetischer Unordnung, starker Korrelations- und Gedächtniseffekte und nichtlinearer Reibung"
  "Anomalous diffusion and transport processes in the presence of spatial and energetic disorder, strong correlation and memory effects, and nonlinear friction"
  German Science Foundation (DFG)
  Applicant: **Priv.-Doz. Dr. Igor Goychuk**

- "Controlled disorder in nanostructured materials: coupling experiments and simulations"
  German Science Foundation (DFG)
  Applicant: **Dr. Alberto Leonardi**

- "Modellierung der Aggregation und Selbstorganisation von Einzelpartikeln in optimale Strukturen"
  German Science Foundation (DFG)
  Applicant: **Prof. Michael Engel**

- "Selbstorganisation kolloidaler Partikel in Emulsionstropfen: Aggregationsmechanismus, Struktur und resultierende optische Eigenschaften "
  German Science Foundation (DFG)
  Applicant: **Prof. Michael Engel**

- "Mechanical Properties of Granular Metamaterials"
  German Science Foundation (DFG) and Agence Nationale de la Recherche (ANR)
  Applicants: **Prof. Thorsten Pöschel** and Dr. Jonathan Barés

- "SALTED – Sequential Particle Deposition – A High Performance Simulator for Granular Packings
  German Science Foundation (DFG)
  Applicant: **Prof. Thorsten Pöschel**

- ROBIN - "Entwicklung und Einsatz robuster elektrischer Mess- und Bildgebungsverfahren zur hochaufgelösten Erfassung von thermohydraulischen Parametern in Großversuchsanlagen der nuklearen Sicherheitsforschung"
  ("Development and application of robust electrical measurement and imaging techniques for high-resolution acquisition of thermal-hydraulic parameters in large-scale nuclear safety research test facilities")
  Federal Ministry of Education and Research (BMBF)
  (7. Energieforschungsprogramms der Bundesregierung in der nuklearen Sicherheitsforschung und der Strahlenforschung)
  (7th Federal government's energy research program in nuclear safety research and radiation research)
  Applicant: **Prof. Thorsten Pöschel**

- "Behaviour of Granular Matter under Vibrations (SPACE GRAINS)"
  European Space Agency (ESA)
  Applicants: J. Anthony (Leeds, UK), Sébastien Aumaitre (Saclay, France), Michaël Berhanu (Paris, France), É. Clement (Paris, France), D. Durian (U. Pennsylvania, USA), E. Falcon (Paris, France), S. Fauve (Paris, France), A. Garcimartin (Pamplona, Spain), Y. Garrabos (Bordeaux, France), M. Hou (Beijing, China), X. Jia (Marne, France), C. Lecoutre (Bordeaux, France), S. Luding (Twente, Netherlands), D. Maza (Pamplona, Spain), **T. Pöschel** (Erlangen, Germany), M. Sperl (Cologne, Germany), N. Vandewalle (Liège, Belgium)

- Return fellowship 2022/2023 for Dr. Leopoldo Gómez (Humboldt Fellow at MSS)
  Alexander von Humboldt Foundation
  Applicant: **Dr. Leopoldo Gómez**

- "Multiscale modeling of additive manufacturing processes" – Application for a Humboldt Fellowship
  Alexander von Humboldt Foundation
  Applicant: **Dr. Sudeshna Roy**

- "Understanding Hydraulic Fracture with X-ray Tomography"
  "CONICET/BAYLAT start-up financing 2021-2022"
  Applicants: **Prof. Thorsten Pöschel**, **Prof. Leopoldo Gómez** (Universidad Nacional del Sur, Argentina)

- "Catastrophe Theory in Low-strength Vibrated Granular Matter" – Scholarship
  Chinese Academy of Science, China Scholarship Council
  Applicant: **Dr. Zhiyuan Cui**

- "Implementation of Multiscale X-DFA – a Fourier Analysis for X-ray Radiograms"
  Kompetenznetzwerk für wissenschaftliches Höchstleistungsrechnen in Bayern (KONWIHR-IV)
  Applicants: **Dr. Manuel Baur**, **Prof. Thorsten Pöschel**

- "Scattering Tool to Advance Research of Materials Structure (STAR-MiSt)"
  Kompetenznetzwerk für wissenschaftliches Höchstleistungsrechnen in Bayern (KONWIHR-IV)
  Applicants: **Dr. Alberto Leonardi**, **Prof. Thorsten Pöschel**

- "Optimizing and Parallelizing a 3D freeze drying simulation"
  Kompetenznetzwerk für wissenschaftliches Höchstleistungsrechnen in Bayern (KONWIHR-IV)
  Applicants: **Christopher Bross**, **Prof. Thorsten Pöschel**

- "Laser beam melting of metals using Incompressible Smoothed Particle Hydrodynamics and a ray tracing approach"
  Gauss Centre for Supercomputing (GCS)
  Applicants: **Michael Blank**, **Prof. Thorsten Pöschel**

- "Modellbasierte Optimierung von Zwangsdurchlaufverdampfern in der Kältetechnik"
  Energie Campus Nürnberg
  Applicant: **Dr. Patric Müller**

- "Growth Instabilities for Porous Medium Formation and Evolution of Clathrate Crystals"
  Humboldt Research Fellowship for Postdocs, Alexander von Humboldt Foundation
  Applicant: **Dr. Carlos L. Bassani**

- "NORTH-CLAYS: characterisatioN Of paRTicle morpHology for quick-CLAYS"
  EXCITE Network (European Research Council)
  Transnational access to nano-CT X-ray facilities (2nd call)
  Applicant: **Dr. Vasileios Angelidakis**

- “Thermodynamic and structural characterization of pathways for crystal nucleation in solutions”
  German Academic Exchange Service (DAAD) and Programmes for Project-Related Personal Exchange (PPP) with India
  Applicant: **Prof. Michael Engel**

- “Building functional supraparticles through directed assembly of nonspherical nanoparticles”
  NSF-DFG Lead Agency Activity on Chemistry and Transport in Confined Spaces
  Applicant: **Prof. Michael Engel**

Cooperations with Industry (Funding)

- “Tomographic Investigation of Failure in Ceramic Feedthroughs”
  Fa. BIOTRONIK SE & Co. KG, Berlin
  Entwicklungsservice CRM Komponenten, Nürnberg
  project lead **Dr. Michael Heckel**, **Dr. Achim Sack**

- “Simulationen der Warmeleitfähigkeit von Keramikschäumen und weiteren Dämmstoffen” (“Simulations of the thermal conductivity of ceramic foams and other insulating materials")
  Fa. Schlagmann Poroton GmbH & Co. KG, Zeilarn
  project lead **Dr. Patric Müller**

- “Traceability of malware propagation on computer networks using statistical properties of social networks”
  Deutsche Telekom AG, Berlin
  project lead **Prof. Thorsten Pöschel**

13. Publications

Scientific papers published by the MSS in peer-reviewed journals in 2022

1. H. Götz, A. A. Santarossa, A. Sack, T. Pöschel, P. Müller, *Soft particles reinforce robotic grippers: Robotic grippers based on granular jamming of soft particles*. Granular Matter **24**, 31, DOI 10.1007/s10035-021-01193-4 (2022).
2. S. Takada, D. Serero, T. Pöschel, *Transport coefficients for granular gases of electrically charged particles*. Journal of Fluid Mechanics **935**, A38, DOI 10.1017/jfm.2022.37 (2022).
3. S.-C. Zhao, T. Pöschel, *Collective motion in two-dimensional swirling granular matter*. Physical Review E **105**, L022902, DOI 10.1103/PhysRevE.105.L022902 (2022).
4. H. Torres Menéndez, E. Altshuler, N. V. Brilliantov, T. Pöschel, *Lack of collective motion in granular gases of rotators*. New Journal of Physics **24**, 073002, DOI 10.1088/1367-2630/ac78fb (2022).
5. D. C. Marques, C. L. Bassani, C. Kakitani, M. A. Marcelino Neto, A. K. Sum, R. E. Morales, *Mapping Wall Deposition Trends of Gas Hydrates: I. Gas-Water-Hydrate Systems*. Industrial & Engineering Chemistry Research **61**, 2333, DOI 10.1021/acs.iecr.1c04723 (2022).
6. H. Xiao, A. J. Liu, D. J. Durian, *Probing Gardner physics in an active quasithermal pressure-controlled granular system of noncircular particles*. Physical Review Letters **128**, 248001, DOI 10.1103/PhysRevLett.128.248001 (2022).
7. G. Zhang, H. Xiao, E. Yang, R. J. Ivancic, S. A. Ridout, R. A. Riggleman, D. J. Durian, A. J. Liu, *Structuro-elasto-plasticity model for large deformation of disordered solids*. Physical Review Research **4**, 043026, DOI 10.1103/PhysRevResearch.4.043026 (2022).
8. O. D'Angelo, F. Kuthe, K. van Nieuwland, C. Ederveen Janssen, T. Voigtmann, M. Jalaal, *Spreading of droplets under various gravitational accelerations*. Review of Scientific Instruments **93**, 115103, DOI 10.1063/5.0105624 (2022).
9. O. D'Angelo, A. Horb, A. Cowley, M. Sperl, W. T. Kranz, *Granular piston-probing in microgravity: Powder compression, from densification to jamming*. npj Microgravity **8**, 48, DOI 10.1038/s41526-022-00235-2 (2022).

10. V. Angelidakis, S. Nadimi, M. Garum, A. Hassanpour, *Nano-Scale Characterization of Particulate Iron Pyrite Morphology in Shale*. Particle & Particle Systems Characterization **39**, 2200120, DOI 10.1002/ppsc.202200120 (2022).

11. S. Nadimi, V. Angelidakis, M. Otsubo, A. Ghanbarzadeh, *How can the effect of particle surface roughness on the contact area be predicted?*, Computers and Geotechnics **150**, 104890, DOI 10.1016/j.compgeo.2022.104890 (2022).

12. A. Leonardi, R. Neder, M. Engel, *Efficient solution of particle shape functions for the analysis of powder total scattering data*. Journal of Applied Crystallography **55**, 329–339 (2022).

13. J. Wang, Y. Liu, G. Bleyer, E. S. Goerlitzer, S. Englisch, T. Przybilla, C. F. Mbah, M. Engel, E. Spiecker, I. Imaz, D. Maspoch, N. Vogel, *Coloration in Supraparticles Assembled from Polyhedral Metal-Organic Framework Particles*. Angewandte Chemie International Edition **61**, e202117455, DOI 10.1002/anie.202117455 (2022).

14. S. L. Bueno, A. Leonardi, N. Kar, K. Chatterjee, X. Zhan, C. Chen, Z. Wang, M. Engel, V. Fung, S. E. Skrabalak, *Quinary, Senary, and Septenary High Entropy Alloy Nanoparticle Catalysts from Core@Shell Nanoparticles and the Significance of Intraparticle Heterogeneity*. ACS nano **16**, 18873–18885, DOI 10.1021/acsnano.2c07787 (2022).

15. I. Goychuk, *Memory can induce oscillations of microparticles in nonlinear viscoelastic media and cause a giant enhancement of driven diffusion*. Proceedings of the National Academy of Sciences **119**, e2205637119, DOI 10.1073/pnas.2205637119 (2022).

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32. S. Roy, H. Xiao, M. Y. Shaheen, T. Pöschel, *Local structural anisotropy in particle simulations of powder spreading in additive manufacturing*. Casablanca International Conference on Additive Manufacturing (2022).
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Patent Application

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Soft particles reinforce robotic grippers: Robotic grippers based on granular jamming of soft particles

Holger Götz, Angel Santarossa, Achim Sack, Thorsten Pöschel, *and* ***Patric Müller***

Abstract:

Granular jamming has been identified as a fundamental mechanism for the operation of robotic grippers. In this work we show, that soft particles like expanded polystyrene beads lead to significantly larger gripping forces in comparison to rigid particles. In contradiction to naive expectation, the combination of jamming and elasticity gives rise to very different properties of the jammed phase, compared to hard-particle systems. This may be of interest also beyond the application in robotic grippers.

Figure: Experimental setup for automatic holding force measurements.

1. H. Götz, A. A. Santarossa, A. Sack, T. Pöschel, P. Müller, *Soft particles reinforce robotic grippers: Robotic grippers based on granular jamming of soft particles*. Granular Matter **24**, 31, DOI 10.1007/s10035-021-01193-4 (2022).

Transport coeffcients for granular gases of electrically charged particles

Satoshi Takada, ***Dan Serero****, and* ***Thorsten Pöschel***

Abstract:
We consider a dilute gas of electrically charged granular particles in the homogeneous cooling state. We derive the energy dissipation rate and the transport coefficients from the inelastic Boltzmann equation. We find that the deviation of the velocity distribution function from the Maxwellian yields overshoots of the transport coefficients, and especially, the negative peak of the Dufour-like coefficient, μ, in the intermediate granular temperature regime. We perform the linear stability analysis and investigate the granular temperature dependence of each mode, where the instability mode is found to change against the granular temperature. The molecular dynamics simulations are also performed to compare the result with that from the kinetic theory.

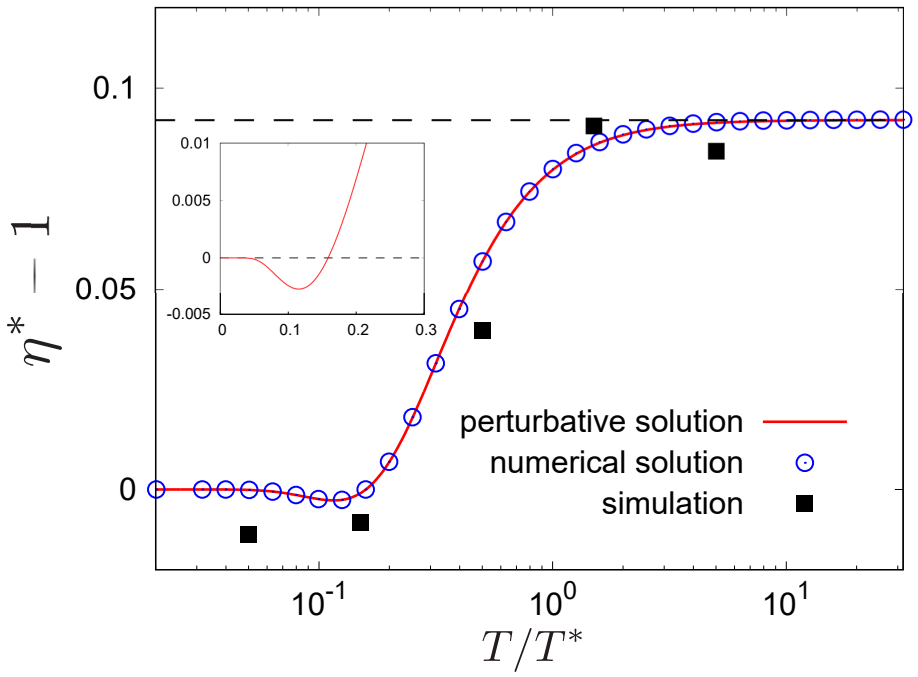

Figure: Shear viscosity as a function of granular temperature obtained from the kinetic theory perturbatively (solid line) and numerically (open circles) for $e^* = 0.8$. The filled squares show results obtained from an event-driven molecular dynamics simulation. The dashed line is the shear viscosity of a hard-sphere gas. The inset shows a magnification of the intermediate regime.

2. S. Takada, D. Serero, T. Pöschel, *Transport coefficients for granular gases of electrically charged particles*. Journal of Fluid Mechanics **935**, A38, DOI 10.1017/jfm.2022.37 (2022).

Collective motion in two-dimensional swirling granular matter

Song-Chuan Zhao *and* ***Thorsten Pöschel***

Abstract:

A two-dimensional granular packing under horizontally circular shaking exihibits various collective motion modes depending on the strength of oscillation and the packing density. For intermediate packing density and oscillation strength, a high density area travels along the container's side wall clockwisely, while the oscillation itself is anti-clockwise. For the system close to the hexagon packing, at small oscillation amplitudes, the whole packing rotates collectively in the clockwise direction around its center of mass. The central part of the packing rotates as a solid-like core and is separated from the boundary by a fluid-like layer. Further increasing the oscillation amplitudes, the two-dimensional scenario breaks down near the side wall, while the center becomes dilute. This reclaims the possibility of spontaneous clustering at high oscillation amplitude, as reported in our previous work. The rotational frustration which occurs in dense neighborhood is supposed to play a crucial role in the motion modes studied here.

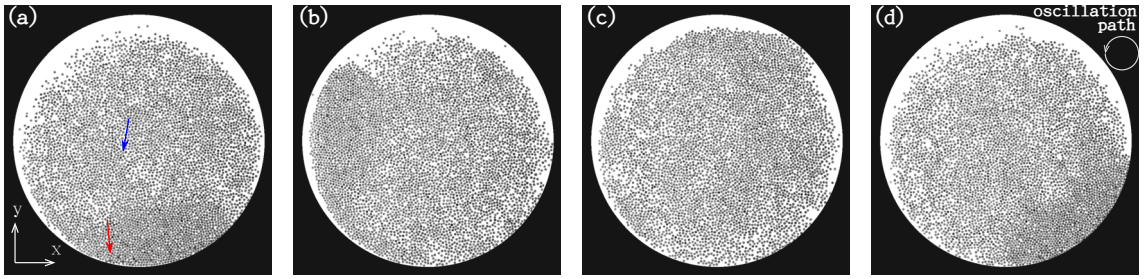

Figure: Snapshots of the packing of $\varphi = 0.57$ and $A = 7\,\mathrm{mm}$ at the middle of (a) cycle 1, (b) cycle 5, (c) cycle 9 and (d) cycle 13. In the inset of (d) the oscillation path of the amplitude $A = 10\,\mathrm{mm}$ is drawn up to scale.

3. S.-C. Zhao, T. Pöschel, *Collective motion in two-dimensional swirling granular matter*. Physical Review E **105**, L022902, DOI 10.1103/PhysRevE.105.L022902 (2022).

Lack of collective motion in purely rotating granular gases

Harol Torres Menéndez, *Ernesto Altshuler, Nikolai V. Brilliantov, and* ***Thorsten Pöschel***

Abstract:

The dynamics of gases made of particles interacting dissipatively –known as granular gases– is fully described by the translational and rotational motion of the individual particles. However, research in the field concentrates in the limit of smooth particles, where the rotational degrees of freedom are suppressed. Here we investigate experimentally and theoretically the opposite limit: a granular gas where the translational degrees of freedom are eliminated, and the key degrees of freedom are rotational. We demonstrate that the lattice topology does not play any noticeable rôle in the dynamics of the system, which is mainly governed by the lattice constant. Surprisingly, our results reveal that the removal of translational degrees of freedom suppresses the collective motion of the system: the dynamics is dominated by uncorrelated random collisions.

