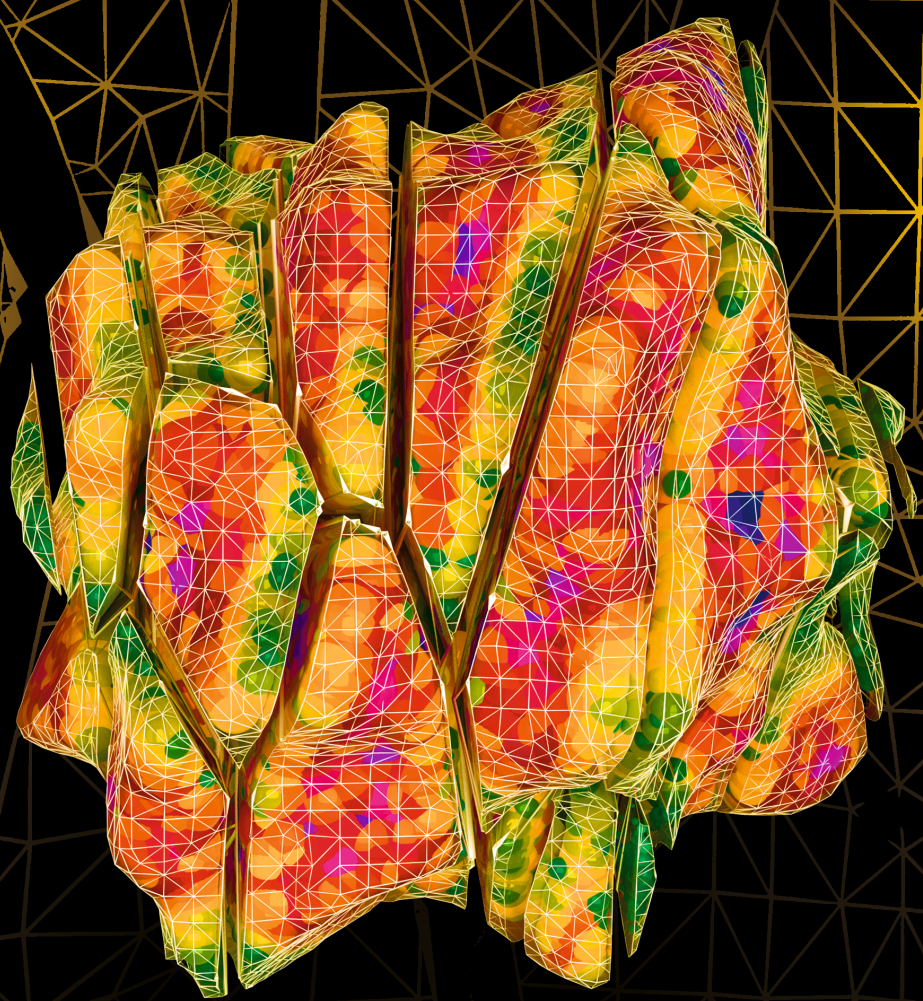
Institute for Multiscale Simulation

Prof. Thorsten Pöschel
Prof. Michael Engel

Friedrich-Alexander-Universität Erlangen-Nürnberg

2023 Annual Report



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)
Cauerstraβe 3, 91058 Erlangen

Editor: Utku Canbolat

Front cover: Fragmentation of a complex shaped particles using the multi-sphere approach for DEM applications.
Image by Ali Mauricio Velasco Sabogal, cover design by Gerd Beck

Back cover: Formation of cracks in a drying suspension.
Image by Meysam Bagheri

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Institute for Multiscale Simulation

Annual Report 2023

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 2023.

Erlangen, December 2023
Thorsten Pöschel, Michael Engel

1. Staff Members

Professors

Prof. Dr.
Thorsten Pöschel

Prof. Dr.
Michael Engel

Visiting Researchers

Assoc. Prof. Dr.
Tomoko Mizuguchi

Dr.
Anabella Abate

Assistant Professor (Privatdozent) and Habilitation Candidates

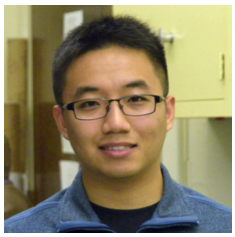
Priv.-Doz. Dr. rer. nat.
Patric Müller

Dr.-Ing.
Sudeshna Roy

Dr.-Ing.
Carlos Lange Bassani

Dr.
Alberto Leonardi

Postdoctoral Researchers



Dr.-Ing
Hongyi Xiao

Dr.-Ing.
Vasileios Angelidakis

Dr.-Ing.
Olfa D'Angelo

Dr. Aswathy
Muttathukattil
Narayanan

Dr. rer. nat.
Achim Sack

Dr. Artem
Panchenko

PhD Students

M. Eng.
Felix Buchele

M. Sc.
Meysam Bagheri

M. Sc.
Holger Götz

M. Sc.
Sarthak Jadhav

M. Sc.
Atharva Pandit

M. Sc.
Angel Santarossa

M. Sc.
Federico Tomazic

M. Sc.
Navid Panchi

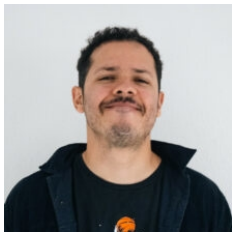
M. Sc.
Huzaif Rahim

M. Sc.
Utku Canbolat

M. Sc.
Nicolas Pechler

M. Sc.
Kaijie Zhao

M. Sc.
Nydia Roxana
Varela-Rosales



M. Sc.
Geovane de Jesus
Rodrigues

Visiting Students

M.Sc.
Laureano Ortellado
PhD Student
Department of Physics
Universidad Nacional
del Sur Argentina

Carlos Andrés del Valle
Bachelor's Student
Department of Physics
National University
of Colombia

Adriana Enriquez
Bachelor's Student
Department of Physics
University of Havana

Master and Bachelor Students

Nadja Al Akkam
Master student

Chandrew Aseervatham
Master student

Deniz Fakioglu
Master student

Qing Yu
Master student

Yasmin Gerlach
Master student

Sahib Abdullayev
Master student

Prashanth Prakash
Kamath
Master student

Isabella Schneider
Bachelor student

Yazan Alzaghah
Bachelor student

Frederik Keil
Bachelor student

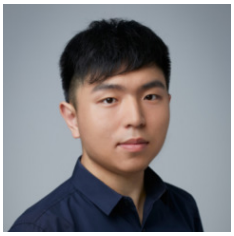
Valentin Hartinger
Bachelor student

Technical and Administrative Staff

System Administrator

Ulrike Hansl
Team Assistant

Walter Pucheanu
Master Technician & Head of the Mechanics Workshop

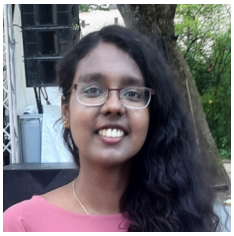


Hao Sheng
System administrator, Technician for X-ray tomography, Radiation safety officer

Student Assistants

Priyanka Singh

Zheng Yu Siah



Paavai Rajasekar

Mohammed Ubaid

Lara Delevic

Yi-Ting Chiang

Fatima Tanvir

Santhwana Thadavantavida

2. MSS Seminar

159. **Dr. Jonathan Kollmer**
Faculty of Physics, University of Duisburg-Essen
"Dense granular gases and tribocharging in microgravity"
January 18, 2023