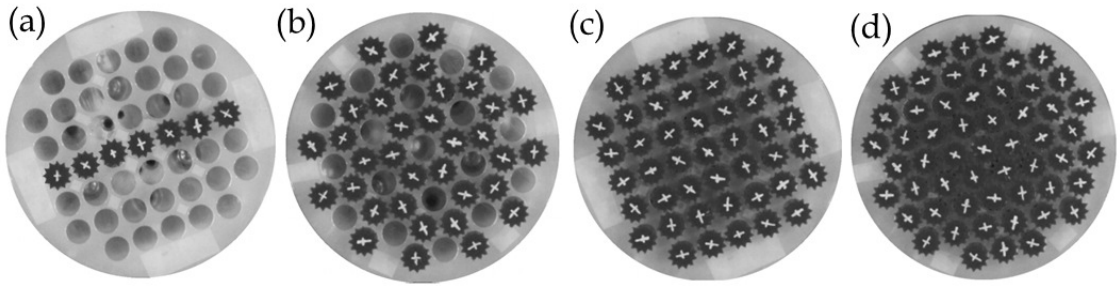

Figure: Rotational granular gas lattices. (a) two neighbors; (b) three neighbors; (c) four neighbors; (d) six neighbors. Also, the lattice constant, a, and the clearance, $R = r_h - r_l$, can be chosen

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Mapping Wall Deposition Trends of Gas Hydrates: I. Gas-Water-Hydrate Systems

Daniela C. Marques, ***Carlos L. Bassani****, Celina Kakitani, Moisés A. Marcelino Neto, Amadeu K. Sum, and Rigoberto E.M. Morales*

Abstract:

Measurements of gas hydrate deposition under sheared conditions are reported in this study. In Part I of this series, experiments with a 100% water cut (gas-water-hydrate systems, without oil) are analyzed. A total of 35 experiments are presented for methane hydrates (sI structure) and for a gas mixture composed of 74.7 mol % methane and 25.3 mol % ethane (sII structure) for subcooling ranging from 1.3 to 11.9 °C, liquid loadings from 20 to 60 vol %, and oscillation rates from 6 to 18.75 rpm. Visual observation of the macromorphology of the systems, before and after the onset of gas hydrate formation, is made possible by polycarbonate windows that resist the imposed pressure. Results point out that wall deposition occurs within the first hour after the onset of hydrate formation for the measured conditions. The location of the wall deposits-in the lateral or upper walls, enduring gravity-is mapped in terms of the hydrodynamics of water and its ability to reach the different walls of the cell. Quantitative results for the molar amount of gas consumed during hydrate formation are presented, and mathematical insights are given into how growth kinetics change once the system undergoes wall deposition in the 1 h-timescale, as well as deposit hardening (annealing) in longer timescales.

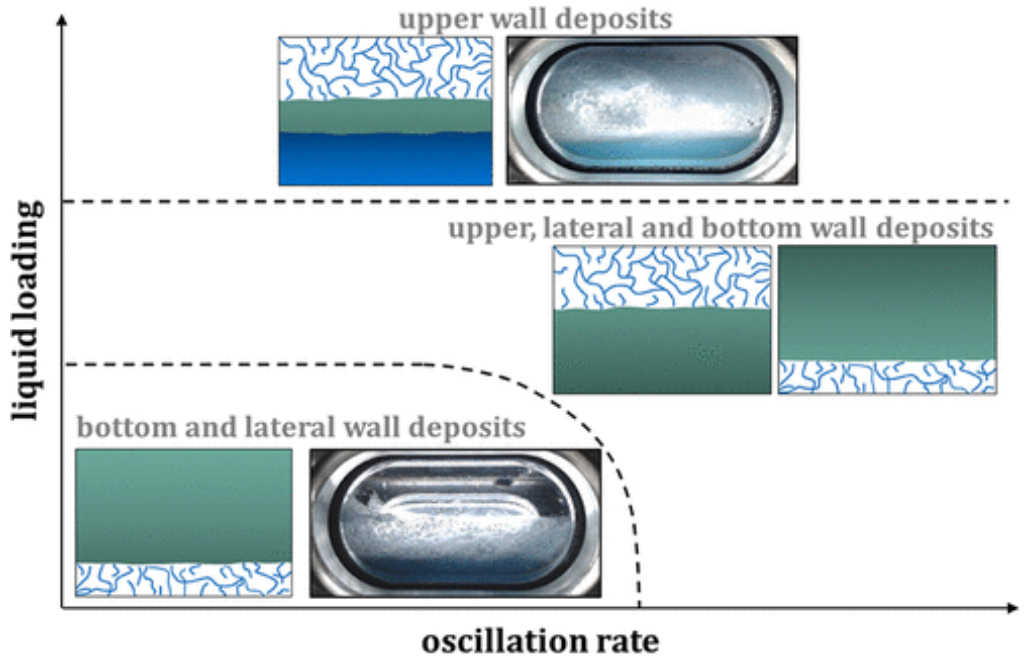


Figure: Map of deposit behavior of gas hydrates regarding liquid loading and oscillation rate, for 100% water cut systems, for crystalline structure II and gas composition of 74.7 mol % methane and 25.3 mol % ethane.

5. D. C. Marques, C. L. Bassani, C. Kakitani, M. A. Marcelino Neto, A. K. Sum, R. E. Morales, *Mapping Wall Deposition Trends of Gas Hydrates: I. Gas-Water-Hydrate Systems*. Industrial & Engineering Chemistry Research **61**, 2333, DOI `10.1021/acs.iecr.1c04723` (2022).

Probing Gardner physics in an active quasithermal pressure-controlled granular system of noncircular particles

***Hongyi Xiao**, Andrea Liu, and Douglas Durian*

Abstract:

To search for experimental signals of the Gardner crossover, an active quasithermal granular glass is constructed using a monolayer of air-fluidized star-shaped particles. The pressure of the system is controlled by adjusting the tension exerted on an enclosing boundary. Velocity distributions of the internal particles and the scaling of the pressure, density, effective temperature, and relaxation time are examined, demonstrating that the system has key features of a thermal system. Using a pressure-based quenching protocol that brings the system into deeper glassy states, signals of the Gardner crossover are detected via cage size and separation order parameters for both particle positions and orientations, offering experimental evidence of Gardner physics for a system of anisotropic quasithermal particles in a low spatial dimension.

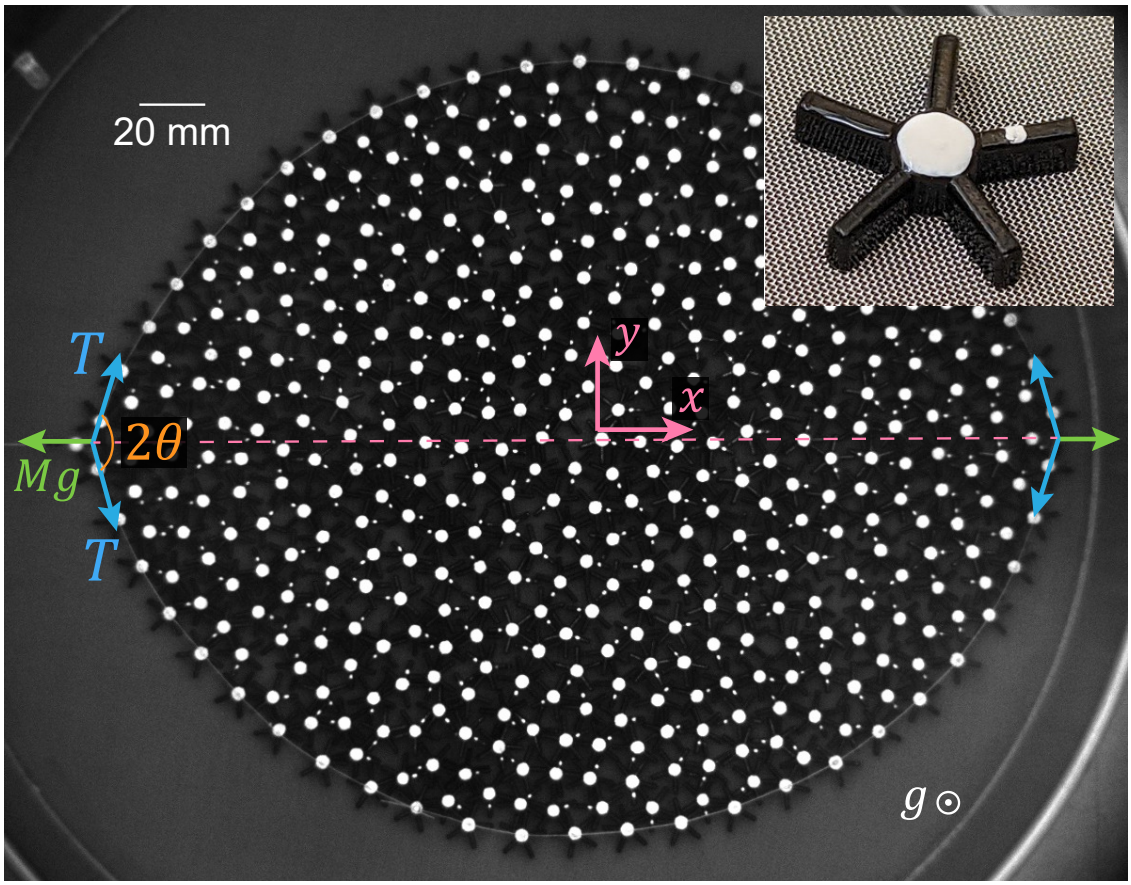


Figure: Photograph of the pressure-controlled experiment with star-shaped particles (inset). Air-fluidized particles are enclosed by a boundary made of a chain of particles on a thin flexible thread. The left end is pulled with a controlled force while the right end is anchored.

6. H. Xiao, A. J. Liu, D. J. Durian, *Probing Gardner physics in an active quasithermal pressure-controlled granular system of noncircular particles*. Physical Review Letters **128**, 248001, DOI 10.1103/PhysRevLett.128.248001 (2022).

Structuro-elasto-plasticity model for large deformation of disordered solids

Ge Zhang, ***Hongyi Xiao****, Entao Yang, Robert Ivancic, Sean Ridout, Robbert Riggleman, Douglas Durian, and Andrea Liu*

Abstract:

Elastoplastic lattice models for the response of solids to large-scale deformation typically incorporate structure only implicitly via a local yield strain that is assigned to each site. However, the local yield strain can change in response to a nearby or even distant plastic event in the system. This interplay is key to understanding phenomena such as avalanches in which one plastic event can trigger another, leading to a cascade of events, but is typically neglected in elastoplastic models. To include the interplay one could calculate the local yield strain for a given particulate system and follow its evolution, but this is expensive and requires knowledge of particle interactions that aren't necessarily pairwise additive or possible to extract from experiments. Instead, we use a structural quantity, "softness," obtained using machine learning to correlate with imminent plastic rearrangements. We show that softness correlates with local yield strain and use it to construct a "structuro-elasto-plasticity" model that reproduces particle simulation results reasonably well for several observable quantities, confirming that we capture the influence of the interplay of local structure, plasticity, and elasticity on material response.

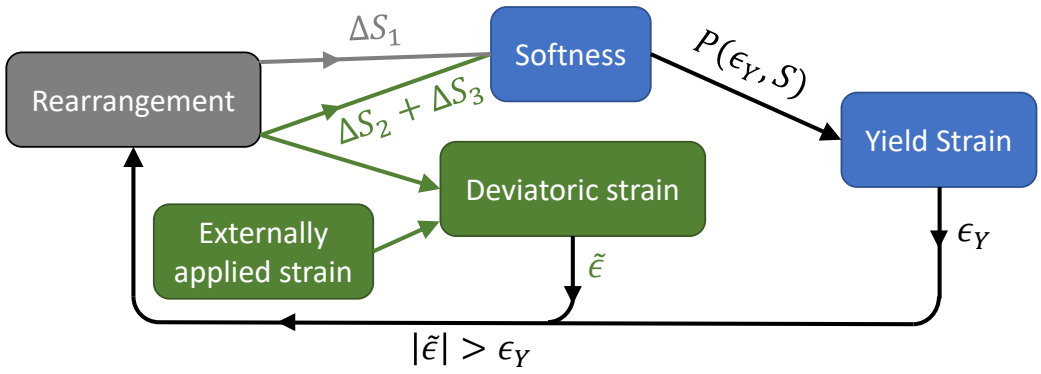


Figure: The general scheme for the Structuro-elasto-plastic model depicting interplays between the three element for plastic deformation of disordered solids.

7. G. Zhang, H. Xiao, E. Yang, R. J. Ivancic, S. A. Ridout, R. A. Riggleman, D. J. Durian, A. J. Liu, *Structuro-elasto-plasticity model for large deformation of disordered solids*. Physical Review Research **4**, 043026, DOI 10.1103/PhysRevResearch.4.043026 (2022).

Spreading of droplets under various gravitational accelerations

***Olfa D'Angelo**, Felix Kuthe, Kasper van Nieuwland, Clint Ederveen Janssen, Thomas Voigtmann, and Maziyar Jalaal*

Abstract:

We describe a setup to perform systematic studies on the spreading of droplets of complex fluids under microgravity conditions. Tweaking the gravitational acceleration under which droplets are deposited provides access to different regimes of the spreading dynamics, as quantified through the Bond number. In particular, microgravity allows us to form large droplets while remaining in the regime where surface tension effects and internal driving stresses are predominant over hydrostatic forces. The VIP-DROP^2 (VISCO-Plastic DROPlets on the DROP tower) experimental module provides a versatile platform to study a wide range of complex fluids through the deposition of axisymmetric droplets. The module offers the possibility to deposit droplets on a precursor layer, which can be composed of the same or a different fluid. Furthermore, it allows us to deposit four droplets simultaneously while conducting shadowgraphy on all of them and observing either the flow field (through particle image velocimetry) or the stress distribution inside the droplet in the case of stress birefringent fluids. It was developed for a drop tower catapult system, is designed to withstand a vertical acceleration of up to 30 times the Earth's gravitational acceleration in the downward direction, and is capable of operating remotely under microgravity conditions. We provide a detailed description of the module and an exemplary data analysis for droplets spreading on-ground and in microgravity.

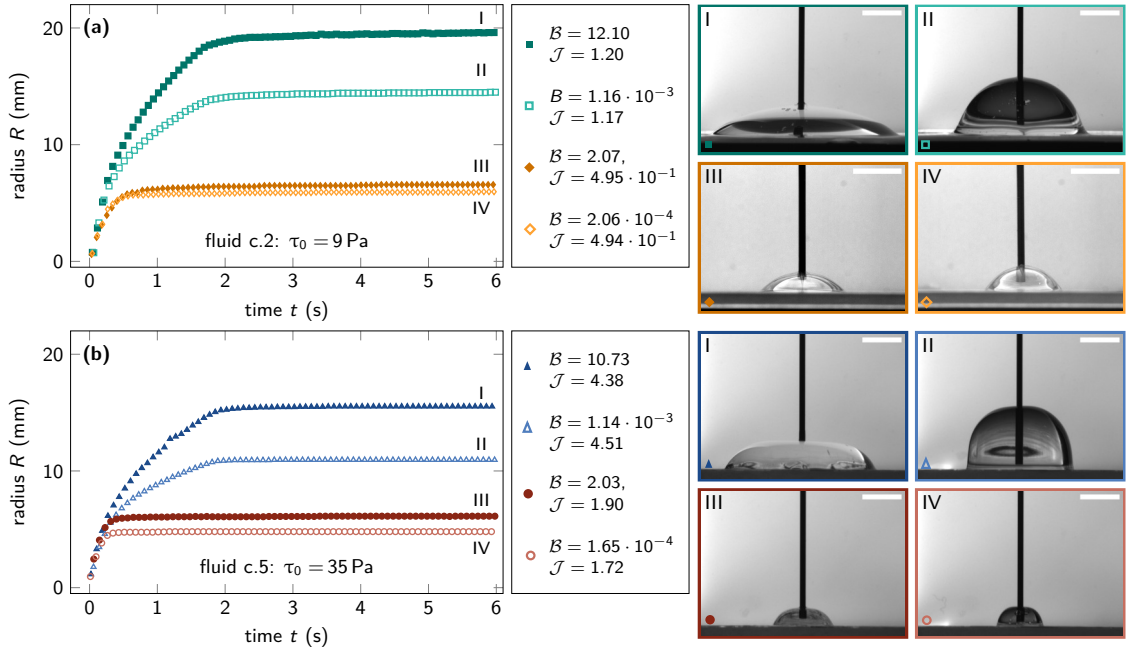


Figure: Radius $R(t)$ of the droplets as a function of time, comparing the same fluids on-ground (labeled $1g$, filled marks) and under microgravity conditions (μg, empty marks). Pictures are taken at the last instant before the end of the experiment. In all pictures, the scale bar represents 8 mm.

8. O. D'Angelo, F. Kuthe, K. van Nieuwland, C. Ederveen Janssen, T. Voigtmann, M. Jalaal, *Spreading of droplets under various gravitational accelerations*. Review of Scientific Instruments **93**, 115103, DOI `10.1063/5.0105624` (2022).

Granular piston-probing in microgravity: powder compression, from densification to jamming

***Olfa D'Angelo**, Anabelle Horb, Aidan Cowley, Matthias Sperl, W. Till Kranz*

Abstract:

The macroscopic response of granular solids is determined by the microscopic fabric of force chains, which, in turn, is intimately linked to the history of the solid. To query the influence of gravity on powder flow behavior, a granular material is subjected to compression by a piston in a closed container, on-ground and in microgravity (on parabolic flights). Results show that piston-probing densifies the packing, eventually leading to jamming of the material compressed by the piston, regardless of the gravitational environment. The onset of jamming is found to appear at lower packing fraction in microgravity ($\varphi_J^{\mu-g} = 0.567 \pm 0.014$) than on-ground ($\varphi_J^{gnd} = 0.579 \pm 0.014$). We interpret these findings as the manifestation of a granular fabric altered by the gravitational force field: in absence of a secondary load (due to gravitational acceleration) to stimulate reorganization in a different direction to the major compression stress, the particles' configuration becomes stable at lower density, as the particles have no external drive to promote reorganization into a denser packing. This is coupled with a change in interparticular force balance which takes place under low gravity, as cohesive interactions become predominant. We propose a combination of microscopic and continuum arguments to rationalize our results.

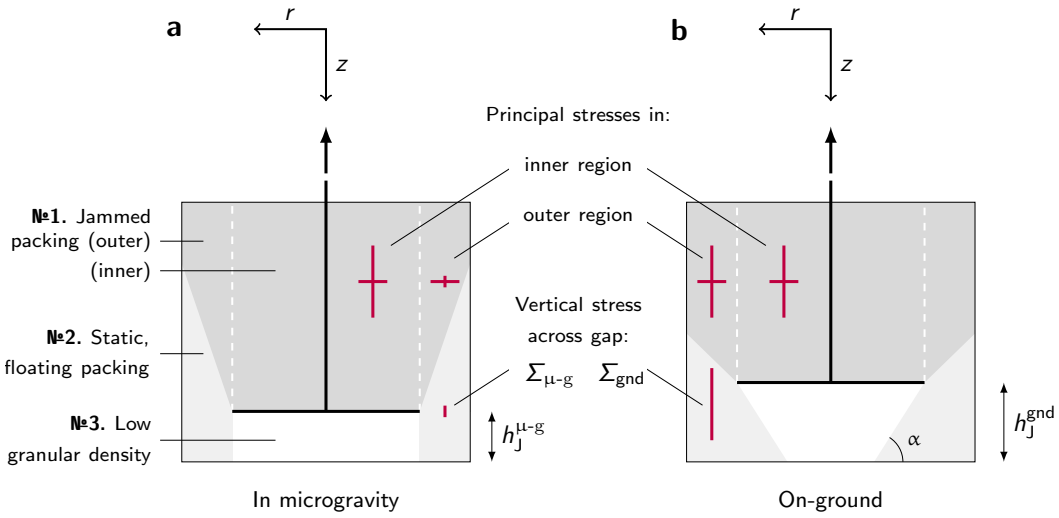


Figure: Schematic representation of the regions appearing in powder container as the piston rises, (a) in microgravity ($\mu - g$) and (b) on-ground (gnd). On-ground, the powder forms a slope at its angle of repose α with the horizontal. Stress magnitudes in arbitrary units are depicted by red lines. The height $h_J^{\mu-g,gnd}$ denotes the height at which the piston is stopped by the jammed material above it, respectively under microgravity and on-ground conditions. The difference in force chain configuration between microgravity and ground leads to drastically different vertical stresses in the outer region. The load Σ on the material below the piston is, as a consequence, much lower in microgravity compared to the ground.

9. O. D'Angelo, A. Horb, A. Cowley, M. Sperl, W. T. Kranz, *Granular piston-probing in microgravity: Powder compression, from densification to jamming*. npj Microgravity **8**, 48, DOI 10.1038/s41526-022-00235-2 (2022).

Nano-scale characterization of particulate iron pyrite morphology in shale

***Vasileios Angelidakis**, Sadegh Nadimi, Mohamed Garum, and Ali Hassanpour*

Abstract:

This study analyzes the morphology of iron pyrite particles within a shale sample captured using nano-computed tomography (Nano-CT). The complex, framboidal morphology of the iron pyrite particles is characterized using various metrics, and comparisons are drawn on their effectiveness to quantify their observed morphological characteristics. Then, simplified representations of selected iron pyrite particles are generated to facilitate a sensitivity analysis of the effect of imaging resolution on morphological parameters of particle form. A discussion is developed on the required number of pixels per particle diameter for particle shape characterization. It is shown that shape indices that rely on the simplified main particle dimensions can be accurately calculated even for low fidelity levels of 10 pixels per particle diameter. More complex shape indices that use vertices, volume, and surface area, are more sensitive to image resolution, even for 40 pixels per particle diameter.

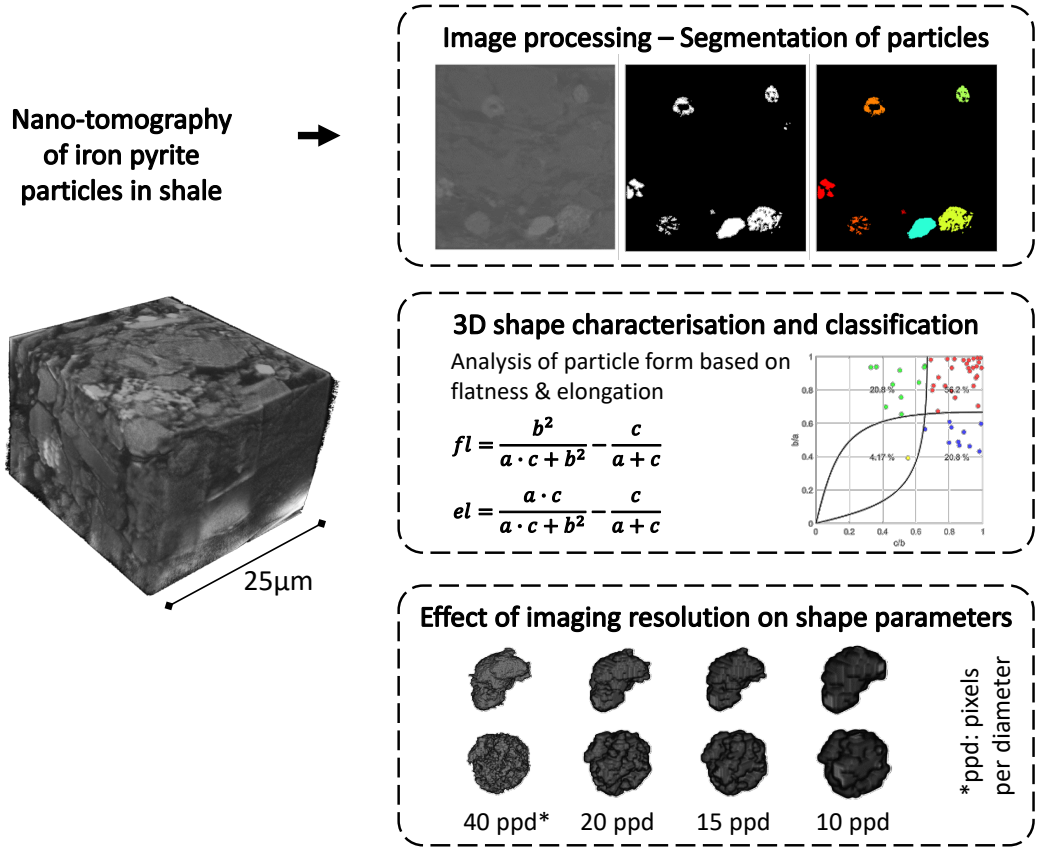


Figure: Shape characterisation and classification of iron-pyrite particles using Nano-CT.

10. V. Angelidakis, S. Nadimi, M. Garum, A. Hassanpour, *Nano-Scale Characterization of Particulate Iron Pyrite Morphology in Shale*. Particle & Particle Systems Characterization **39**, 2200120, DOI 10.1002/ppsc.202200120 (2022).

How can the effect of particle surface roughness on the contact area be predicted?

Sadegh Nadimi, ***Vasileios Angelidakis****, Masahide Otsubo, and Ali Ghanbarzadeh*

Abstract:

This paper describes a systematic study of the effect of fractal rough surfaces on the contact area with the aim of advancing contact constitutive laws used in the Discrete Element Method. An in-house Boundary Element code is adopted to investigate the mechanical behaviour of computer-generated surface roughness. Surfaces are generated to have methodically controlled root mean square height (S_q), root mean square gradient (S_{dq}), short wavevector (q_0), large wavevector (q_1), Hurst exponent (H) and fractal dimension (D_f). The effect of each parameter on the contact area is investigated. Two recently proposed analytical solutions in tribology (i.e. Persson-Tosatti and Pastewka-Robbins) are applied to predict the real contact area. A parameter based on S_q, q_0, and H is proposed and its sensitivity for real contact area prediction is demonstrated. Surfaces of natural sand are simulated and their mechanical response shows similar trend as the computer-generated surfaces, albeit more complex.

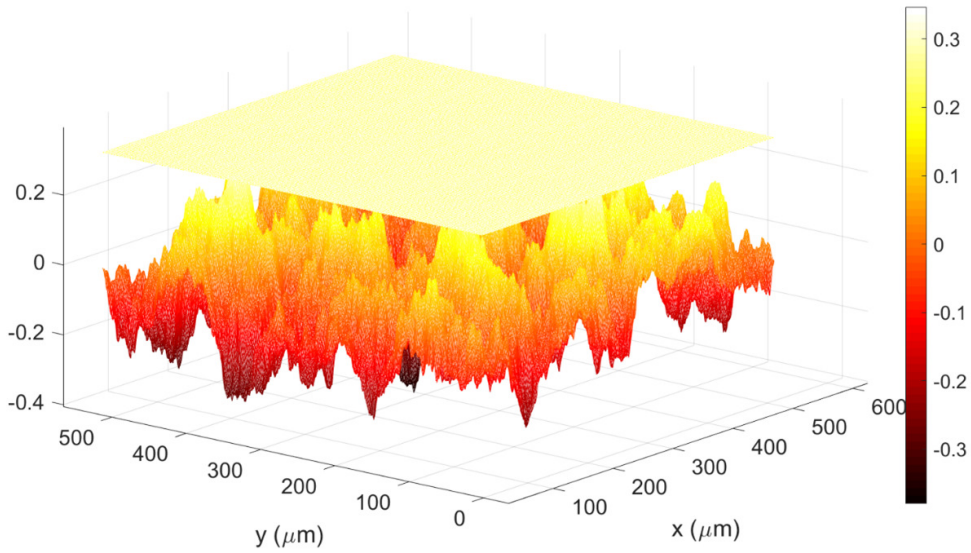


Figure: Contact between a smooth and a rough surface. The colour map shows the elevation in μm measuring from the average height of the rough surface.

11. S. Nadimi, V. Angelidakis, M. Otsubo, A. Ghanbarzadeh, *How can the effect of particle surface roughness on the contact area be predicted?*, Computers and Geotechnics **150**, 104890, DOI 10.1016/j.compgeo.2022.104890 (2022).

Efficient solution of particle shape functions for the analysis of powder total scattering data

Alberto Leonardi, Reinhard Neder, and Michael Engel

Abstract:

Structural characterization of powder samples via total scattering methods, in either real or reciprocal space, must take into account the effect of particle shape. Here, the shape contribution of a set of ideally isolated particles to the small-angle scattering (SAS) component of the intensity profile is modelled using the shape function Svergun and Koch (2003). The shape function is obtained by orientational averaging of common volume functions (CVFs) for a discrete set of directions. The effects of particle size and size dispersity are accounted for via scaling of the CVFs and their convolution with the underlying probability distribution. The method is applied to shapes with CVFs expressed analytically or by using discrete tables. The accurate calculation of SAS particle shape contributions up to large momentum transfer demonstrates the reliability and flexibility of modelling shape functions from sets of CVFs. The algorithm presented here is computationally efficient and can be directly incorporated into existing routines for analysis of powder total scattering data.

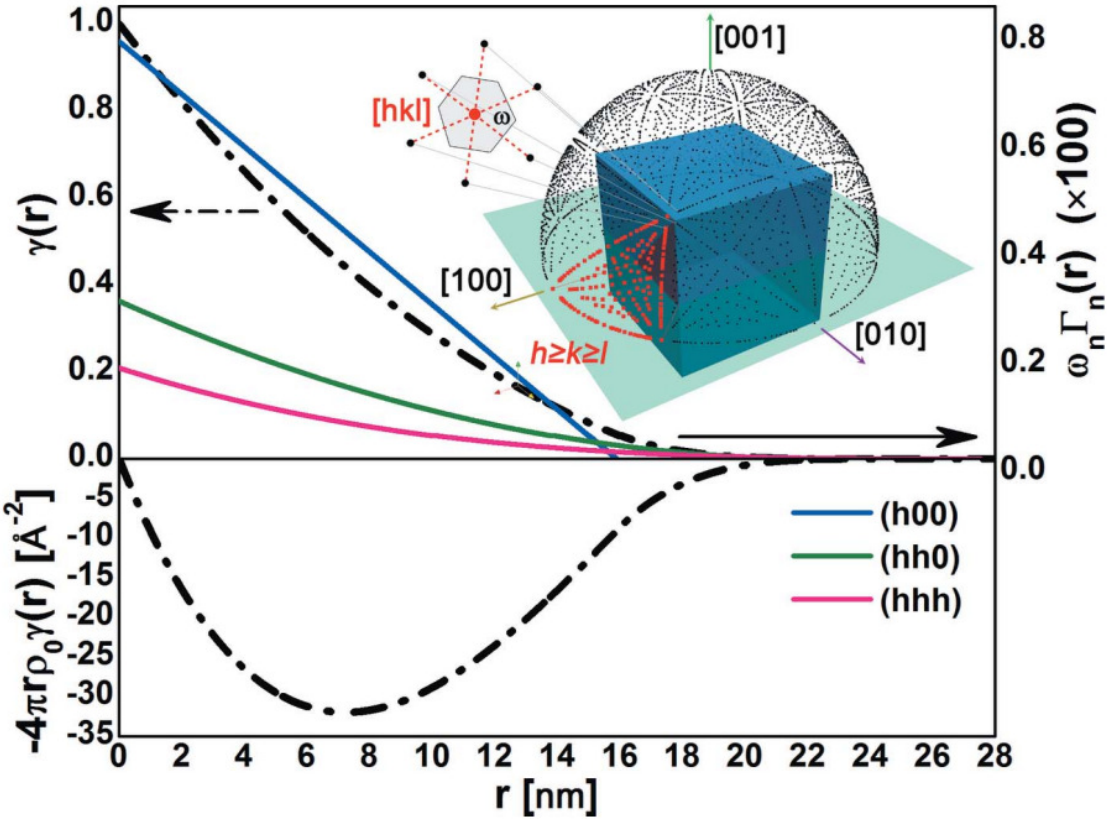


Figure: Modelling the shape function for a cube of edge length 16*nm*.

12. A. Leonardi, R. Neder, M. Engel, *Efficient solution of particle shape functions for the analysis of powder total scattering data*. Journal of Applied Crystallography **55**, 329–339 (2022).

Coloration in Supraparticles Assembled from Polyhedral Metal-Organic Framework Particles

Junwei Wang, Yang Liu, Gudrun Bleyer, Eric S. A. Goerlitzer, Silvan Englisch, Thomas Przybilla, ***Chrameh Fru Mbah****,* ***Michael Engel****, Erdmann Spiecker, Inhar Imaz, Daniel Maspoch, and Nicolas Vogel*

Abstract:

Supraparticles are spherical colloidal crystals prepared by confined self-assembly processes. A particularly appealing property of these microscale structures is the structural color arising from interference of light with their building blocks. Here, we assemble supraparticles with high structural order that exhibit coloration from uniform, polyhedral metal–organic framework (MOF) particles. We analyse the structural coloration as a function of the size of these anisotropic building blocks and their internal structure. We attribute the angle-dependent coloration of the MOF supraparticles to the presence of ordered, onion-like layers at the outermost regions. Surprisingly, even though different shapes of the MOF particles have different propensities to form these onion layers, all supraparticle dispersions show well-visible macroscopic coloration, indicating that local ordering is sufficient to generate interference effects.

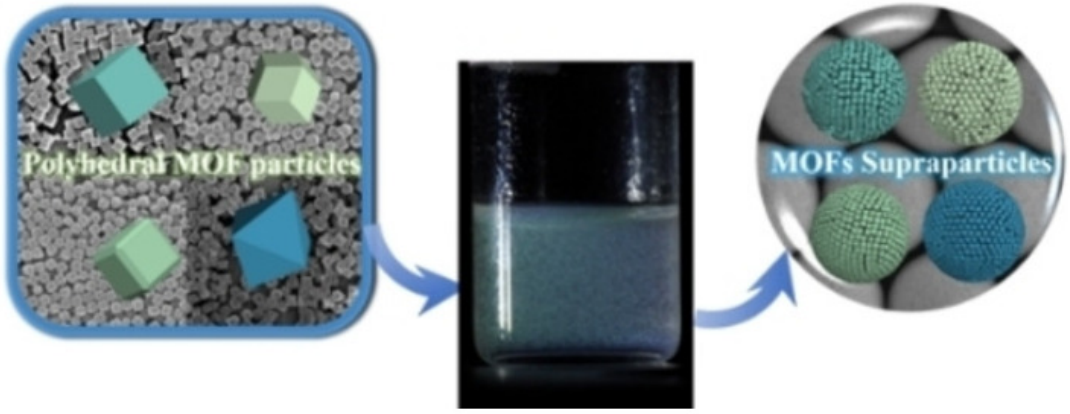


Figure: Supraparticles exhibiting coloration and high structural order are assembled from four different uniform, polyhedral metal-organic framework (MOF) particles. In these supraparticles, the macroscopic color originates from constructive interference of light reflected at ordered surface layers of the polyhedral particles.

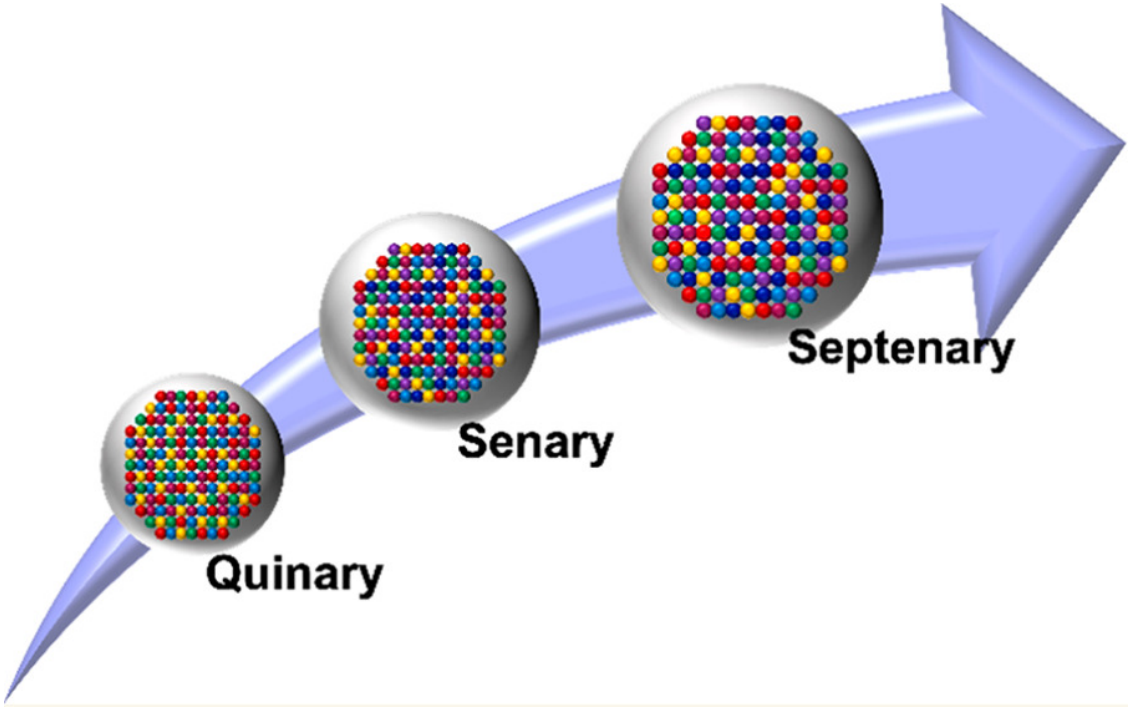
13. J. Wang, Y. Liu, G. Bleyer, E. S. Goerlitzer, S. Englisch, T. Przybilla, C. F. Mbah, M. Engel, E. Spiecker, I. Imaz, D. Maspoch, N. Vogel, *Coloration in Supraparticles Assembled from Polyhedral Metal-Organic Framework Particles*. Angewandte Chemie International Edition **61**, e202117455, DOI `10.1002/anie.202117455` (2022).