160. **Dr. Thomas Lynn**
Argonne National Laboratory
"Contributions of cutting-and-shuffling to mixing in granular systems: analysis of a model system and outlook for optimization"
January 25, 2023

161. **Prof. Thomas Voigtmann**
German Aerospace Center (DLR), Cologne
"Yield surfaces and residual stresses in granular and colloidal materials"
March 22, 2023

162. **Dr. Hongyi Xiao**
Institute for Multiscale Simulation
"Important aspects for a junior experimental scientist"
April 12, 2023

163. **Prof. Miguel Ruiz García**
School of the Physical Sciences, Universidad Complutense de Madrid
"Emerging collective phenomena: from nonlinear flow networks to active matter"
April 19, 2023

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Otto-von-Guericke-Universität Magdeburg
"Intermittent flow of soft particles passing through orifices"
April 26, 2023

165. **Prof. Joshua Dijksman**
Van der Waals-Zeeman Institute, University of Amsterdam
"What HARD physics can we learn from soft hydrogel suspensions?"
May 10, 2023

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Friedrich-Alexander-Universität Erlangen-Nürnberg
"Characterization of feedstock materials for powder bed fusion Additive Manufacturing"
May 17, 2023
167. **Prof. Matthias Sperl**
German Aerospace Center, Institute of Materials Physics in Space
"Multiple amorphous states in granular packings and glasses - With some comments on quantum computing"
June 28, 2023
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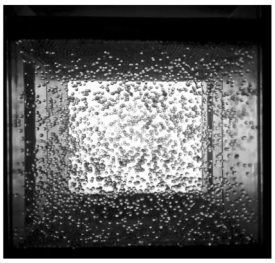
Imperial College London, UK
"Current challenges in particle scale modelling in geomechanics"
July 5, 2023
169. **Prof. José Daniel Muñoz**
National University of Colombia
"Elementary volumes and forces in equilibrium statistical mechanics descriptions of granular media"
July 12, 2023
170. **Prof. Kai Huang**
Duke Kunshan University, China
"Granular Drag: From fundamentals to applications"
July 19, 2023
171. **Prof. Tomoko Mizuguchi**
Kyoto Institute of Technology, Japan
"Free energy analysis of the molecular transport into amphiphilic self-assembly Systems"
October 3, 2023
172. **Prof. Sudeep N. Punnathanam**
Indian Institute of Science, Bengaluru, India
"A molecular theory of crystal nucleation from dilute phases"
October 18, 2023
173. **Dr. Dominik Krengel**
University of Tsukuba, Japan
"The importance of particle shape in granular materials"
December 20, 2023

159th MSS Seminar
Wednesday, January 18, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Dense granular gases and tribocharging in microgravity

Dr. Jonathan Kollmer
Faculty of Physics, University of Duesburg-Essen

In the early phases of planet formation small grains of dust collide and form growing aggregates in the gaseous environment of a protoplanetary disk. I will present experimental work characterizing the behaviour of colliding grains in microgravity and how their clustering is influenced by interstitial gas and tribocharging.

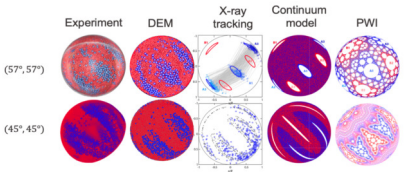


160th MSS Seminar
Wednesday, January 25, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Contributions of cutting-and-shuffling to mixing in granular systems: Analysis of a model system and outlook for optimization

Dr. Thomas Lynn
Argonne National Laboratory

Granular materials are a common industrial intermediate and product. The final homogeneity of a mixing process is important to the quality of a product or material. Well-studied fluid-like approximations capture a limited view of these materials. Mixing by cutting-and-shuffling (like that for a deck of cards or a Rubik's cube) is a paradigm that has not been studied in detail but can be applied in a variety of situations, particularly for understanding the mixing of granular materials. Mathematically, cutting-and- shuffling is described by piecewise isometries (PWIs), which rearrange solid pieces cut from an original object. Here, mixing is created by the cut discontinuities in the PWI. The accumulated discontinuities due to a PWI create an intricate fractal structure that estimates the potential for mixing in a simple spherical tumbler of granular material, but this potential for mixing does not always result in real mixing. However, cut-and-shuffle dynamics can be used to locate barriers to mixing. The discontinuous nature of mixing from cuts or discontinuities in these systems makes formulating the cut-and-shuffle mixing problem for optimization challenging, but an application of supervised learning for copying an existing mixing methodology shows a promising future for the improvement of cut-and-shuffle mixing using machine learning methods.

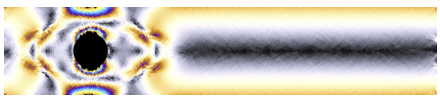


161st MSS Seminar
Wednesday, March 22, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Yield surfaces and residual stresses in granular and colloidal materials

Prof. Thomas Voigtmann
Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln

To flow or not to flow - our everyday life is filled with fluids that seem to probe the boundary of this question. In physicists' terms, they show a wide range of complex rheological characteristics that defy the usual notions of "fluid" and "solid". Their ubiquity notwithstanding, the associated phenomena are anything but simple to describe from microscopic principles.
In this talk, we will investigate specifically the role that macroscopic geometry plays in determining the flow and deformation behavior. I will discuss how microscopic theory and some fundamental principles of continuum mechanics can inform rheological models to predict the yield surfaces that separate the flowing from the non-flowing states of a glass-forming and a granular fluid.
Looking further at the stresses that remain frozen into a glassy material long after any flow has ceased, we will see how microscopic dynamics and macroscopic geometry conspire to produce residual-stress distributions that are behind the colorful birefringence displays of many an amorphous solid. Through this I hope to convince you that nonequilibrium statistical physics, through the integration-through transients framework, helps us to define a range of qualitative features of complex-fluid flows that would be difficult to guess right in empiricial models.



162nd MSS Seminar
Wednesday, April 12, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Important aspects for a junior experimental scientist

Dr. Hongyi Xiao
Institute for Multiscale Simulation, University of Erlangen-Nuremberg

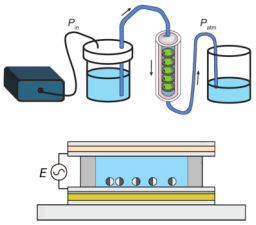
Starting a scientific career as an experimentalist is often exciting but sometimes frustrating, as barriers for a transition from learning to creating knowledge and technologies are seldom mentioned in education curriculum. In this presentation, I will address the challenges in such a transition and discuss important aspects of conducting experimental research as a junior scientist. This covers evaluating research ideas, transforming research goals to testable hypotheses, identifying key measurable, etc. Accumulating knowledge and skills is also important, and effective methods will be identified beyond classroom-type learning. The presentation will serve as the first lecture in a series aiming to help young experimental scientists, with the rest of the lectures focusing more on executing experimental plans, evaluating results, and developing more specialized skills.

163rd MSS Seminar
Wednesday, April 19, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Emerging collective phenomena: from nonlinear flow networks to active matter

Prof. Miguel Ruiz Garcia
Universidad Complutense de Madrid

Nature is full of examples where individual components, exhibiting simpler behavior, self- organize and generate emerging complex behavior as a group. Such collective behavior emerges at every level and scale, from the self-sustained oscillations in the brain vasculature to the mesmerizing behavior of a flock of birds. In this talk, we will approach the physics of nonlinear flow networks and active matter from opposite points of view. We will learn how passive nonlinear ducts that transport fluid can display emerging phenomena when arranged in a complex network, and will discuss how we have built such a nonlinear flow network in the lab. In the case of active matter we will go in the other direction, from the collective behavior to the local rules that support it. We propose a graph-neural-network-based scheme that takes the collective movement of the particles and learns the forces present in the system. After training the network, one can extract both active and passive interactions between particles. We validate this approach with numerical data, and extract physical conclusions from experiments of synthetic active particles.

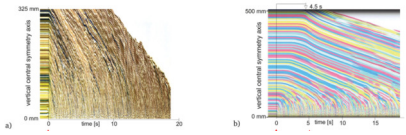


164th MSS Seminar
Wednesday, April 26, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Intermittent flow of soft particles passing through orifices

Jing Wang
Otto-von-Guericke-Universität Magdeburg

Soft, low-friction particles in silos show peculiar features during the discharges from silos. The outflow rate is found to become increasingly fluctuating and even intermittent with decreasing orifice size and with decreasing filling height. In orifices narrower than two particle diameter, the outflow can be stopped completely but can be dissolved spontaneously. We suppose this phenomenon is caused by viscoelasticity of soft particles. Besides, we investigate the force on a spherical obstacle in discharges of cylinder silos. The force grows quadratically with the sphere diameter in the case of soft particles.

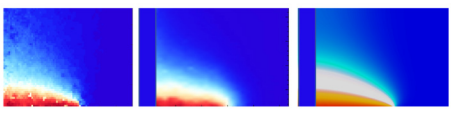


165th MSS Seminar
Wednesday, May 10, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

What hard physics can we learn from soft hydrogel suspensions?

Prof. Joshua Dijksmann
Van der Waals-Zeeman Institute, University of Amsterdam, Amsterdam, The Netherlands

Granular fows are often spatially heterogeneous featuring characteristic shear bands when strain accumulates. Understanding how such shear band localizaton emerges from microscopics is stll a major challenge. One class of so-called non-local theories identfed that the width of the shearing zone should depend on the local stress. I will discuss work in which we explicitly test this picture by introducing a uniquely stress-sensitve suspension: hydrogel suspensions. Such suspensions can be probed in a classic boundary-driven fow geometry in which shear bands can be well-tuned and characterized: the Split- Botom Shear Cell (SBSC). The stress-sensitve suspension is composed of mildly polydisperse sof, slippery hydrogel spheres submersed in water. We measure their fow profles and rheology while controlling the confnement stress via hydrostatc efects and compression. We determine the average angular velocity profles in the quasi-statc fow regime using MRI-PIV and probe a range of fow speeds using discrete element method (DEM) simulatons. We explicitly match a pressure-sensitve non-local granular fuidity (NGF) to the observed fow behavior. We fnd that shear bands for this type of suspension become extremely broad under the low confning stresses from the almost density-matched fuid partcle mixture, while collapsing to a narrow shear zone under fnite, externally imposed compression levels. The DEM and NGF results match the observatons quanttatvely, confrming the conjectured pressure sensitvity for suspensions and its role in NGF. To further emphasize the unique pressure sensitvity of the suspensions in general and the usefulness of the hydrogel suspension system in partcular, we demonstrate a transiton from yield stress to power law fow behavior from the rheology of the suspension.

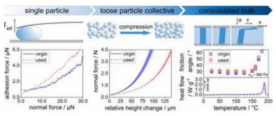


166th MSS Seminar
Wednesday, May 17, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Characterization of Feedstock Materials for Powder Bed Fusion Additive Manufacturing

Dr. Jochen Schmidt[1,2]
[1] Institute of Particle Technology, Department of Chemical and Biological Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany
[2] Colloborative Research Center 814 "Additive Manufacturing", Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

In this talk, powder requirements for PBF-AM processes will be addressed and established state-of-the-art methods, as well as novel approaches for characterization of bulk solid properties of AM feedstock powders under process conditions will be reviewed and assessed with respect to the method's predictability of the feedstock's AM processability. Moreover, some important plastic powder production and functionalization methods will be briefly sketched and the effect of particle (c.f. size distribution, shape) and bulk solid properties on part properties and processability, i.e. structure-property relationships along the AM process chain will be demonstrated for selected examples.



Hesse et al., Additive Manufacturing Vol. 41 (2021) 101957

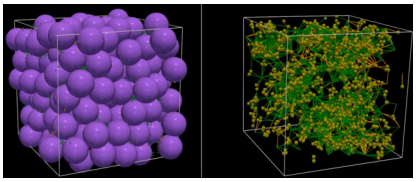
167th MSS Seminar
Wednesday, June 28, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Multiple Amorphous States in Granular Packings and Glasses - With Some Comments on Quantum Computing

Prof. Matthias Sperl

German Aerospace Center Institute of Materials Physics in Space

Asymmetric binary mixtures of granular particles, i.e. involving particles with widely different sizes, exhibit an additional jamming transition inside the already mechanically stable regime. The talk shall explain what that has to do with glasses, concrete, water, and quantum computing.



168th MSS Seminar
Wednesday, July 5, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Current challenges in particle scale modelling in geomechanics

Prof. Catherine O'Sullivan

Faculty of Engineering, Imperial College London

This presentation will introduce some current challenges in particle scale modelling from a geomechanical perspective. Recent developments on simulating both granular materials and clay will be introduced. The talk will firstly focus on coupled thermal-hydro-mechanical behaviour of granular materials. The potential to use thermal DEM to develop new experimental protocols and to advance understanding of material response to thermal cycles will firstly be outlined. Then challenges associated with developing effective frameworks for coupled fluid-particle simulations will be considered, focusing both on accuracy and computational efficiency. The second half of the presentation will introduce the challenges associated with simulating assemblies of clay particles. The focus will be on kaolinite. Key concepts that will be introduced include the need to simulate large system sizes, the importance of considering the non-monotonic nature of the force-separation relationship and the challenges associated with considering particles that have a heterogeneous surface charge distribution.

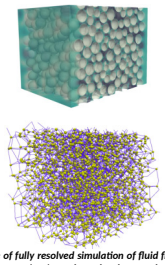
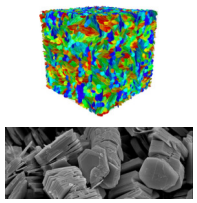


Image of fully resolved simulation of fluid flow in pore space (top) used to develop conductance models for pore network model (bottom)



Coarse grained molecular dynamics model of kaolinite (top) and SEM image of kaolinite (bottom, from Mineralogical Society of Great Britain and Ireland)

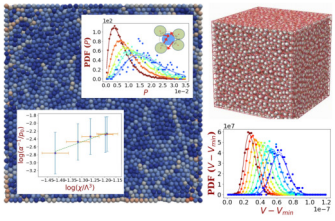
169th MSS Seminar
Wednesday, July 12, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Elementary volumes and forces in equilibrium statistical mechanics descriptions of granular media

Prof. Jose Daniel Muñoz

Simulation of Physical Systems group, CoE-SciCo Excellence Center on Scientific Computation, Department of Physics, National University of Colombia.

Volumes and force networks have been used to build statistical descriptions of granular media. In this talk we will discuss how both descriptions can be based on statistically independent elementary units, either volumes or forces, and how they can predict the distributions of Voronoi volumes and pressures per grain observed in both experiments and simulations for the special case of isotropic random arrays of monodisperse grains. Furthermore, we approximate how to join both descriptions and maximize total entropy to obtain from first principles an equation of state relating pressures and forces for this granular medium. Those results are further steps to modelling granular media from equilibrium statistical mechanics.