Quinary, Senary, and Septenary High Entropy Alloy Nanoparticle Catalysts from Core@Shell Nanoparticles and the Significance of Intraparticle Heterogeneity

Sandra L. A. Bueno, ***Alberto Leonardi****, Nabojit Kar, Kaustav Chatterjee, Xun Zhan, Changqiang Chen, Zhiyu Wang,* ***Michael Engel****, Victor Fung, and Sara E. Skrabalak*

Abstract:

Colloidally prepared core@shell nanoparticles (NPs) were converted to monodisperse high entropy alloy (HEA) NPs by annealing, including quinary, senary, and septenary phases comprised of PdCuPtNi with Co, Ir, Rh, Fe, and/or Ru. Intraparticle heterogeneity, i.e., subdomains within individual NPs with different metal distributions, was observed for NPs containing Ir and Ru, with the phase stabilities of the HEAs studied by atomistic simulations. The quinary HEA NPs were found to be durable catalysts for the oxygen reduction reaction, with all but the PdCuPtNiIr NPs presenting better activities than commercial Pt. Density functional theory (DFT) calculations for PdCuPtNiCo and PdCuPtNiIr surfaces (the two extremes in performance) found agreement with experiment by weighting the adsorption energy contributions by the probabilities of each active site based on their DFT energies. This finding highlights how intraparticle heterogeneity, which we show is likely overlooked in many systems due to analytical limitations, can be leveraged toward efficient catalysis.



14. S. L. Bueno, A. Leonardi, N. Kar, K. Chatterjee, X. Zhan, C. Chen, Z. Wang, M. Engel, V. Fung, S. E. Skrabalak, *Quinary, Senary, and Septenary High Entropy Alloy Nanoparticle Catalysts from Core@Shell Nanoparticles and the Significance of Intraparticle Heterogeneity*. ACS nano **16**, 18873–18885, DOI 10.1021/acsnano.2c07787 (2022).

Memory can induce oscillations of microparticles in nonlinear viscoelastic media and cause a giant enhancement of driven diffusion

Igor Goychuk

Abstract:

We investigate analytically and numerically a basic model of driven Brownian motion with a velocity-dependent friction coefficient in nonlinear viscoelastic media featured by a stress plateau at intermediate shear velocities and profound memory effects. For constant force driving, we show that nonlinear oscillations of a microparticle velocity and position emerge by a Hopf bifurcation at a small critical force (first dynamical phase transition), where the friction's nonlinearity seems to be wholly negligible. They also disappear by a second Hopf bifurcation at a much larger force value (second dynamical phase transition). The bifurcation diagram is found in an analytical form confirmed by numerics. Surprisingly, the particles' inertial and the medium's nonlinear properties remain crucial even in a parameter regime where they were earlier considered entirely negligible. Depending on the force and other parameters, the amplitude of oscillations can significantly exceed the size of the particles, and their period can span several time decades, primarily determined by the memory time of the medium. Such oscillations can also be thermally excited near the edges of dynamical phase transitions. The second dynamical phase transition combined with thermally induced stochastic limit cycle oscillations leads to a giant enhancement of diffusion over the limit of vast driving forces, where an effective linearization of stochastic dynamics occurs.

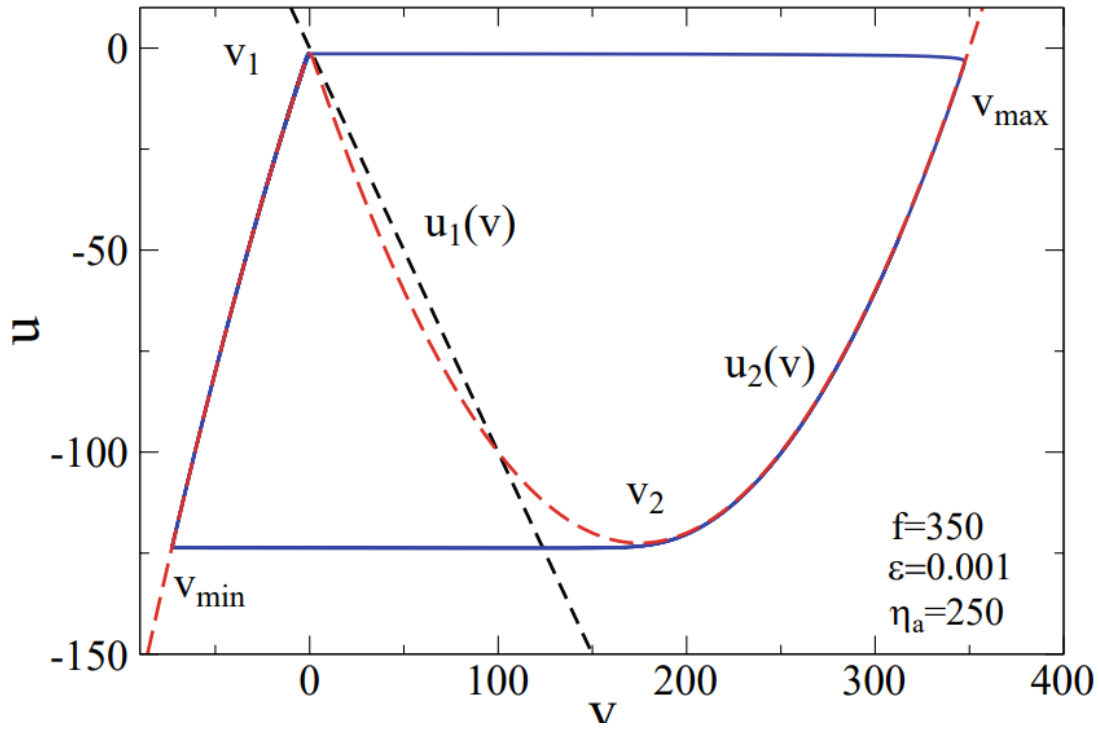


Figure: Dynamics in (v,u) phase plane at $T=0$, $\eta_a=250$, $f_c=250$, $f=350$, $\varepsilon=0.001$. Two nullclines are depicted together with a trajectory accomplishing several cycles.

15. I. Goychuk, *Memory can induce oscillations of microparticles in nonlinear viscoelastic media and cause a giant enhancement of driven diffusion*. Proceedings of the National Academy of Sciences **119**, e2205637119, DOI `10.1073/pnas.2205637119` (2022).

Resonance-like enhancement of forced nonlinear diffusion as a nonequilibrium phase transition

Igor Goychuk

Abstract:

We describe the phenomenon of a resonance-like, giant enhancement of diffusion in a basic model of nonlinear diffusion featured by a nonlinear in velocity friction and the corresponding multiplicative thermal noise. The model is consistent with thermal equilibrium in the absence of driving. Different from previous studies of this phenomenon, where the crucial nonlinearity originates from a periodic external potential while friction is linear, we focus on the case of a constant force driving, whereas the crucial nonlinearity stems from the friction. The basic model of such friction considered interpolates between linear viscous Stokes friction at small velocities and dry Coulomb-like friction at large velocities corresponding to a stress plateau in some nonlinear viscoelastic materials. Recently, a nonequilibrium phase transition to super-diffusion and super-transport was discovered within this basic model. We show that adding a tiny viscous friction part to major nonlinear friction regularizes in part this behavior. Diffusion becomes asymptotically normal. However, the phase transition translates into a giant enhancement of normal diffusion and mobility of particles at the transition point over the intuitively expected large force limit, where the linearization of friction occurs. Such a giant enhancement of diffusion is closely related to the largely enhanced kinetic temperature of the particles at and beyond the critical point. We provide analytical results obtained within an effective mass approximation which nicely agree with stochastic numerics.

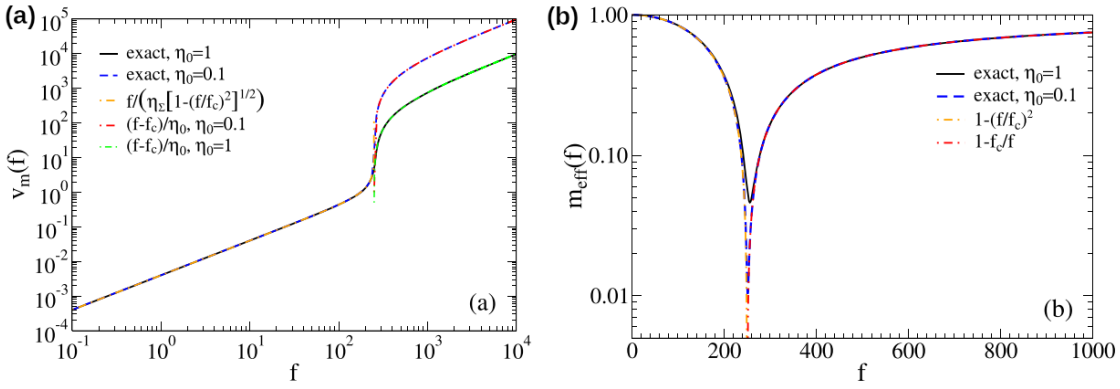


Figure: Dependencies of v_m (a) and m_{eff} (b) on force f. In (a), the exact expression in equations (B.2)–(B.11) is compared with the discussed in text approximations for two values $\eta_0 = 1$ and $\eta_0 = 0.1$ at fixed $\eta_a = 250$ and $f_c = 250$ with $v_c = 1$. The existence of two very different regimes, left and right of f_c, is clearly seen. The approximations work very well except for a small neighborhood of f_c, which shrinks with diminishing η_0. In (b), the exact result in equations (26), (B.2)–(B.11) is compared with two approximations.

16. I. Goychuk, *Resonance-like enhancement of forced nonlinear diffusion as a nonequilibrium phase transition*. New Journal of Physics **24**, 043018, DOI 10.1088/1367-2630/ac614f (2022).

Round robin test on angle of repose: DEM simulation results collected from 16 groups around the world

Hidetaka Saomoto, Naotaka Kikkawa, Shuji Moriguchi, Yukio Nakata, Masahide Otsubo, ***Vasileios Angelidakis****, Yi Pik Cheng, Kevin Chew, Gabriele Chiaro, Jérôme Duriez, Sacha Duverger, Joaquín Irazábal González, Mingjing Jiang, Yohei Karasaki, Akiko Kono, Xintong Li, Zhuyuan Lin, Asen Liu, Sadegh Nadimi, Hitoshi Nakase, Daisuke Nishiura, Utsa Rashique, Hiroyuki Shimizu, Kumpei Tsuji, Takashi Watanabe, Xiaomin Xu, Mourad Zeghal*

Abstract:

The round robin test (the simultaneous analysis of the same problem) is a method to investigate the variance and sensitivity of results provided by different analysts for a given problem and the reliability of the particular software used by each group participating in the test. A round robin test has been conducted for the traditional numerical method (e.g., finite difference method), but not yet for the discrete element method (DEM). This paper presents the results of the first ever round robin test on the DEM simulation for the angle of repose, involving 16 groups from around the world using different softwares. Within the scope of this round robin test, most groups reported similar simulation results for the angle of repose that differed only by a few degrees from the average of the experimental values, which was initially concealed from participants. There was also good agreement on the degree of variance of the angle of repose. In addition, this paper revealed the recent trends on the interparticle constitutive models and DEM softwares by considering the reports obtained from the participants.

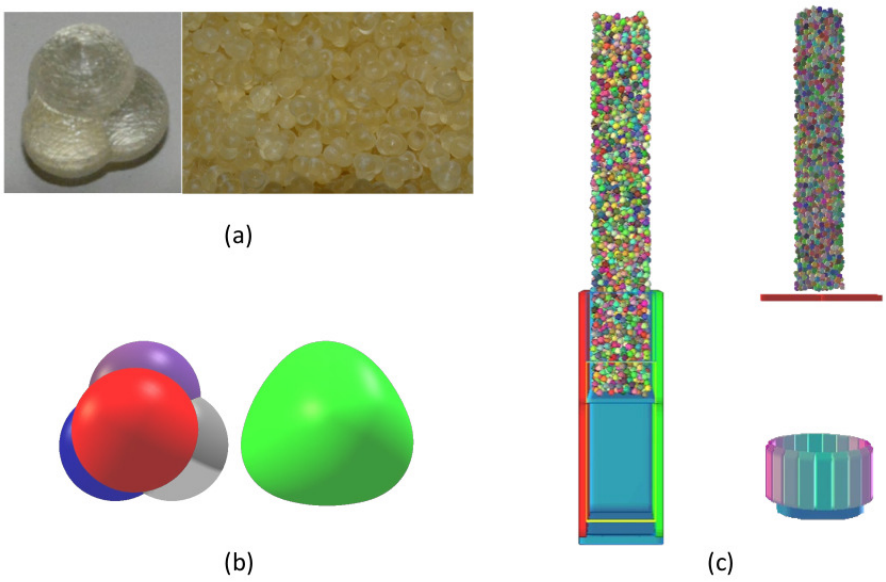


Figure: Angle of repose simulations (a) 3D-printed material (b) multisphere and potential particle representations (c) simulations for plane-strain and axisymmetric repose states.

17. H. Saomoto, N. Kikkawa, S. Moriguchi, Y. Nakata, M. Otsubo, V. Angelidakis, Y. Pik Cheng, K. Chew, G. Chiaro, J. Duriez, S. Duverger, J. I. González, M. Jiang, Y. Karasaki, A. Kono, X. Li, Z. Lin, A. Liu, S. Nadimi, H. Nakase, D. Nishiura, U. Rashique, H. Shimizu, K. Tsuji, T. Watanabe, X. Xu, M. Zeghal, *Round robin test on angle of repose: DEM simulation results collected from 16 groups around the world*. Soils and Foundations **63**, 101272, DOI `10.1016/j.sandf.2023.101272` (2023).

Effect of Particle Size on the Suction Mechanism in Granular Grippers

Angel Santarossa, Olfa D'Angelo, Achim Sack, and Thorsten Pöschel

Abstract:

Granular grippers are highly adaptable end-effectors that exploit the reversible jamming transition of granular materials to hold and manipulate objects. Their holding force comes from the combination of three mechanisms: frictional forces, geometrical constraints, and suction effects. In this workt, we experimentally study the effect of particle size on the suction mechanism. Through X-ray computed tomography, we show that small particles (average diameter d = 120 micrometers) achieve higher conformation around the object than larger particles (d = 4mm), thus allowing the formation of air-tight seals [1]. When the gripper is pulled off, mimicking lifting of an object, vacuum pressure is generated in the sealed cavity at the interface gripper–object. If the particles used as filling material are too large, the gripper does not conform closely around the object, leaving gaps between the gripper's membrane and the object. These gaps prevent the formation of sealed vacuum cavities between the object and the gripper and in turn hinder the suction mechanism from operating.

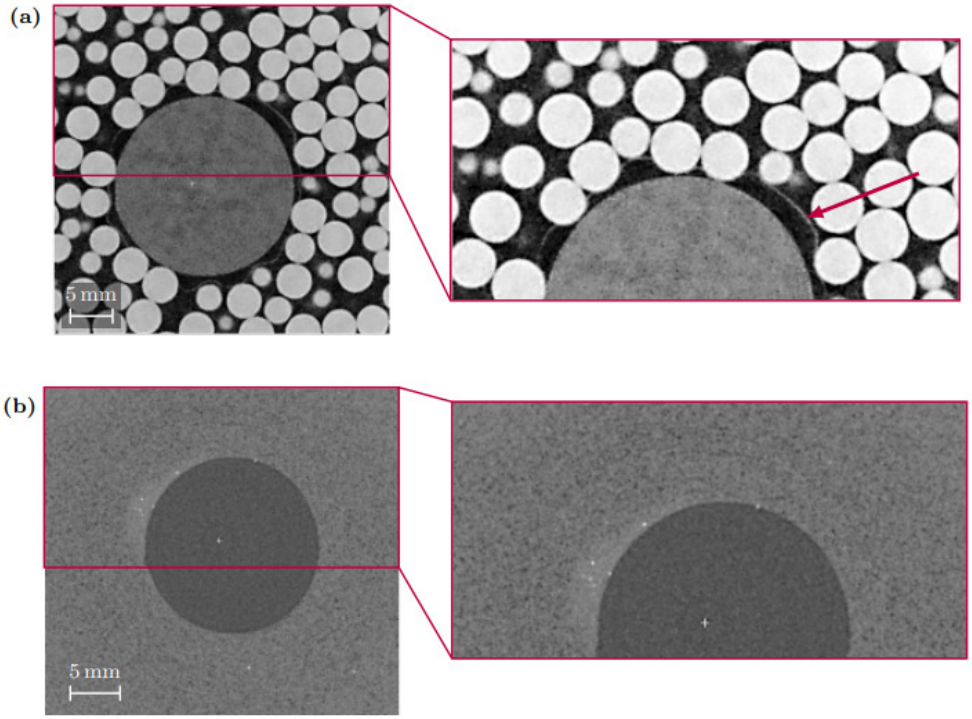


Figure: Tomogram slices for (a) (d = 4.0 mm) particles and (b) (d = 120 μm) particles after evacuation of the gripper. The images on the right side are magnifications of the original tomogram slices. The arrow notes a region where the membrane is not in contact with the surface of the object.

18. A. Santarossa, O. D'Angelo, A. Sack, T. Pöschel, *Effect of Particle Size on the Suction Mechanism in Granular Grippers*. Granular Matter **25**, 16, DOI 10.1007/s10035-022-01306-7 (2023).

Rheology of dilute granular gas mixtures where the grains interact via a square shoulder and well potential

Kiwamu Yoshii, Satoshi Takada, Kosuke Kurosawa, and ***Thorsten Pöschel***

Abstract:

We develop the rheology of a dilute granular gas mixture. Motivated by the interaction of charged granular particles, we assume that the grains interact via a square shoulder and well potential. Employing kinetic theory, we compute the temperature and the shear viscosity as functions of the shear rate. Numerical simulations confirm our results above the critical shear rate. At a shear rate below a critical value, clustering of the particles occurs.