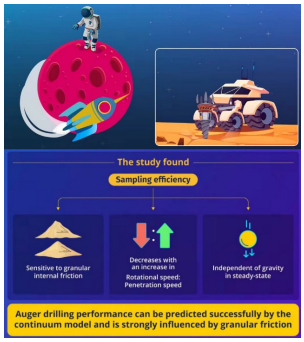
170th MSS Seminar
Wednesday, July 19, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Granular Drag: From fundamentals to applications

Prof. Kai Huang

Collective Dynamics Lab, Division of Natural and Applied Sciences, Duke Kunshan University

In this talk, I will use projectile impact and auger drilling as two examples to illustrate how granular media respond to external intruders with an emphasis on applications in space exploration. In addition, I will also provide a brief overview of how to effectively trace objects embedded in a granular medium with an overview of challenges and opportunities associated.



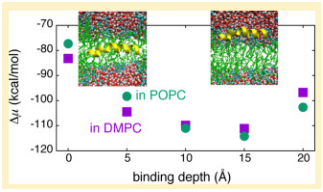
171st MSS Seminar
Wednesday, October 4, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Free energy analysis of the molecular transport into amphiphilic self-assembly systems

Prof. Tomoko Mizuguchi

Faculty of Materials Science and Engineering, Kyoto Institute of Technology

Self-assemblies of amphiphilic molecules, such as lipid membranes and micelles, can flexibly change their local structures while maintaining their whole shape. This property enables them to take up and transport materials. Understanding intermolecular interactions, including solvents and ions, is essential to finding ways to control the distribution and transport of substances. In this talk, I will show the free-energy analysis of the binding and transport of a molecule in micelle and bilayer membrane by molecular dynamics simulations. In the micelle system, we control the diffusion of surfactant molecules to make a sharp boundary. By calculating the free-energy profile in transporting of a hydrophobic molecule into the micelle, we investigate the effect of boundary roughness on the transport property. The results reveal that a sharp boundary induces the free energy barrier at the interface and the stableness of a molecule in the center of micelle. In the membrane system, we examine the stabilities of a variety of binding configurations of a small peptide in two kinds of bilayers. The binding free energy is calculated, and it is seen that the transmembrane configuration is stable in both membranes. A surface-bound state is also found to be stable due to the balance between the attractive and repulsive interactions of the peptide with lipid and water.



172nd MSS Seminar
Wednesday, October 18, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

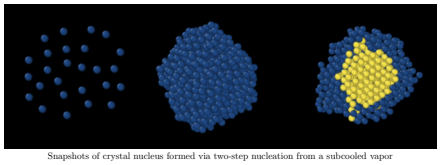
A Molecular Theory of Crystal Nucleation from Dilute Phases

Prof. Sudeep N. Punnathanam

Department of Chemical Engineering, Indian Institute of Science, India

In a typical molecular simulation, the occurrence of nucleation is a rare event. Hence, simulating a nucleation event requires sophisticated enhanced sampling techniques such as umbrella sampling, transition path sampling, metadynamics, etc. While there has been a tremendous progress in the development of techniques to simulate crystal nucleation from melts, technical challenges persist in our ability to simulate crystal nucleation of solutes from solutions. These difficulties are rooted in the need to maintain constant chemical potential of the solute in the solution during the formation of the nucleus. Towards addressing these issues, we present a molecular theory of crystal nucleation from dilute phases such as vapors or dilute solutions. Using statistical mechanics, we derive an exact expression for free energy of formation of the nucleus. The molecular theory of nucleation is then developed from this expression, which is applicable when the concentration of the nucleating species is very dilute. The theory can model the nonclassical two-step crystal nucleation seen in many systems. We have applied the theory to study and analyze the crystal nucleation pathways from Lennard-Jones vapor and NaCl solution. We find that prior explanations of the two-step mechanism based on lower barrier height for liquid nuclei is incomplete. The analysis from the molecular theory reveal that a complete explanation would also require consideration of anisotropy in the diffusion constants for growth of liquid droplets vis-á-vis the crystal nuclei.

Keywords: Crystal Nucleation, Lennard-Jones, NaCl solution, Fokker-Planck



Snapshots of crystal nucleus formed via two-step nucleation from a subcooled vapor

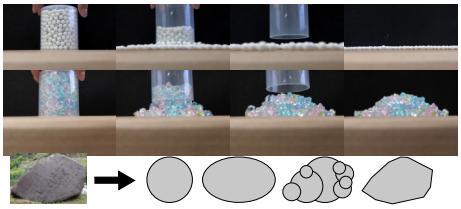
173rd MSS Seminar
Wednesday, December 20, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

The importance of particle shape in granular materials

Dr. Dominik Krengel

Department of Engineering Mechanics and Energy, University of Tsukuba, Japan

Granular materials are assemblies of particles with a wide variety of shapes. For the individual particles it is their shape that determines their kinematics: round particles will prefer rolling, while elongated particles will prefer sliding. Differences in particle mobility will then lead to differences in derived bulk properties, such as packing density or shear resistance, where in soil mechanics, stability is desirable, while in chemical engineering, good fluidity is sought.
Lamentably, the majority of Discrete Element simulations still make use of simplified, spherical models, where shape is, at best, treated by introducing some sort of unphysical rolling friction. While in the last several years some researchers have begun to use non-spherical particle models, such as super-quadrics or rigid clumps of spheres, it is polygonal or polyhedral shapes that best describe realistic granular materials.
In this talk I will explore the role of particle shape for some geotechnical examples across multiple scales and discuss some of the difficulties implementing additional forces, such as friction or Van-der-Waals forces, for polygonal particles in DEM simulations.



3. Conference Presentations

- Angel Santarossa and Holger Götz:
  Adaptive metamaterials based on granular jamming (poster presentation)
  CBI Symposium 2023
  February 3, 2023, Erlangen, Germany
- Utku Canbolat:
  Plastic deformation, wear and heat transfer in fracture of complex-shaped particles (poster presentation)
  CBI Symposium 2023
  February 3, 2023, Erlangen, Germany
- Angel Santarossa:
  Effect of particle size on the suction mechanism in granular grippers (oral presentation)
  DPG spring meeting of the condensed matter section (SKM)
  March 26-31, 2023, Dresden, Germany
- Michael Engel:
  Modeling the effect of ligands on growth and assembly of nanocrystals (oral presentation)
  Material Research Society Meeting
  April 12, 2023, San Francisco, The United States
- Carlos Lange Bassani:
  Understanding kinetic Wulff shapes from particle to nanoparticle scales via lattice-gas simulations (oral presentation)
  Workshop: Nanoparticle assemblies: a new form of matter with classical structure and quantum function
  May 01-12, 2023, Santa Barbara, CA/USA
- Thorsten Pöschel:
  Electrical impedance tomography for bubble flow diagnosis (oral presentation)
  Workshop robust instrumentation for thermal-hydraulic experiments
  May 15-17, 2023, Aix-en-Provence, France
- Carlos Lange Bassani:
  Semi-Gibbs ensemble describes kinetic nanocrystal Wulff shapes (poster presentation)
  Structure design and emerging phenomena in nanoparticle assemblies: what's next?
  May 15-18, 2023, Santa Barbara, CA/USA

- Holger Götz:
  Simulation of flexible membranes for granular systems (oral presentation)
  Workshop on open source software and granular matter
  May 31 – June 1, 2023, University of Twente, The Netherlands
- Thorsten Pöschel:
  Patient zero tracking (oral presentation)
  BOWW - Berlin open RAN working week
  June 13-15, 2023, Berlin, Germany
- Michael Engel:
  Colloidal quasicrystals (oral presentation)
  ICQ15 - The 15th International Conference on Quasicrystals
  June 18-23, 2023, Tel Aviv University, Israel
- Thorsten Pöschel:
  Collective behavior and self-organization of active granular particles (oral presentation)
  Getting into Shape. Pushing for Exotic Particulate Media Mechanics
  June 19-23, 2023, Lorentz Center Leiden, The Netherlands
- Carlos Lange Bassani:
  Transient model of hydrate pore sealing applied to oil-dominant systems (oral presentation)
  10th International Conference on Gas Hydrates (ICGH10)
  July 9-14, 2023, Singapore
- Carlos Lange Bassani:
  A new approach for gas hydrate slurry flow based on a multiscale model for multiphase flow (poster presentation)
  10th International Conference on Gas Hydrates (ICGH10)
  July 9-14, 2023, Singapore
- Carlos Lange Bassani:
  Simulation of porous medium evolution of gas clathrate hydrates (oral presentation)
  14th European Congress of Chemical Engineering and 7th European Congress of Applied Biotechnology (ECCE&ECAB2023)
  September 17-21, 2023, Berlin, Germany
- Olfa D'Angelo:
  How do granular media deform? – Particles properties and their influence on deformation mechanism (oral presentation)
  XIX International Congress on Rheology (ICR 2023)
  July 19-August 4, 2023, Athens, Greece
- Olfa D'Angelo:
  The manifold rheology of granular fluids (poster presentation)
  XIX International Congress on Rheology (ICR 2023)
  July 19-August 4, 2023, Athens, Greece
- Michael Engel:
  Packing aspects when self-assembling spheres (oral presenation)
  GeomPack: Geometry and packing in material structure and biology
  August 14 - September 25, 2023, Isaac Newton Institute for Mathematical Sciences, United Kingdom
- Michael Engel:
  Thermodynamically stable quasicrystal and dense dimer packings from tetrahedron colloids (oral Presentation)
  5th International Conference on Packing Problems: Packing and patterns in granular mechanics

August 22-24, 2023, Isaac Newton Institute for Mathematical Sciences, United Kingdom

- Thorsten Pöschel:
  Geometry of structures in granular systems with dissipation and friction (oral presentation)
  SPP2265: Random Geometric Systems
  August 29, 2023
- Olfa D'Angelo:
  The manifold rheology of granular fluids (poster presentation)
  7th International Soft Matter Conference (ISMC 2023)
  September 4-8, 2023, Osaka, Japan
- Federico Tomazic:
  Coarse-grained simulations of ligand-tethered nano-plates (poster presentation)
  International Soft Matter Conference
  September 4-8, 2023, Osaka, Japan
- Utku Canbolat:
  Image-informed fracture model for complex-shaped particles in discrete element simulations (oral presentation)
  9th International Conference on Discrete Element Methods (DEM9)
  September 17-21, 2023, Erlangen, Germany
- Angel Santarossa:
  Tomographic imaging-based finite element analysis of 3D mixed-mode cracks (poster presentation)
  9th International Conference on Discrete Element Methods (DEM9)
  September 17-21, 2023, Erlangen, Germany
- Holger Götz:
  Jammed granular metamaterials (oral presentation)
  9th International Conference on Discrete Element Methods (DEM9)
  September 17-21, 2023, Erlangen, Germany
- Huzaif Rahim:
  Alignment, stress, and packing density: Unravelling the granular Weissenberg effect (poster presentation)
  9th International Conference on Discrete Element Methods (DEM9)
  September 17-21, 2023, Erlangen, Germany
- Meysam Bagheri:
  Physics of drying suspensions: Modeling crack formation through microscopic interactions (oral presentation)
  9th International Conference on Discrete Element Methods (DEM9)
  September 17-21, 2023, Erlangen, Germany
- Sudeshna Roy:
  Powder spreading of irregular particles with thermal properties (oral presentation)
  9th International Conference on Discrete Element Methods (DEM9)
  September 17-21, 2023, Erlangen, Germany
- Patric Müller:
  Soft particles reinforce robotic grippers – robotic grippers based on granular jamming of soft particles (oral presentation)
  9th International Conference on Discrete Element Methods (DEM9)
  September 17-21, 2023, Erlangen, Germany
- Vasileios Angelidakis:
  Mechanical characterisation of highly interlocked granular metamaterials (oral presentation)
  9th International Conference on Discrete Element Methods (DEM9)

September 17-21, 2023, Erlangen, Germany

- Vasileios Angelidakis:
  Research-led Teaching of Discrete Element Simulations (poster presentation)
  9th International Conference on Discrete Element Methods (DEM9)
  September 17-21, 2023, Erlangen, Germany
- Carlos del Valle:
  Stable integration of rotations for non-spherical particles in the Discrete Element Method (oral presentation)
  9th International Conference on Discrete Element Methods (DEM9)
  September 17-21, 2023, Erlangen, Germany
- Thorsten Pöschel:
  Granular convection in micro-gravity (oral presentation)
  9th International Conference on Discrete Element Methods (DEM9)
  September 17-21, 2023, Erlangen, Germany
- Vasileios Angelidakis:
  An open-Source software for sequential particle deposition (oral presentation)
  9th International Conference on Discrete Element Methods (DEM9)
  September 17-21, 2023, Erlangen, Germany
- Hongyi Xiao:
  Propulsion of a scallop-like swimmer in granular matter (oral presentation)
  9th International Conference on Discrete Element Methods (DEM9)
  September 17-21, 2023, Erlangen, Germany
- Thorsten Pöschel:
  SALTED – A high-performance simulator for granular packings (oral presentation)
  9th International Conference on Discrete Element Methods (DEM9)
  September 17-21, 2023, Erlangen, Germany
- Frederik Keil:
  Random packings of Meissner tetrahedra (poster presentation)
  9th International Conference on Discrete Element Methods (DEM9)
  September 17-21, 2023, Erlangen, Germany
- Michael Engel:
  Taming entropy in colloidal crystallization (oral presenation)
  SLAM Seminar - Institute of Science and Technology Austria
  September 29, 2023, Klosterneuburg, Austria
- Federico Tomazic:
  Simulation of layer formation during crystallization of supraparticles in spherical confinement (oral presentation)
  Particle-Based Materials Symposium
  October 5-6, 2023, Braunschweig Germany
- Michael Engel:
  Structural complextity in colloidal self-assembly (online)
  Statistical Thermodynamics and Molecular Simulations (STMS) Seminar Series
  November 17, 2023

4. Selected Postdoc Projects

Dr. Sudeshna Roy, "DEM simulations of powder spreading considering the thermal properties of surface molten materials."
This project aims to enhance our understanding of thermal effects in additive manufacturing powder spreading setups, focusing on four key objectives. Firstly, a microscale thermal model will be developed in the 'MercuryDPM' code, incorporating temperature-dependent mechanical properties of powder particles and extending the code for the powder spreading setup. Secondly, the thermal effects on powder layer structure will be elucidated, studying structural anisotropy, temperature distribution, and flowability. Thirdly, the project will reconstruct melted areas from particle data, assessing their impact on subsequent powder layers and contributing to understanding melting and solidification processes. Lastly, the effects of particle geometry and thermal properties will be investigated under varying conditions, leading to the derivation of improved process strategies and enhanced part quality. This comprehensive approach, spanning from fundamental modeling to practical optimization, aims to provide valuable insights for advancing additive manufacturing processes.