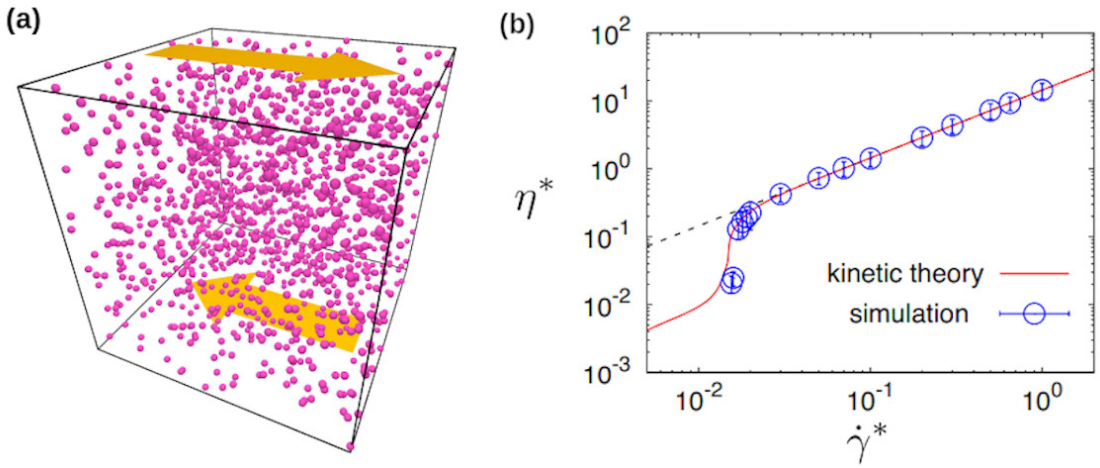


Figure: (a) Snapshot of the system. The arrows indicate the directions of shear at $y = -L/2$ and $L/2$, (b) Viscosity as a function of the shear rate for $e = 0.99$, $\lambda = 1.5$, and $x_1 = 3/4, x_2 = 1/4$. The dashed line shows Bagnolds' scaling.

19. K. Yoshii, S. Takada, K. Kurosawa, T. Pöschel, *Rheology of dilute granular gas mixtures where the grains interact via a square shoulder and well potential*. Physics of Fluids **35**, 013327, DOI 10.1063/5.0132127 (2023).

Modeling surface tension in Smoothed Particle Hydrodynamics using Young-Laplace pressure boundary condition

Michael Blank, ***Prapanch Nair***, *and* ***Thorsten Pöschel***

Abstract:

We introduce a surface tension model for Smoothed Particle Hydrodynamics (SPH) using a Young-Laplace pressure boundary condition. In this novel approach, at free surfaces the truncated kernel contribution is supplemented analytically by a term that acts as a Dirichlet pressure boundary condition. This analytical approach is in contrast to several scaling approaches prevalent in the SPH literature. Below figure illustrates this model. The external pressure p is composed out of the constant ambient pressure p^{amb} and the curvature dependent Young-Laplace pressure difference Δp^{YL} across a liquid-gas interface. We demonstrate its robustness and accuracy by simulating several notoriously difficult three-dimensional free surface flow problems driven by surface tension.

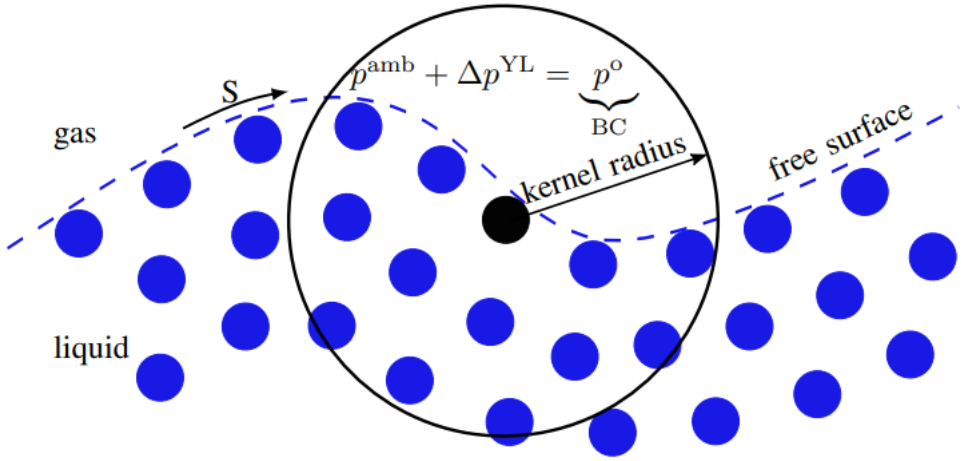


Figure: Illustration of the *Young-Laplace pressure based boundary condition* applied at a free surface (S) separating a liquid and a gaseous phase. The sampled volume of the kernel function centered at the black particle is not sufficiently sampled by neighboring (blue) particles. We apply the Dirichlet boundary condition for pressure analytically to account for the volume within the kernel radius beyond the free surface.

20. M. Blank, P. Nair, T. Pöschel, *Modeling surface tension in Smoothed Particle Hydrodynamics using Young-Laplace pressure boundary condition*. Computer Methods in Applied Mechanics and Engineering **406**, 115907, DOI `10.1016/j.cma.2023.115907` (2023).

Boltzmann equation in aggregation kinetics

Nikolai V. Brilliantov, Alexander I. Osinsky, and ***Thorsten Pöschel***

Abstract:

We consider an application of the Boltzmann equation to aggregation kinetics, where the transport mechanism is the ballistic motion of particles. This refers to such systems as molecular gases, granular gases and even dark matter. Two aggregation models are analyzed – random and impact-energy dependent agglomeration. The latter is associated with different inter-particle forces responsible for the merging. We start from the Boltzmann equation governing the evolution of the mass-velocity distribution functions of different species – the agglomerates of different sizes and derive generalized Smoluchowski equations. These describe the time-dependence of the agglomerates densities and their partial temperatures. We obtain exact solutions to these equations for simplified cases and develop a scaling theory for the asymptotic behavior of the system. To explore numerically the agglomeration kinetics, we elaborate a couple of simulation techniques, including the variation of DSMC and a combination of Monte Carlo and low-rank approximation methods for reaction-rate kernels. We observe a very rich behavior of the system, with new surprising regimes and construct the corresponding kinetic phase diagram. Finally, we demonstrate that the results of the scaling theory are in excellent agreement with the simulation results.

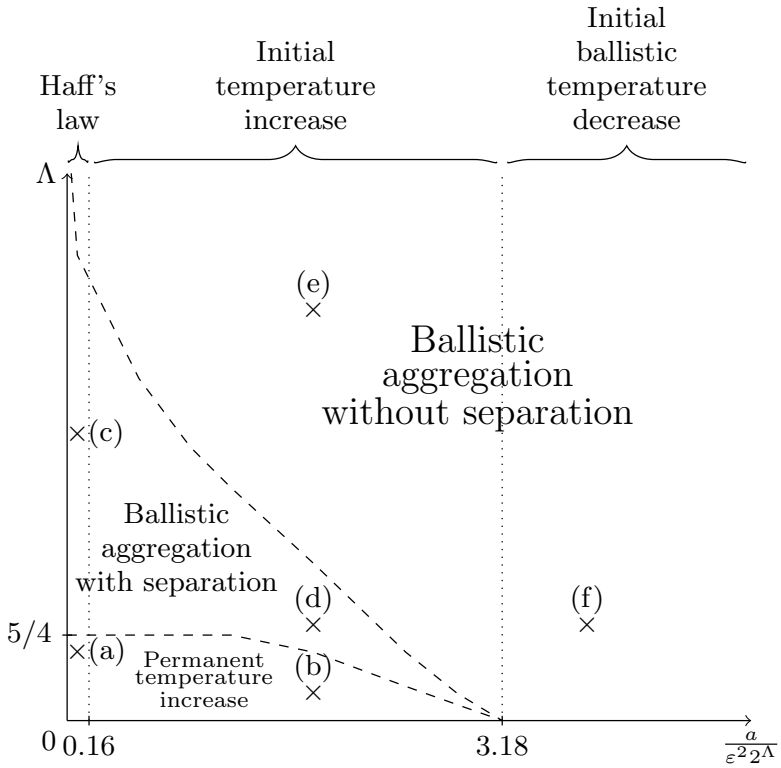


Figure: Phase diagram for the temperature-dependent Smoluchowski equations. Different kinetic regimes are demarcated by dashed lines. The simulations were performed for $\varepsilon = 0.99$, $m_1 = 1$, and $\sigma_1 = 1$, for mono-disperse initial conditions, initial dimensionless density $(\pi/6)n_1(0){\sigma_1}^3 = 0.05$ and initial temperature $T_1(0) = 1$.

21. N. V. Brilliantov, A. I. Orsinsky, T. Pöschel, *Boltzmann equation in aggregation kinetics - Nonequilibrium Thermodynamics and Fluctuation Kinetics* (Cham, 2022), DOI 10.1007/978-3-031-04458-8_10.

Stochastic Resonance and Optimal Clustering for Assemblies of ion Channels

Gerhard Schmid, ***Igor Goychuk****, Peter Hänggi, S Zeng, and Peter Jung*

Abstract:
We consider the statistical properties of action potentials generated by clusters of sodium and potassium channels due to channel noise and/or external stimulation. Since the fluctuations are related to the cluster size, a size-resonance effect - analogto stochastic resonance - is observed that facilitates optimal decodingof small external stimuli at optimal cluster sizes. Furthermore, in analogy to the coherence resonance effect, the channel-noise induced firingpatterns exhibit a resonant-like temporal coherence as a function of the cluster size even in the absence of a periodic stimulus. In the presence of additional synaptic noise, SR occurs only for large cluster sizes which possess suboptimal internal noise levels.

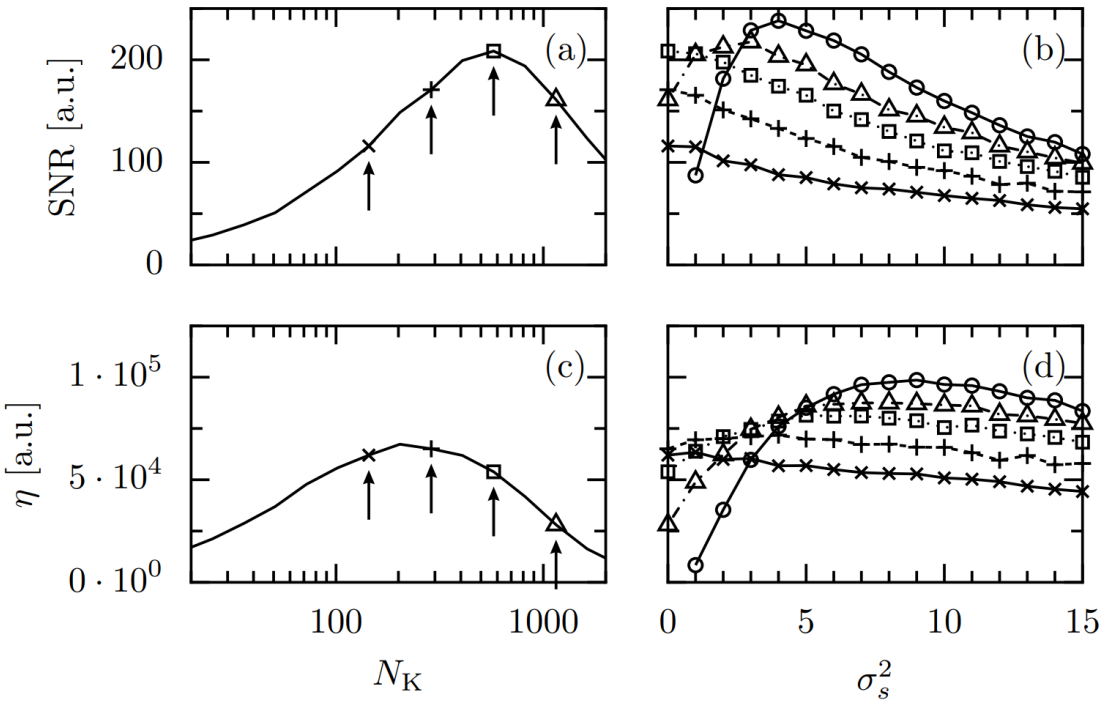


Figure: The signal-to-noise ratio SNR and the spectral amplification η of an external subthreshold sinusoidal stimulus with amplitude $A = 1.0\mu_A/cm^2$ and angular driving frequency $\Omega = 0.3ms^{-1}$ for different observation areas: (a) and (c) no synaptic noise; (b) and (d) the SNR and η versus the synaptic noise for the system sizes indicated by the arrows in (a) and (c): $N_K = 144$, solid lines through the crosses; $N_K = 288$, longdashed line connecting the pluses; $N_K = 576$, short dashed line through squares; $N_K = 1152$, dotted line connectingthe triangles. The situation with no internal noise (i.e. formally $N_K \longrightarrow \infty$) is depicted by the dotted line connectingthe circles.

22. G. Schmid, I. Goychuk, P. Hänggi, S. Zeng, P. Jung, *Stochastic Resonance and Optimal Clustering for Assemblies of ion Channels - The Random and Fluctuating World: Celebrating Two Decades of Fluctuation and Noise Letters* (Singapore, 2022), DOI 10.1142/9789811252143_0031.

X-ray multiaxes reconstruction of granular flows

Luis Armando Torres Cisneros

Abstract:
In the present dissertation, a novel x-ray-based imaging method for studying granular materials is proposed, i.e., the x-ray multiaxes method. The method is applied to an experiment to study the height-dependent diffusivity of particles in granular flows within split-bottom geometry under periodical shear. One type of granular system that can be studied by means of the x-ray multiaxes method is granular flows. Granular flows can be produced by shear. A device used to produce shear bands is the so-called split-bottom cell. Nonetheless, nowadays there are still open questions concerning the properties of the shearing zone within a split-bottom cell at ratios $H/R_s > 0.65$. Here, H and R_s are filling height and split-radius, respectively. Then, common studies on particulate flows, for instance, on particles diffusing, are not straightforward. Since the introduced x-ray multiaxes method allows to inspect systems as granular flows, an experiment on particles diffusing under periodical shear within a split-bottom cell is proposed. The results of this experiment show that it is possible to define a height-dependent effective diffusivity in such a granular flow.

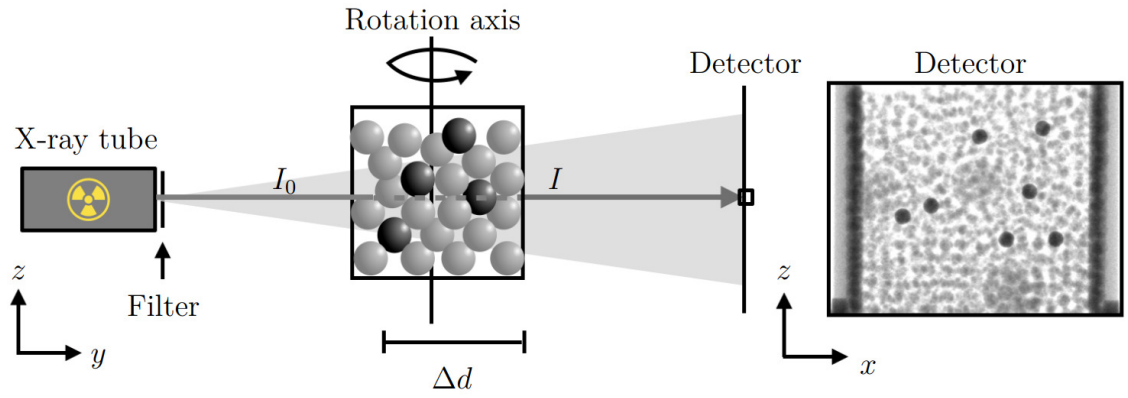


Figure: Sideview of a common x-ray device and example of a radiogram. On the left side the x-rays tube (gray color), the studied granular sample composed by grains of different materials (gray and black spheres), and the x-rays detector are shown. The gray line (dashed and non-dashed) indicates a x-ray emerging out of the tube, passing through the sample and impinging onto the detector. The filter is utilised for minimizing beam hardening. On the right side, a radiogram of a granular material made of steel (black spots) and glass beads (sorrounding speckle) is shown.

23. L. A. Torres Cisneros, *Ph.D. Thesis: X-ray multiaxes reconstruction of granular flows*, URN: urn:nbn:de:bvb:29-opus4-190472 (Erlangen, 2022).

Particle Based Simulation of Granular and Fluid Flow

Patric Müller

Abstract:
In this work, the concept of particles as discrete entities has been used to simulate systems of macroscopic particles, to discretize continuum problems and to represent abstract quantities. It was demonstrated that particle based simulations cover a wide range of applications on all scales and enable promising strategies for the simulation of multiphase flows, phase transitions and the treatment of complicated shaped or free boundaries.

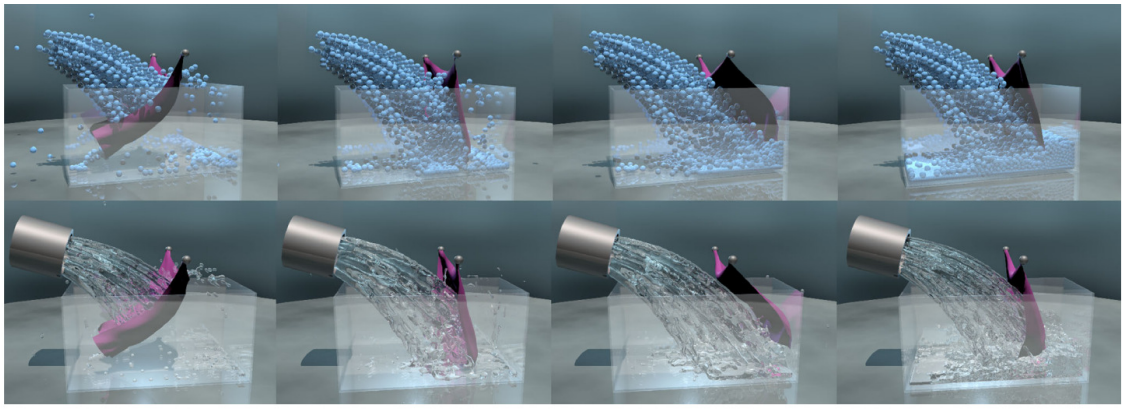


Figure: Coupled simulation of a deformable thin shell and a fluid using our method ($11K$ cloth constraints and $27K$ fluid particles, at 21 fps), where the cloth deforms under the impact of the fluid, while the fluid splashes around. Top row: particle representation of the coupled simulation. Bottom row: rendering of the reconstructed surface of the coupled simulation.

24. P. Müller, *Habilitation Thesis: Particle based simulation of granular and fluid Flow* (Erlangen, 2022).

Simulation of the laser melting process of titanium using Smoothed Particle Hydrodynamics

Michael Blank

Abstract:

The high heating rates generated by focused laser beams are utilized in a range of industrial applications such as laser welding, Selective Laser Melting (SLM), or wire-based Laser Metal Deposition (LMD-w). Inappropriate processing parameters may lead to material defects that deteriorate the mechanical properties of the weld or the manufactured part. To some extent, this is caused by a lack of understanding of the influence of the process parameters on the governing physical effects arising in laser-metal processing. This work presents a three-dimensional numerical model based on the Incompressible Smoothed Particle Hydrodynamics method capable of simulating liquid flow dynamics, heat transfer, and phase transitions of titanium simultaneously. In a series of simulations of single-line laser tracks on titanium metal sheets, the influence of the material's optical properties, laser process parameters, and the emerging vapor on the weld geometry is investigated. Moreover, the influence of the wetting forces on the melt geometry is studied. The fragmentation of the melt, also known as humping in laser welding, is observed when large temperature gradients across the solid-liquid interface occur. Strategies to avoid humping are presented subsequently. Finally, the LMD-w process of titanium is simulated both with and without gravitational forces. A more continuous deposition of titanium can be achieved when using LMD-w in zero-gravity environments.