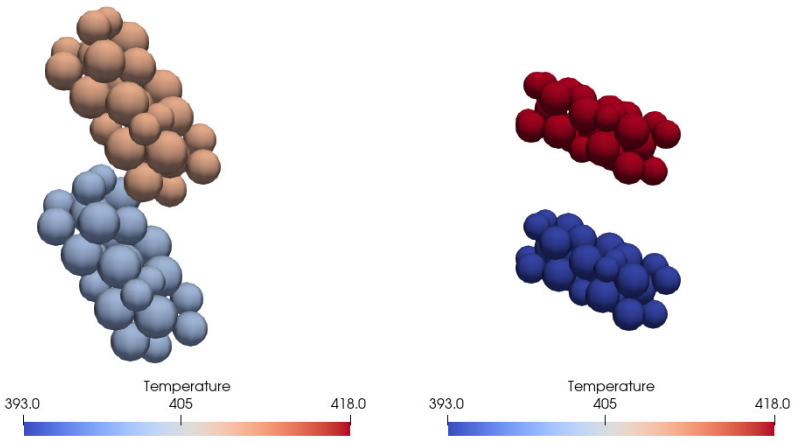


Figure: Results from the merging of multisphere model with thermal contact model showing two multispheres at different temperatures (left) before collision and (right) after collision.

Dr. Olfa D'Angelo, "Granular Rheology In Space (GRIS)"

The success or failure of future space exploration missions will depend on humans' ability to understand and overcome the challenges posed by the Lunar environment – among which, dealing with the overwhelming presence of regolith. With sunlight, regolith is the main *in-situ* resource available on the Moon; all ISRU (*in-situ* resource utilization processes rely on its acquisition, isolation and preparation.

The complexity of Lunar regolith rheology is threefold: the granular material itself exhibits unique physical properties (sharp and abrasive particles with a large amount of fines); the low level of gravity modifies interactions among particles, making cohesive forces predominant; the singular Lunar environment (featuring low gravity but also high vacuum and electrostatic charges from solar winds) has a complex influence on regolith behavior. On ground, existing granular models rely on thousands of years of empirical knowledge. We lack such experience on the Moon. Gravity – more precisely Earth's gravity – is included in current rheological models, although often implicitly. For example, confining pressure and packing fraction indirectly depend on gravitational environment and will redefine soil properties; low gravity also triggers the predominance of cohesive forces, altering granular flowability.

In this project, we will understand the rheology of Lunar regolith *on the Moon*, and translate it into models of regolith flow-behavior. Our models will inform the development of ISRU processes, and provide a benchmark for a future *Lunar regolith rheological simulant*. First, we will make explicit the effect of three factors on regolith rheology: physical properties of regolith, low gravity, and Lunar environment, notably through electrostatic charging.

The combined influence of those factors will be studied through three experiments: an hour-glass experiment, a penetration experiment, and a collapsing wall experiment. Adapted from already existing hardware, they were selected because despite their relative simplicity of implementation, those three experiments combined provide a holistic view of granular behavior. They also directly relate to ISRU processes, past and future: from the tranche collapse and penetration data from Apollo missions, to robotic and human interactions with Lunar soil during the Artemis mission, to provide fuel for Lunar Gateway, and towards the democratization of Lunar activities, notably with NASA's commercial lunar payload services (CLPS). By combining efforts and results from those experiments, we will propose a universal description of granular rheology adapted to low gravity environments, enabling humans to explore sand-covered space bodies: our Moon, asteroids, Mars, and beyond.

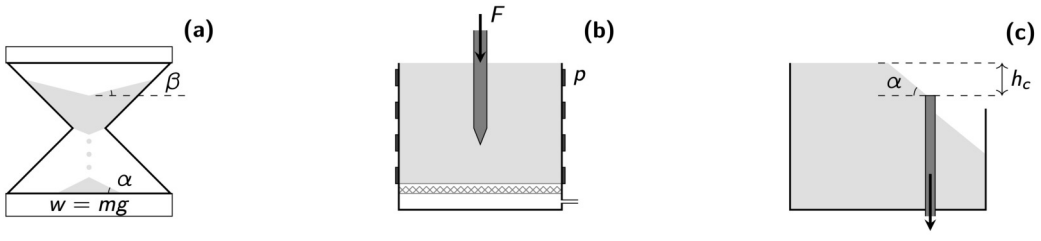
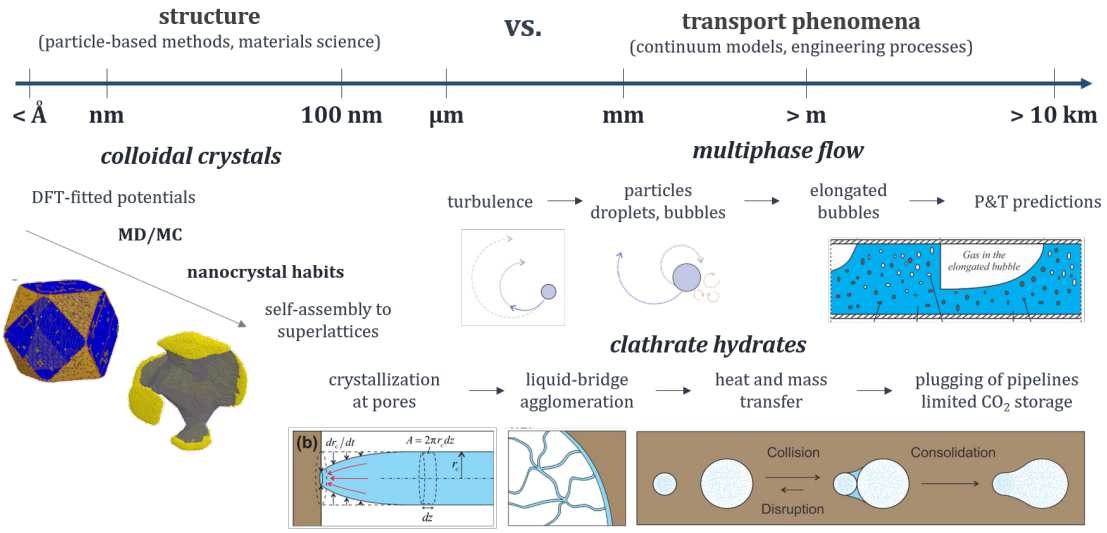


Figure: Concept schematics of the three experiments proposed: (a) hourglass experiment, (b) penetration experiment, (c) vertical wall collapse experiment.