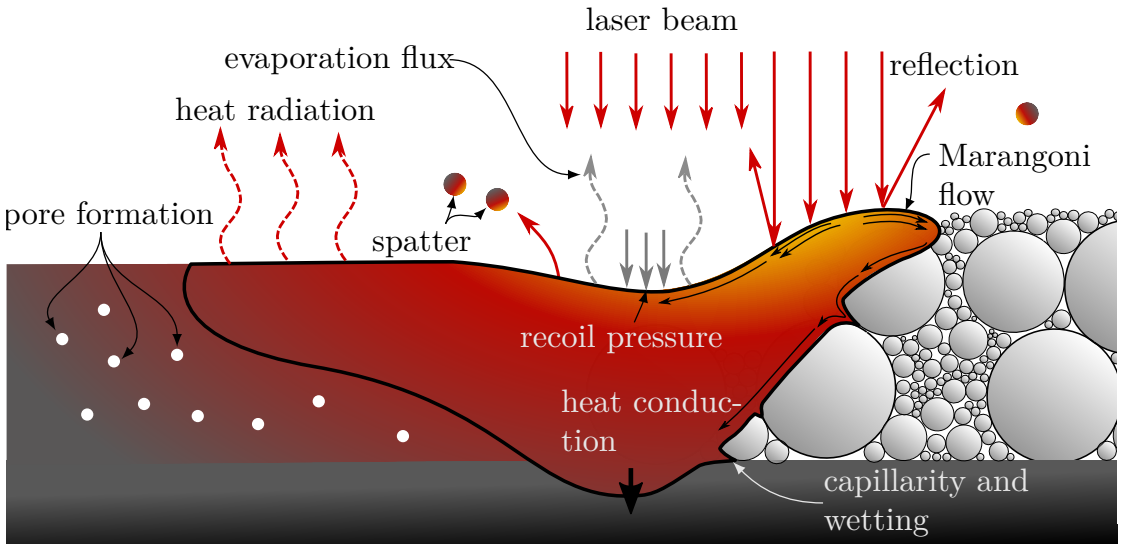


Figure: Physical phenomenon arising in laser-metal processing.

25. M. Blank, *Ph.D. Thesis: Simulation of the laser melting process of titanium using Smoothed Particle Hydrodynamics* (Erlangen, 2022).

Spontaneous Size Segregation in Textured Granular Pipe Flow

Kuang-Wu Lee *and* ***Patric Müller***

Abstract:

A new spontaneous particle segregation mechanism is found in textured granular pipe flow. In contrast to the previous studies in similar geometry, where the particle segregation is caused by air drag differences of different grain sizes in the pipe flow, in this study we found, even in an air-less environment, the particle segregation can be triggerred by the perturbations imposed from the particle collisions on the textured confinement wall. The pipe inner walls in our simulations are assumed frictional, as well as for the embedded wall textures. This system conformation provides external perturbation input to the falling granular particles in the pipe. Previous studies of textured pipe flow have found, for a monodisperse system, the spiral inner wall texture smoothes density waves and jamming plugs. We discover that, for a binary mixture system, the wall spiral textures do not only smoothen the bulk density waves, but also provide effective shaking to the system. This spontaneous shaking causes perturbation input in different frequencies, depending on the inner wall structures. Because particles of different sizes respond differently to this shaking, this effect eventually leads to spontaneous size segregation.

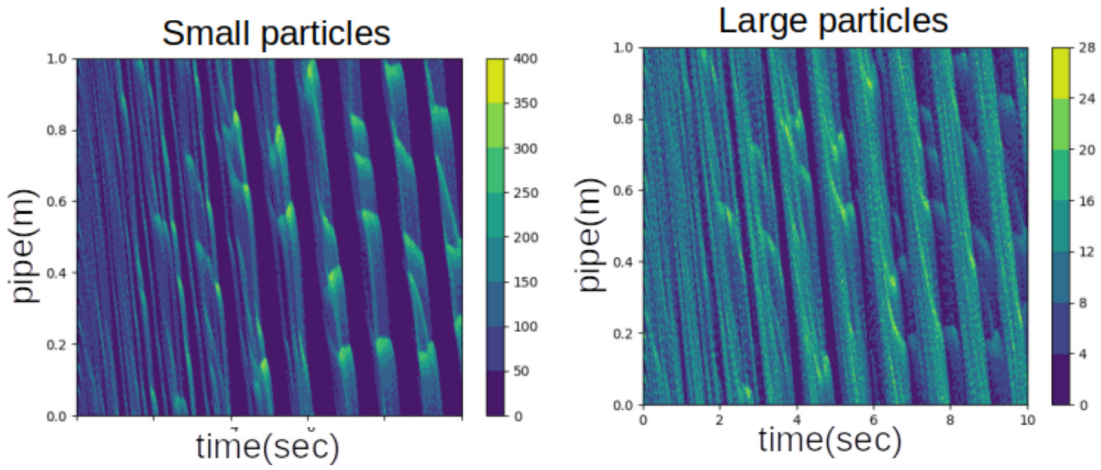


Figure: A typical size segregation of polydisperse granular particles in the pipe flow. The case shown here is for volume fraction $V_\varphi = 0.2$ and aspect ratio $D_\varphi = 5$. The upper panel is the time evolution of small particles, while the lower panel is for large particles. The colormap indicates the line number density $(\#/m)$ of each species.

26. K.-W. Lee, P. Müller, *Spontaneous Size Segregation in Textured Granular Pipe Flow*. in review (2022).

Stochastic Thermodynamics of the Rheology of Granular Media

Seyed Habibollah Ebrahimnazhad Rahbari , Hyunggyu Park, Hor Dashti-Naserabadi, and ***Thorsten Pöschel***

Abstract:

We introduce the concept of forward and reverse flows in a shear flow of dense particulate matter; this is in analogy to forward and reverse processes in stochastic thermodynamics. These notions enable us to investigate flow fluctuations in a novel framework of stochastic thermodynamics in which we focus on those fluctuations that result in entropy consumption. We further investigate the scaling properties of probability for reverse flows as the system undergoes a rigidity transition in the dense regime. Our analysis reveals (1) an enhanced uniformity of flow near jamming and (2) a dichotomy of the underlying mechanisms for entropy consumption. The generality of the framework paves the way to apply the formalism to a wider range of flow fluctuations, such as those in turbulence, which have not yet been investigated with discrimination of the entropy production/consumption.

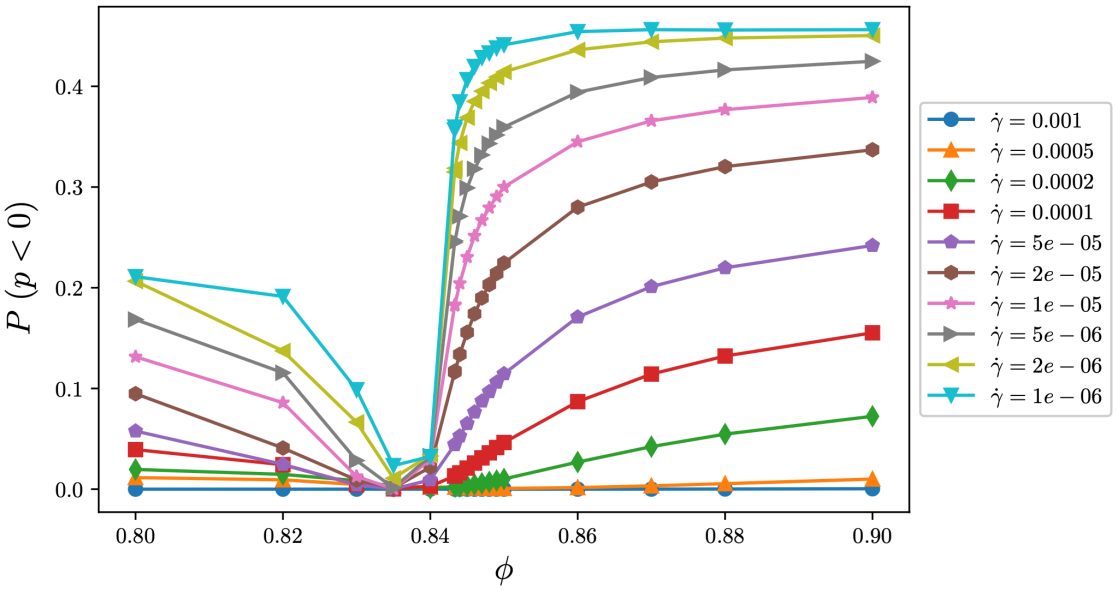


Figure: The probability for negative power $P(p<0)$ vs packing fraction ϕ. Each color corresponds to a shear rate that is given in the legend. The number of particles vary from $N = 61941$ to 69684 for $\phi = 0.8$ and 0.9, respectively, at a fixed system size $L = 300$. Each curve has a global minimum near the jamming transition point. The slope of each curve increases by decreasing the shear rate $\dot{\gamma}$.

27. S. H. E. Rahbari, H. Park, H. Dashti-Naserabadi, T. Pöschel, *Stochastic Thermodynamics of the Rheology of Granular Media*. in review (2022).

Modeling Stratified Segregation in Periodically Driven Granular Heap Flow

***Hongyi Xiao**, Zhekai Deng, Julio M Ottino, Paul B Umbanhowar, and Richard M Lueptow*

Abstract:

We present a continuum approach to model segregation of size-bidisperse granular materials in unsteady bounded heap flow as a prototype for modeling segregation in other time varying flows. In experiments, a periodically modulated feed rate produces stratified segregation like that which occurs due to intermittent avalanching, except with greater layer-uniformity and higher average feed rates. Using an advection-diffusion-segregation equation and characterizing transient changes in deposition and erosion after a feed rate change, we model stratification for varying feed rates and periods. Feed rate modulation in heap flows can create well-segregated layers, which effectively mix the deposited material normal to the free surface at lengths greater than the combined layer-thickness. This mitigates the strong streamwise segregation that would otherwise occur at larger particle-size ratios and equivalent steady feed rates and can significantly reduce concentration variation during hopper discharge. Coupling segregation, deposition and erosion is challenging but has many potential applications.

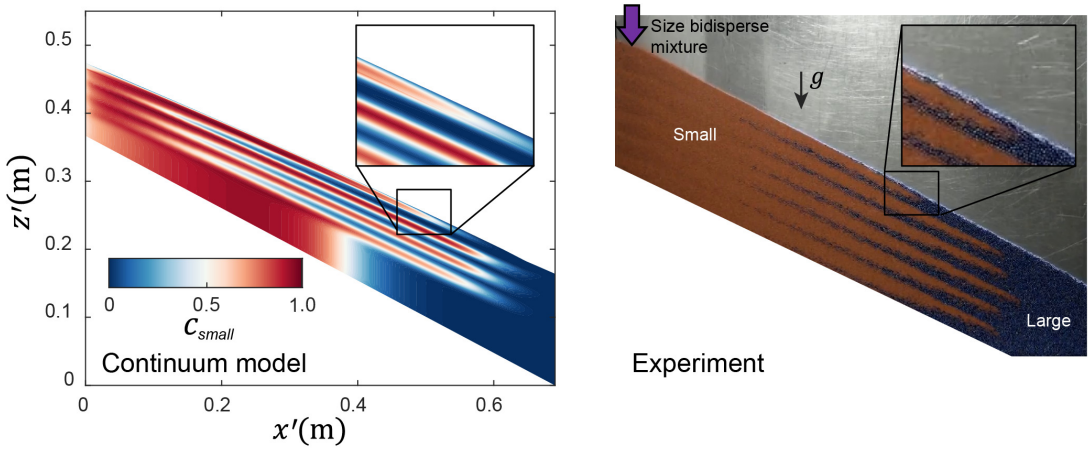


Figure: Comparison of the stratification of large and small particles under flow modulation from the continuum model prediction (left) and from the experimental result (right).

28. H. Xiao, Z. Deng, J. M. Ottino, P. B. Umbanhowar, R. M. Lueptow, *Modeling Stratified Segregation in Periodically Driven Granular Heap Flow*. arXiv:2209.04342, DOI `10.48550/arXiv.2208.00245` (2022).

Effect of cohesion on structure of powder layers in additive manufacturing

Sudeshna Roy**, Mohamad Yousef Shaheen, and **Thorsten Pöschel

Abstract:

Producing a consistent layer quality for different raw-materials is a challenge for powder-based additive manufacturing. Interparticle cohesion plays a key role on the powder spreading process. In this work, we characterise the structure of deposited layers in the powder-base additive manufacturing process by numerical simulations using the Discrete Element Method (DEM). The effect of particle cohesion on the quality of powder bed is evaluated. It is found that higher interparticle cohesion lead to poor spreadability, with more heterogeneous powder layer structure and enhances particle size segregation in the powder layer. We also compare the powder layer quality deposited on a smooth substrate with that on a powder layer. Deposition on a powder layer leads to inferior layer quality of powder layer with higher heterogeneity and higher particle size segregation effects.

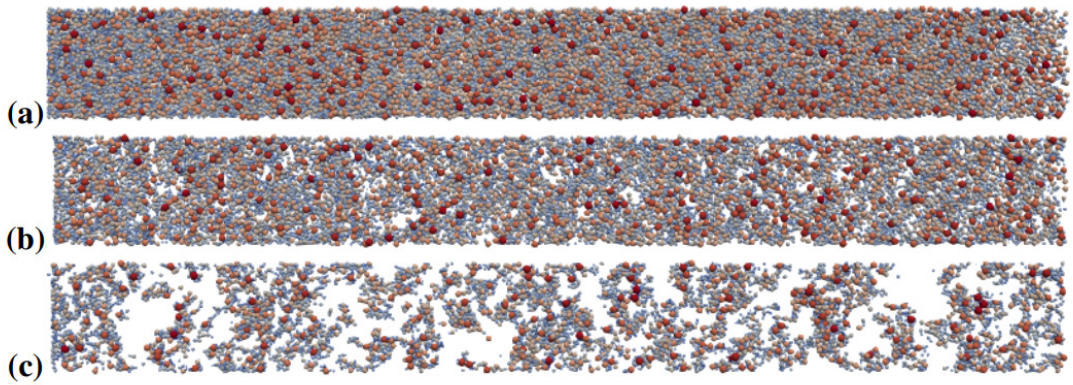


Figure: Top view snapshots of the spread powder layer with $\mu_r = 0.005$ and $\mu_s = 0.1$ for (a) $Bo = 0$, (b) $Bo = 15$ and (c) $Bo = 30$.

29. S. Roy, M. Y. Shaheen, T. Pöschel, *Effect of cohesion on structure of powder layers in additive manufacturing*. in review (2022).

Structure of Entangled Filamentous Matter: Linear vs Rings

Leopoldo R. Gómez**, Nicolás A. García, and **Thorsten Pöschel

Abstract:

While linear polymers are well understood, the structure and dynamics of rings remain elusive. Key concepts such as confining tubes and reptation, which are the cornerstone of polymer physics, could be misleading in the ring dynamics. Here we use commercial rubber bands imaged through X-ray tomography to compare the structural properties of semiflexible linear and ring assemblies. Individual band configurations in the assemblies are obtained through a machine learning segmentation approach, allowing the detailed geometrical and topological characterization of the structures. We found that although rings tend to be more compact and display higher curvature, the topology of rings and linear assemblies are shown to be rather similar, when scaled properly.

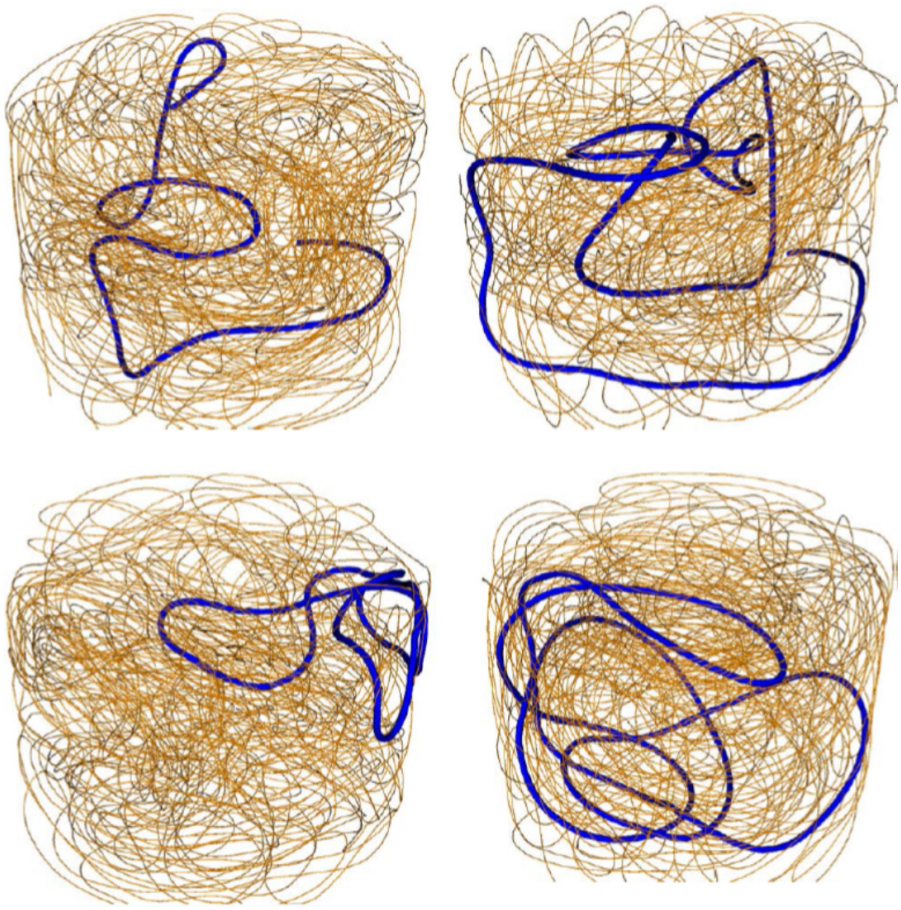


Figure: Packing structure of linear and rings rubber bands. In each assembly a single rubber band is highlighted to better appreciate the configurations.

30. L. R. Gómez, N. A. García, T. Pöschel, *Structure of Entangled Filamentous Matter: Linear vs Rings*. in review (2022).