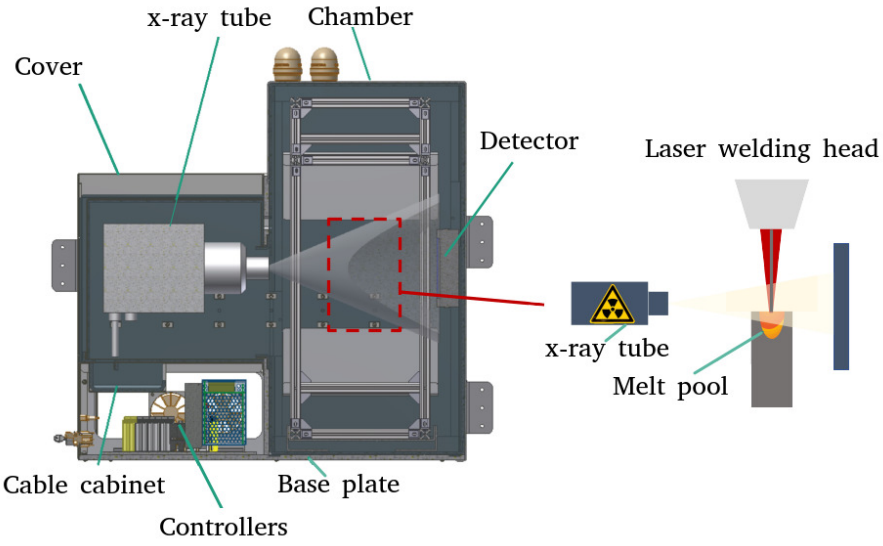
Dr. Carlos Lange Bassani, "Multiscale modeling of crystals from fundamental science to engineering applications"

The repeating patterns inherent in crystals captivate the curiosity of scientists, who were very successful in describing the fundamental scales linking energy (quantum) to the formation of unit cells at the molecular scales. The understanding of phase diagrams, defects, inclusions, and grain boundaries in physical properties at the macroscales allowed the use of crystals in society, which culminated in the machinery technology development in the past century. Such multiscale coupling still harshly relies on curve-fitted models, which hinders the reasons why some engineering recipes work, and blocks the development of new design strategies. Of concern in this project is the emergence of patterns in the mesoscales, such as faceted nanocrystals, dendrites, and porous medium. Whereas (i) the formation of interfaces depends on free energy minimization coming from molecular ordering, requiring structure information described by particle-based methods (molecular dynamics, Monte Carlo), (ii) the environment plays a role in transferring mass (diffusion/convection), momentum (pressure), and energy (temperature) to keep the crystallization process dynamically happening, described by continuum approaches (phase field models, finite volume method). The coupling of structure formation and transport phenomena is therefore key to predicting heterogeneous driving forces over the crystalline surface that lead to different growth pathways, ultimately affecting the outcome of the engineering process. Systems of interest comprise (a) emergent technologies such as the synthesis of nanoparticles of defined shape and their assembly into superstructure (colloidal crystals) as possible new materials for society use, and (b) urgent matters in the reduction of emissions by understanding multiple-component clathrate crystals as potential carbon storage materials, and their agglomeration/deposition in the possibility of reducing environmental impacts in hydrocarbon production.



Dr. Achim Sack, "LADA: LASER Wire Deposition Welding in Zero Gravity"

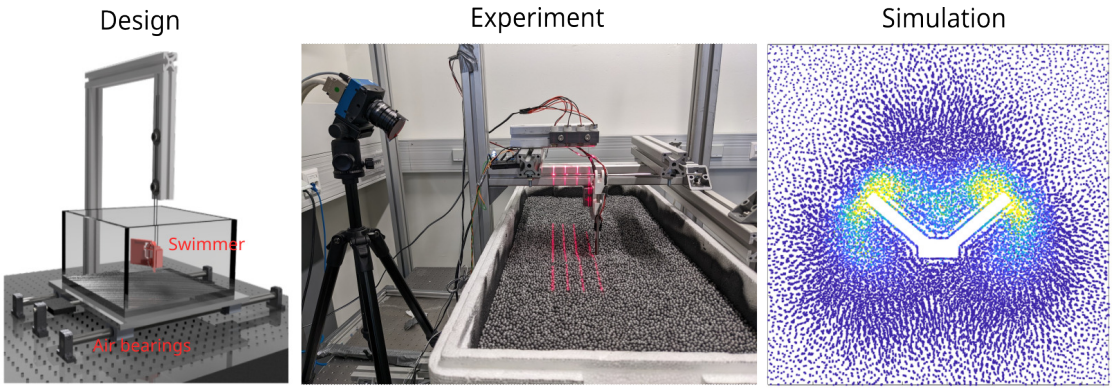
While additive manufacturing of plastics using fused deposition modeling (FDM) is already being tested on the International Space Station, the (technically more important) manufacturing of metal components has not yet been investigated. Specifically, the LASER wire buildup welding process has not yet been applied in microgravity. Therefore, the aim of the planned project is to explore the suitability of the LASER wire deposition welding process for applications under reduced gravity and in zero gravity and to assess its potential. To this end, this process will be mapped by a numerical and experimentally validated method to determine optimal process parameters for specific fabrication tasks. Of particular importance for the development of a stable wire buildup welding process under microgravity conditions is precise knowledge of the behavior of the molten metal for this process. This will be investigated using the recently developed HORUS facility. HORUS allows high-speed X-ray radiography to be performed on parabolic flights. The experience with HORUS as well as the expertise of the applicant on additive manufacturing methods and their numerical simulation provide excellent prerequisites to work on this task. The experimental part is complemented by a computer simulation using SPH to predict the behavior of the melting process. By matching with experimental results obtained by HORUS, the simulation will be improved step by step so that quantitative agreement is achieved. The predictive performance of the simulation will be tested on a series of experiments under different conditions (LASER power, material, feed rate, etc.). Our project should help to open up the extremely important process of LASER wire buildup welding for space missions (in zero gravity) and applications under reduced gravity (Moon, Mars).



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. Vasileios Angelidakis, "Sequential particle deposition and 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.

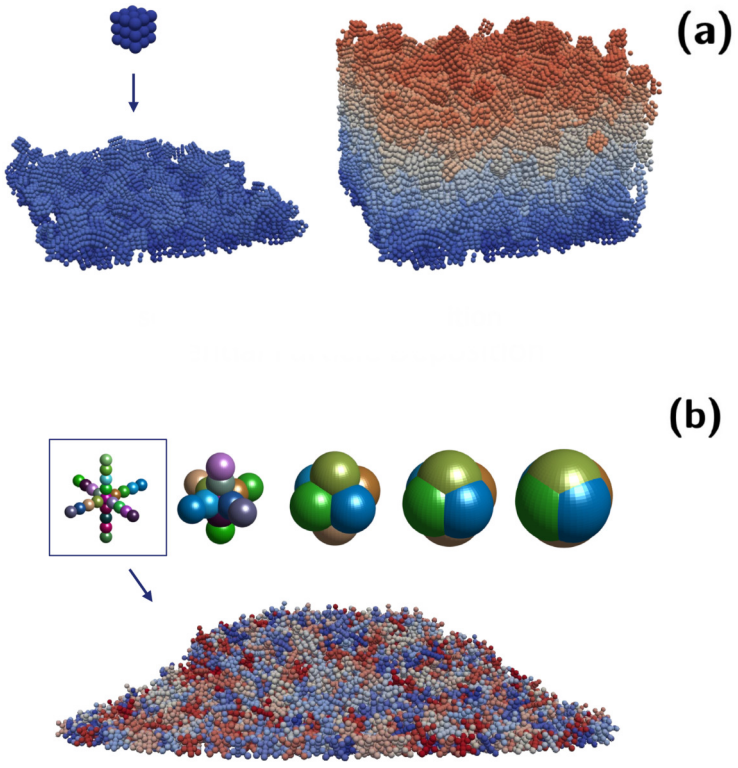
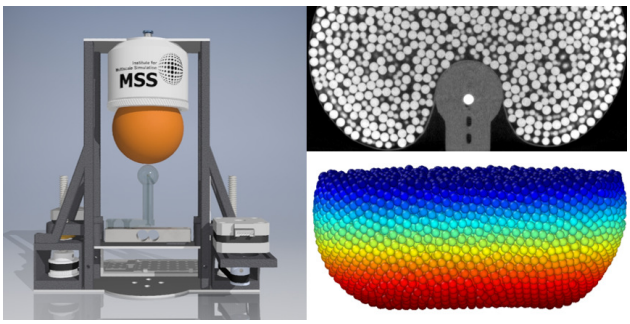


Figure: (a) Sequential particle deposition, (b) mechanical granular metamaterials.