Adaptative Resolution Increase for the Fracture of Brittle Solids with a Multi-sphere Discrete Element Method

Ali Mauricio Velasco**, José-Daniel Muñoz and **Thorsten Pöschel

Abstract:

Discrete Element Methods (DEM) are good alternatives for the study of fractures in brittle solid materials. In contrast to Finite Element Methods (FEM), they solve evolution equations for each grain, avoiding the inversion of huge matrices. However, their resolution is limited by the size of the elements used to represent the material. Hereby we introduce a novel three-dimensional method to study fractures in brittle materials by increasing DEM resolution just on the places where stresses are closer to the breaking thresholds. The solid material is divided into random Voronoï polyhedra, and each polyhedron, each of them a discrete element, is represented by a frozen clump of overlapping spheres, with a similar structure like a sintered material. If two polyhedra share a face, the spheres of one polyhedron in contact with those of the neighbouring one are joined across the face with rigid bars. The forces and torques of such bars are used to compute the strain energy field, who has shown to be adequate to account for fractures in granular media. Once the material is charged with an external load, only discrete elements with high strain energy fields are subdivided into smaller elements, who re-establish bonds between them and with all neighbours. The process iterates until the desired resolution is reached, and those bonds above a threshold break. In this presentation we show how the fracture surface can be retrieved with high accuracy and low computational costs, compared with continuum methods like FEM.

Figure: 15th World Congress on Computational Mechanics (WCCM-XV), 8th Asian Pacific Congress on Computational Mechanics (APCOM-VIII).

31. A. M. Velasco, J.-D. Muñoz, T. Pöschel, *Adaptative Resolution Increase for the Fracture of Brittle Solids with a Multi-sphere Discrete Element Method*. 15th World Congress on Computational Mechanics, 331 (2022).

Local structural anisotropy in particle simulations of powder spreading in additive manufacturing

Sudeshna Roy, ***Hongyi Xiao***, *Mohamad Yousef Shaheen, and* ***Thorsten Pöschel***

Abstract:

Producing consistent and homogeneous packing structure in powder layer deposition for cohesive raw materials under varying thermal conditions is challenging for additive manufacturing. Interparticle cohesion and thermal parameters play key roles on the structure of powder layer deposited on the substrate in additive manufacturing. In this work, we characterize the structural anisotropy of the deposited powder layer and quantify the packing structure on the particle-level using a threshold-free local packing anisotropy based on Voronoi tessellation. Based on the statistics of the local anisotropy, we observe a transition in the structure of the deposited powder layer from homogeneous to heterogeneous for cohesive materials at $Bo = 10$.

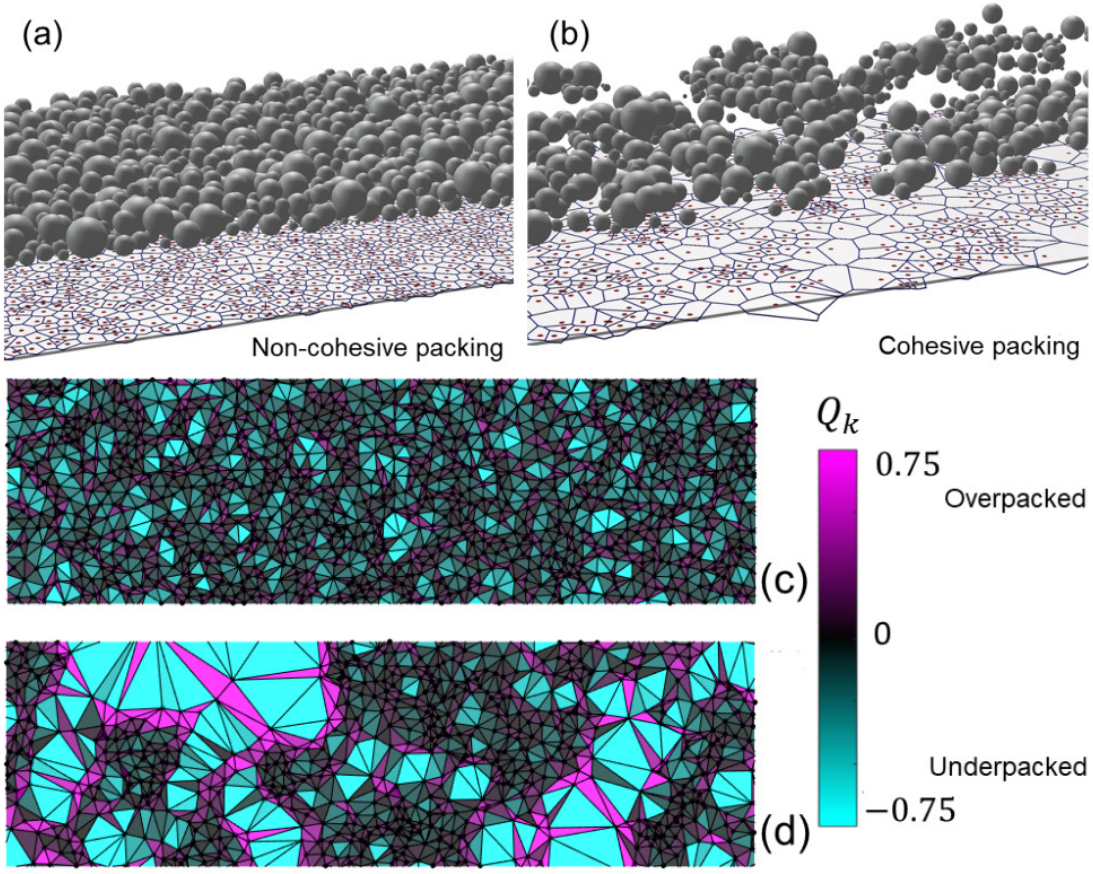


Figure: Granular packing of powder layer for $Bo = 0$ (a), and $Bo = 30$ (b). The points represent the projections of particle centers on the xy plane and the corresponding 2D Voronoi tessellations are also shown on the plane. Delaunay triangles with color representing local values of Q_k for $Bo = 0$ (c), and $Bo = 30$ (d) for a section of deposited layer $(4 \ldots 8)$ mm and $(0.4 \ldots 0.8)$ mm.

32. S. Roy, H. Xiao, M. Y. Shaheen, T. Pöschel, *Local structural anisotropy in particle simulations of powder spreading in additive manufacturing*. Casablanca International Conference on Additive Manufacturing (2022).

Temparature Gradients as a Source of Balling and Humping in Laser Processing of Titanium

Michael Blank**, and **Thorsten Pöschel

Abstract:

The spheroidization of the melt in laser melting processes deteriorates the mechanical properties of the welding seam or the manufactured part. This phenomenon is called humping or balling. To improve the reliability of the product quality a thorough understanding of the occurring physical phenomena is indispensable. By comparison of three-dimensional Smoothed Particle Hydrodynamics simulations of single-line laser tracks of titanium with experiments, we show that high-temperature gradients reduce the wetting forces which act at the three-phase contact line which in turn promotes the fragmentation of the cylindrical melt.

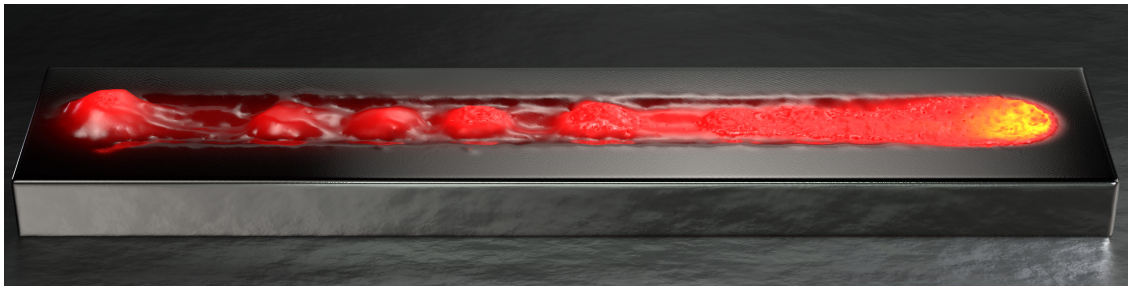


Figure: Simulation snapshot of the laser welding process of titanium using parameter set 4 exhibiting humping.

33. M. Blank, T. Pöschel, *Temparature Gradients as a Source of Balling and Humping in Laser Processing of Titanium*. Casablanca International Conference on Additive Manufacturing (2022).

DEM-Simulation of thin elastic membranes interacting with a granulate

Holger Götz**, and **Thorsten Pöschel

Abstract:
For a wide range of applications, we need DEM simulations of granular matter in contact with elastic flexible boundaries. We present a novel method to describe the interaction between granular particles and a flexible elastic membrane. Here, the standard mass-spring model approach is supplemented by surface patches given by a triangulation of the membrane. In contrast to standard mass-spring models, our simulation method allows for an efficient simulation even for large particle size dispersion. The novel method allows coarsening of the mass-spring system leading to a substantial increase of computation efficiency. The simulation method is demonstrated and benchmarked for a triaxial test.

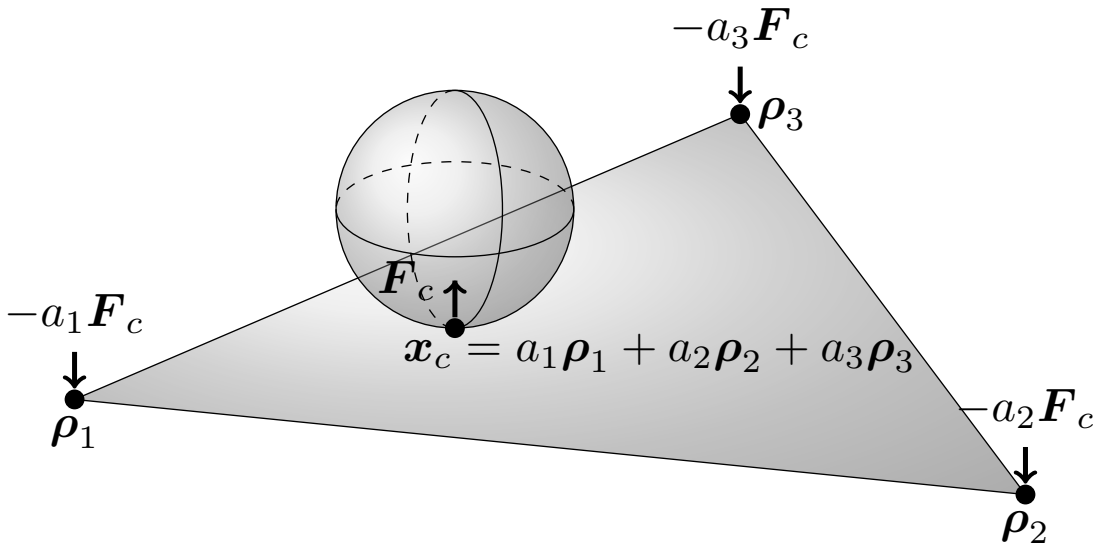


Figure: Sketch of the interaction between a granular particle and a surface patch.

34. H. Götz, T. Pöschel, *DEM-Simulation of thin elastic membranes interacting with a granulate*. arXiv:2210.10222, DOI 10.48550/arXiv.2210.10222 (2022).

Influence of silicon nanocone on cell membrane self-sealing capabilities for targeted drug delivery – computer simulation study

Przemysław Raczyński, Krzysztof Górny, Beata Marciniak, Piotr Bełdowski, ***Thorsten Pöschel****, and Zbigniew Dendzik*

Abstract:

Efficient and non-invasive techniques of cargo delivery to biological cells are the focus of biomedical research because of their great potential importance for targeted drug therapy. Therefore, much effort is being made to study the characteristics of using nano-based biocompatible materials as systems that can facilitate this task while ensuring appropriate self-sealing of the cell membrane. Here, we study the effects of indentation and withdrawal of nanospear on phospholipid membrane by applying steered molecular dynamics (SMD) technique. Our results show that the withdrawal process directly depends on the initial position of the nanocone. The average force and work are considerably more significant in case of the withdrawal starting from a larger depth. This result is attributed to stronger hydrophobic interactions between the nanocone and lipid tails of the membrane molecules. Furthermore, when the indenter was started from the lower initial depth, the number of lipids removed from the membrane was several times smaller than the deeper indentation. The choice of the least invasive method for nanostructure-assisted drug delivery is crucial for possible applications in medicine. Therefore, the results presented in this work might be helpful in efficient and safe drug delivery with nanomaterials.

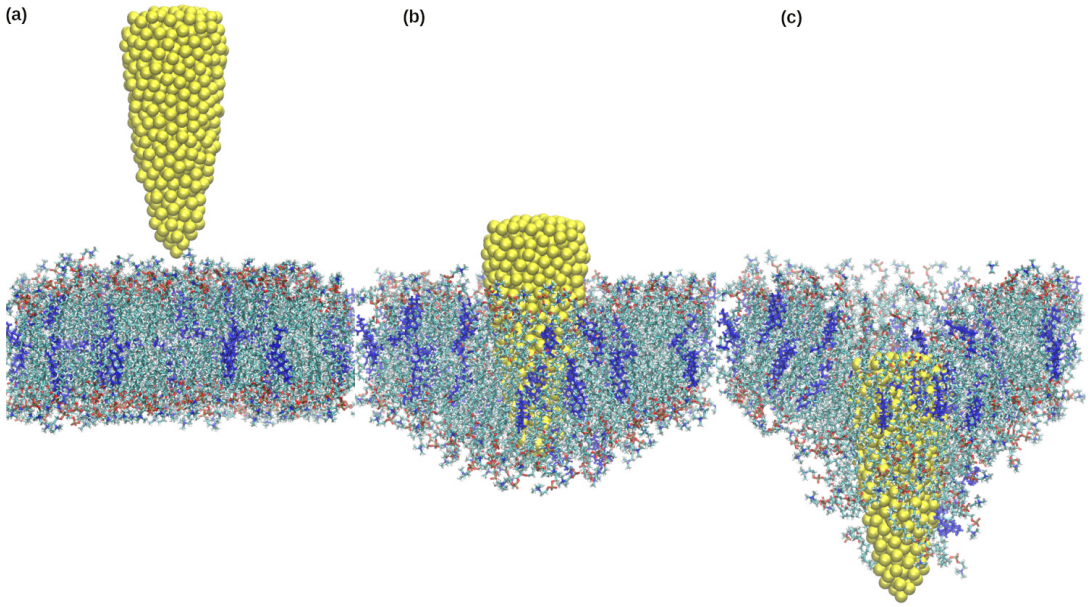


Figure: The snapshots of the instantaneous indentation phases: a) initial configuration, b) nanospear travels the distance approximately 63, c) nanospear travels the distance approximately 105. The cholesterols in the membrane are colored in blue.

35. P. Raczyński, K. Górny, B. Marciniak, P. Bełdowski, T. Pöschel, Z. Dendzik, *Influence of silicon nanocone on cell membrane self-sealing capabilities for targeted drug delivery–computer simulation study*. arXiv:2212.00883, DOI `10.48550/arXiv.2212.00883` (2022).

Granular Meta-Material: Viscoelastic Response of a Bending Beam

Holger Götz**, and **Thorsten Pöschel

Abstract:

Jammed granular matter can be considered as a meta-material that behaves viscoelastically for small deformations. We characterize the properties of the meta-material by means of the response of a simply supported bending beam consisting of jammed granular matter under weak load.

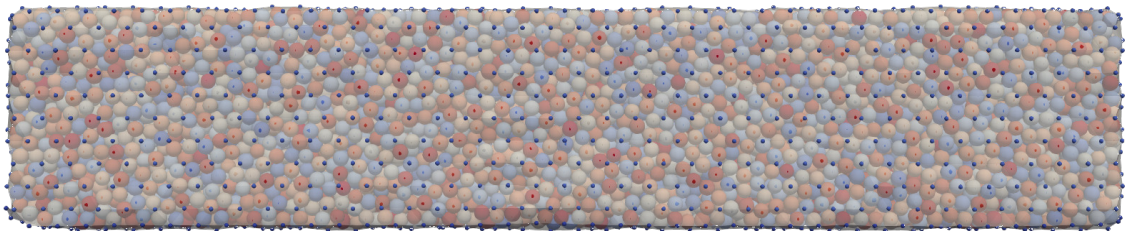
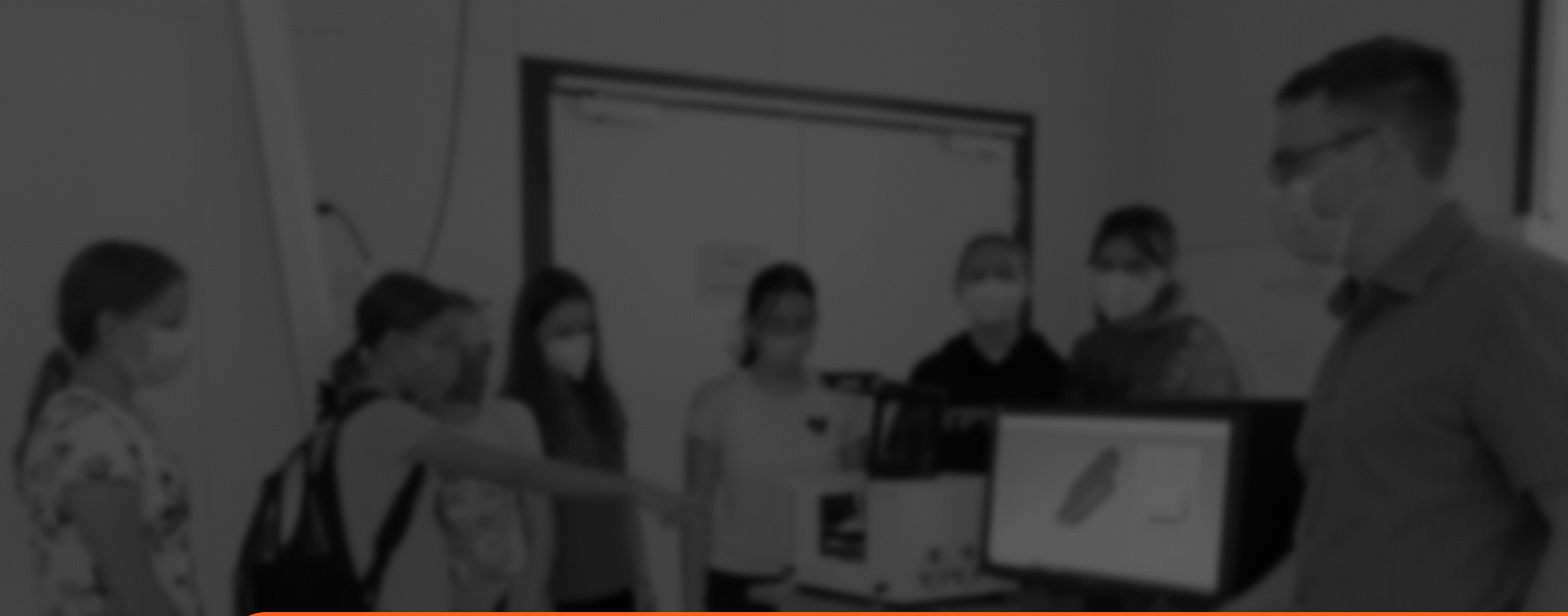


Figure: Setup of the granular bending beam.

36. H. Götz, T. Pöschel, *Granular Meta-Material: Viscoelastic Response of a Bending Beam*. Granular Matter submitted (2022).



14. Public Attention and Public Outreach

MSS actively participated in the Long Night of Science, "Lange Nacht der Wissenschaften"

The tenth Long Night of Science was held on Saturday, May 21, 2022, with many open-air events. The MSS participated with 4 different science presentations at the Erlangen site.

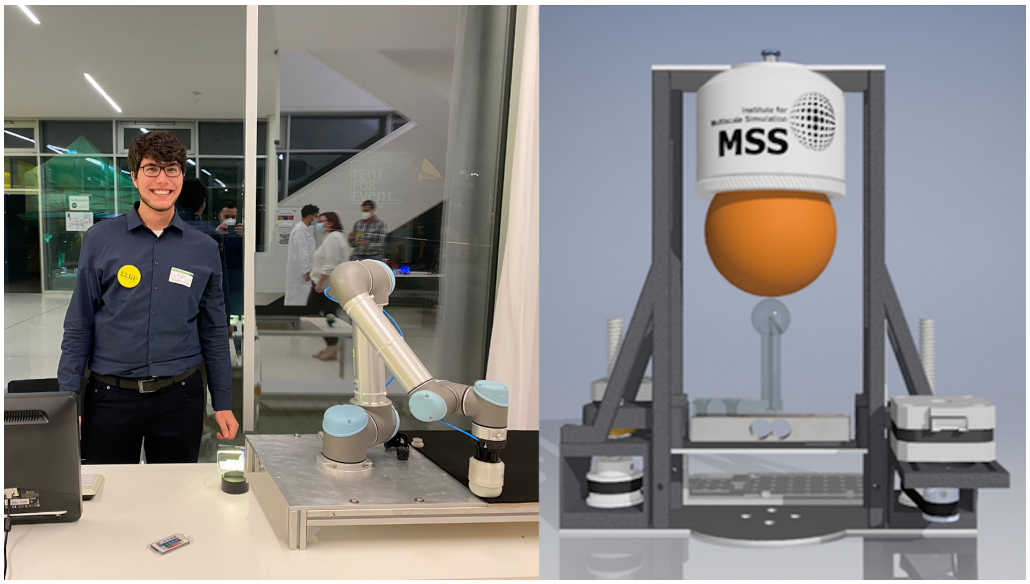
www.fau.de/2022/05/news/lange-nacht-der-wissenschaften-2022-highlights-an-der-fau/

"Lange Nacht der Wissenschaften": Computer Simulations - From Disney to ISS

Michael Blank and Felix Buchele from the MSS group gave a 30-minute talk on how simulations of complex systems are increasingly used in industry and science to investigate physical phenomena and develop new products. The talk explained the basics of these simulations and used examples to show how computer simulations make it possible to measure quantities that cannot be determined experimentally. The examples were from special effects often seen in movies, such as "Lord of the Rings", "Terminator" and "Harry Potter" and also simulation of welding under micro-gravity before it is used on the ISS.

"Lange Nacht der Wissenschaften": Granular Hand - Like 1000 fingers!

In another part of MSS presentations during the Long Night of Science, Angel Santarossa and Yazan Alzaghah showed how a granular robotic hand can grab anything, the objects up to the size of a fist. Our researchers working on soft granular jamming grippers, show the curious visitors the astonishing properties of the reversible jamming transition and its application in robotics.



Left photo by Vasileios Angelidakis

"Lange Nacht der Wissenschaften": Streamlines in moving granules

Achim Sack spoke at the Long Night of Science about the transport process in moving granules and how this can often only be described and observed using technical methods and image processing. In the presented experiment, the change of flow patterns in a rotating granulate was observed with an exciting dynamic phenomenon.

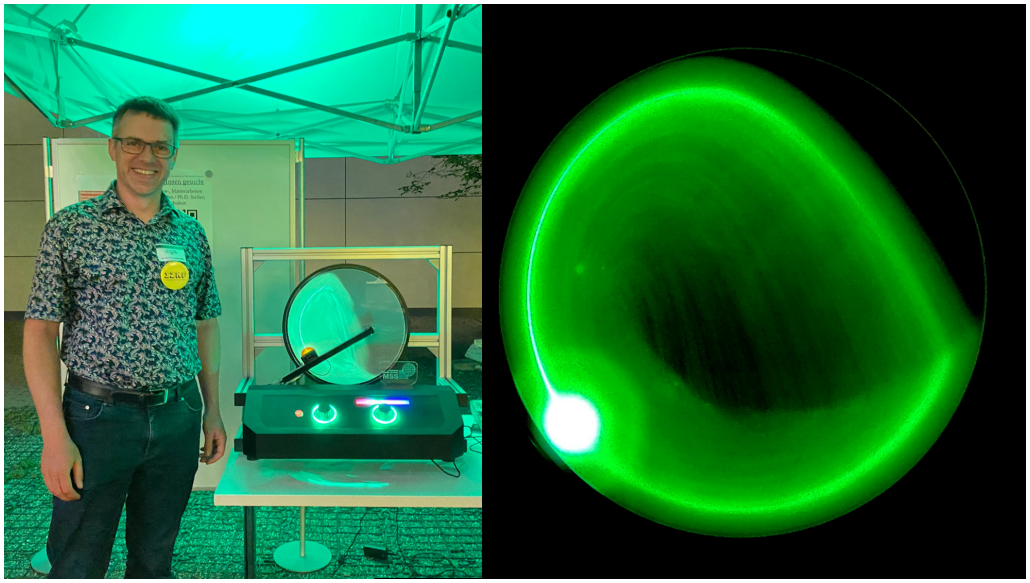


Photo by Vasileios Angelidakis

"Lange Nacht der Wissenschaften": Thermal imaging camera

In the Long Night of Science, Michael Heckel presented experimental show on the infrared thermography as an excellent tool to show temperature differences. In his presentation, he showed how this method can be used to answer questions such as: Which key on a keyboard was pressed last? What does convection look like in a cup of tea? Where do water pipes run? Through which cable does electricity flow?

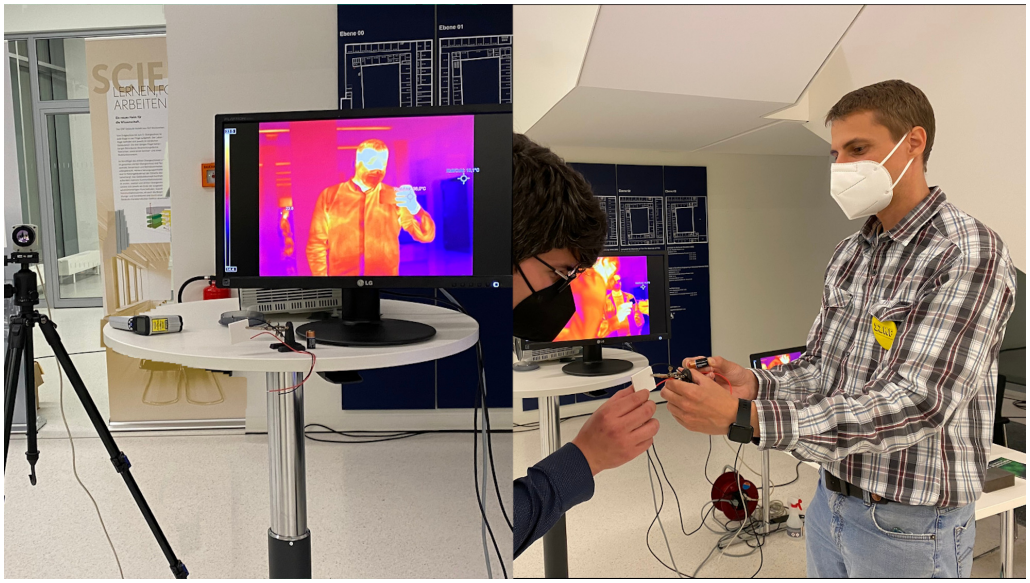
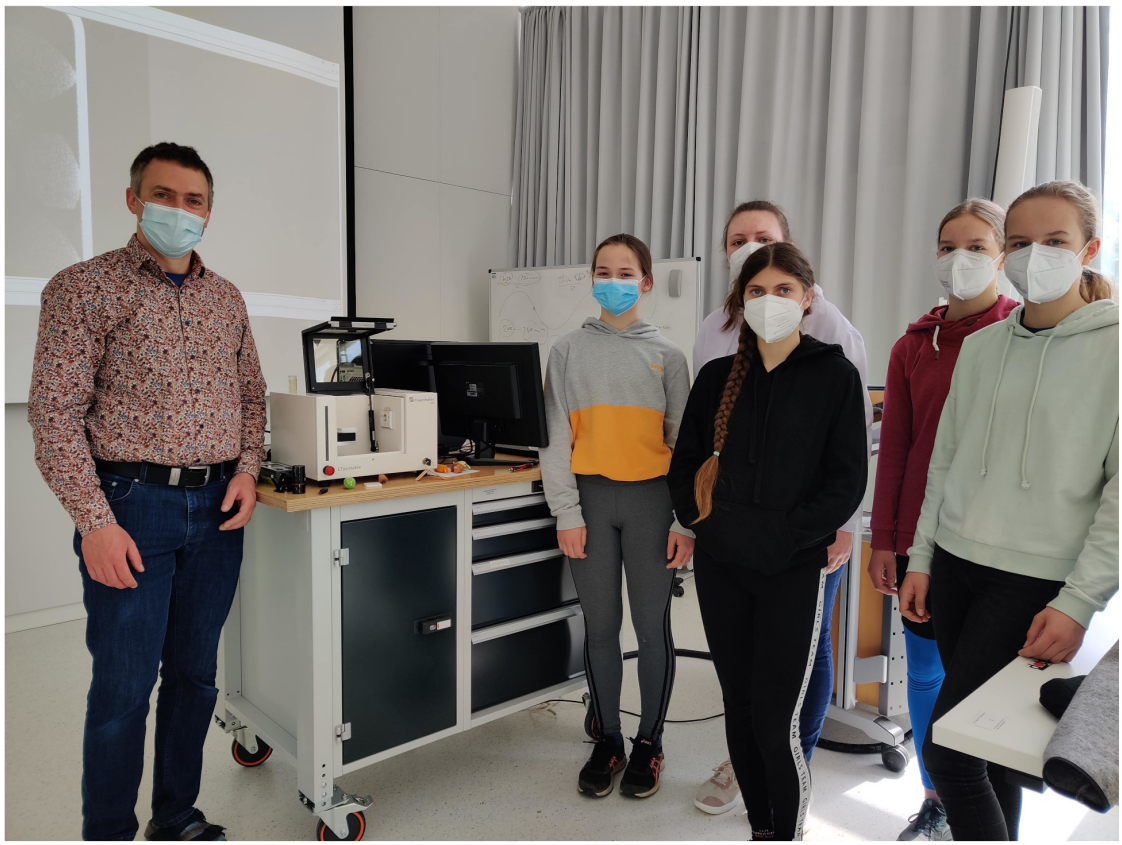


Photo by Vasileios Angelidakis

MSS goes Girls' Day

The Girls' Day is a great opportunity for girls of classes 5-11 to get insights into mostly technical professions. As in the previous years, on 28 April, the MSS presented a two hour long tour (German title: "Licht in's Dunkel bringen", How to bring light into the dark?), where Achim Sack explained how a Computed Tomography is being generated starting from the generation and the properties of X-rays over the generation of a radiograph to a full 3D reconstruction of a Kinder-Surprise egg. The tour took place in attendance. Afterwards, the participants were able to pursue their curiosity about science and technology and, under guidance, make radiographs and X-ray tomographies of objects of their own choosing (e.g. Kinder surprise, headphones and RFID cards). We thank the participants for their attendance, for the in-depth discussions and for the interest in science and technology.
`www.girls-day.de`



Opening ceremony for Futur21 exhibition - Zeche Nachtigall Museum

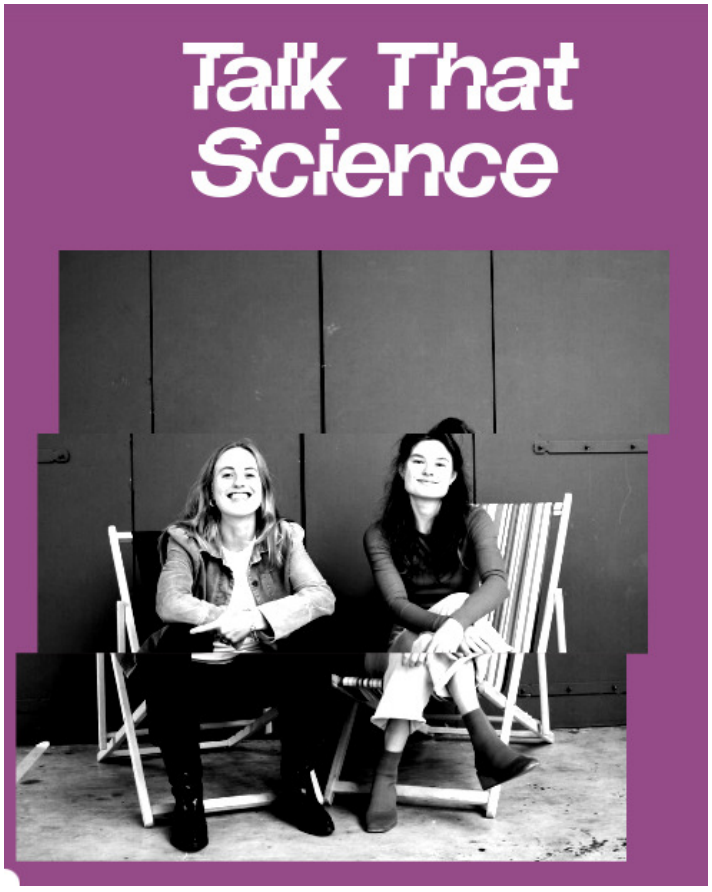
Dr. Olfa D'Angelo had two live discussions on "Technological Progress, from Coal Mining to Lunar Resource Development" and "Moon Bricks" in round tables on May 3, 2022.

`https://futur21.de/orte/zeche-nachtigall-witten`

Talk That Science from Echobox radio

Dr. Olfa D'Angelo was invited with her colleague Maziyar Jalaal from the University of Amsterdam to talk about 3D printing in space on the radio show Talk That Science from Echobox radio.

`www.echobox.radio/shows/talk-that-science`



15. Social Activities

Group Excursion July 2022

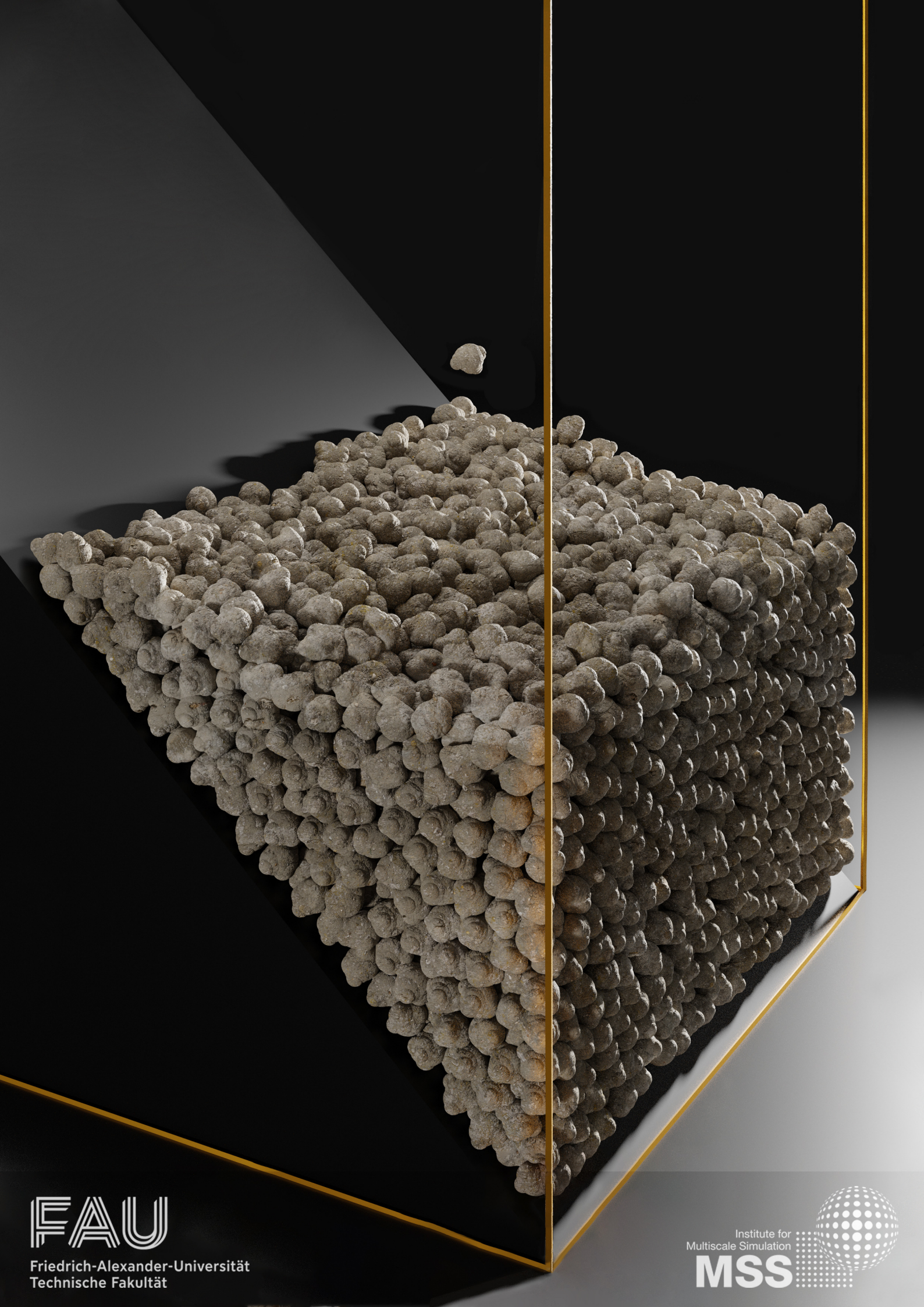
This year we finally had another group excursion. We went hiking at the Schönsteinhöhle near Streitberg. Great fun!

From left to right: Carlos Bassani, Tengda Huang, Federico Tomazic, Michael Engel, Nydia Varela-Rosales, Navid Panchi, Jonathan Martin

MSS Resturant Invitations

This year, MSS invited colleagues to the resturant for several evenings to honor the invited speakers of the MSS seminars.

From left to right: Hongy Xiao, Angel Santarossa, Frederik Keil, Carlos Bassani, Chandrew Aseervatham, Artem Panchenko, Utku Canbolat, Felix Buchele, Huzaif Rahim
Photo by Meysam Bagheri



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Multiscale Simulation
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