5. Ongoing PhD Projects

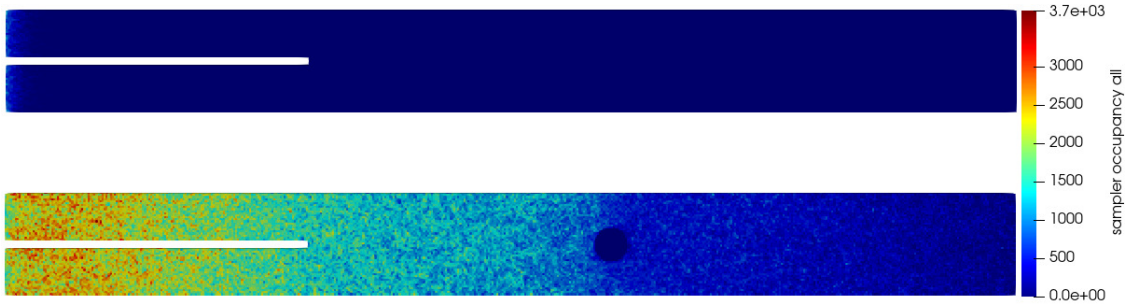
Angel Santarossa, "Jamming-based robotic granular grippers: Experimental study by means of X-ray imaging techniques"

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. 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.



Felix Buchele, "Reactive flow in porous media"

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 catalysts however is limited to microscopic and macroscopic points of view. With tools like Density Functional Theory (DFT), Molecular Dynamics (MD), or Kinetic Monte Carlo (KMC), the properties of catalytic surfaces can be investigated on a microscale. On the other hand, there are rate-based flow solvers and semi-empirical differential equations describing the properties of catalytic systems on a macroscopic, engineering scale. Mesoscopic tools to investigate flow within porous catalysts and chemical reactions based on first principles are virtually non-existent.
The aim of this project 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, precluding the use of continuum methods. Thus, a particle-based Direct Simulation Monte Carlo (DSMC) code is used to simulate flow.
The surface reactions are modeled following energy-barrier-based first principle equations from physical chemistry for Langmuir-Hinshelwood and Eley-Rideal kinetics with detailed, stochastic adsorption and desorption computation. A model for electrochemical reaction kinetics is planned for the future.



Holger Götz, “Jamming and convection in granular systems”

Granular media changes its properties drastically when going through the jamming transition. This effect is used in various applications, ranging from endoscopes for medical purposes to robotics applications such as granular grippers, granular paws, and swarm robots. Many of the applications consist of a granulate that is enclosed by a membrane. To simulate such applications, I developed a method to simulate flexible membranes with the discrete element method (DEM). In this method, the mass-spring approach is supplemented by surface patches, and the interaction between a membrane and a granulate is described by the contacts between the patches and the granulate. This allows for an efficient simulation even with a large particle size dispersion. I used this method to simulate the granular gripper and granular jamming beams and analyzed the connection between the microscopic properties of the individual particles and the macroscopic properties of the jammed granulate. In addition to the properties of jammed granulates, I study granulates in a vertically vibrated container, where the particles undergo convection. Under zero gravity conditions, the expected convection pattern is point-symmetric regarding the center of the container. I investigate deviations from the expected patterns and their driving mechanisms.

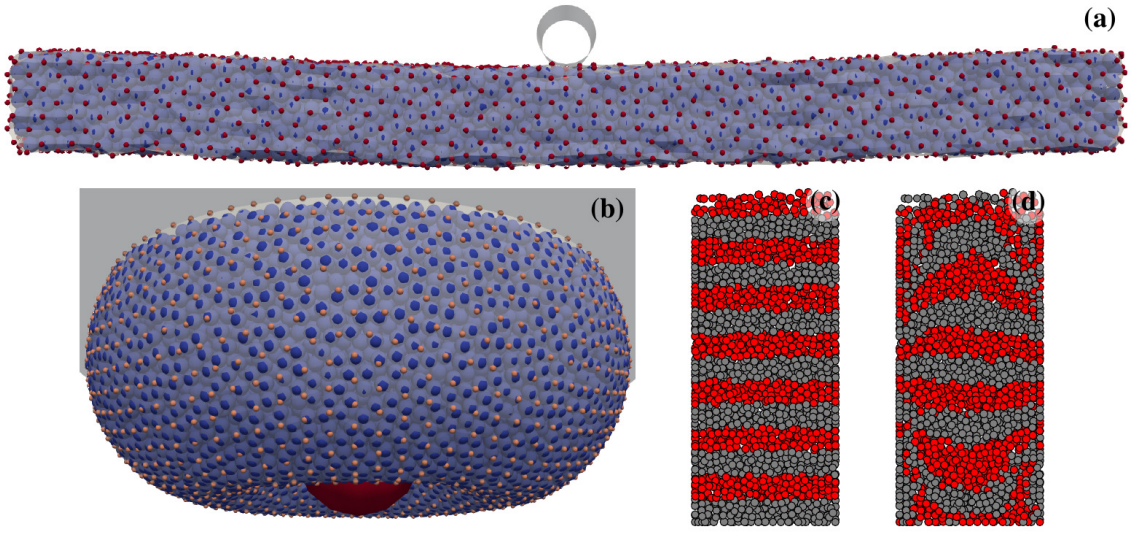


Figure: Exemplary representations of the three investigated systems. A granular bending beam (a), the granular gripper (b), and the initial (c) and final position (d) of particles in a vibrated cylindrical container.

Huzaif Rahim, "The granular Weissenberg effect"

Granular materials with elongated particles exhibit complex flow patterns under shear deformation. Unlike spherical particles, when assemblies with shape-anisotropic particles are sheared, there is an accumulation of material due to secondary convection flows. This effect resembles the Weissenberg effect of non-Newtonian fluids, where secondary flows lead to phenomena such as rod climbing. Although a direct comparison between liquid and granular flow is not prudent, due to the discrete particulate nature of the latter, comparisons of the causes behind each phenomenon can be drawn. The split-bottom shear cell geometry, and linear shear cell geometry with a middle split, are employed in discrete element simulations to study the micromechanical origins of the effect. Systems of spherical and anisotropic particles are simulated in the linear shear cell setups, to facilitate comparisons between materials that do not exhibit heaping and systems that do. The mechanical response is characterized in terms of stress measurements, such as shear stress, normal stress, and the differences between the normal components of the stress tensor. Our results reveal that a granular Weissenberg effect occurs, which is attributed to the components of the normal stress differences; this is also the driving factor for the classical Weissenberg effect. Consequently, this work brings an analogy between the Weissenberg effect observed in non-Newtonian fluids and heap formation in granular fluids composed of discrete particles.

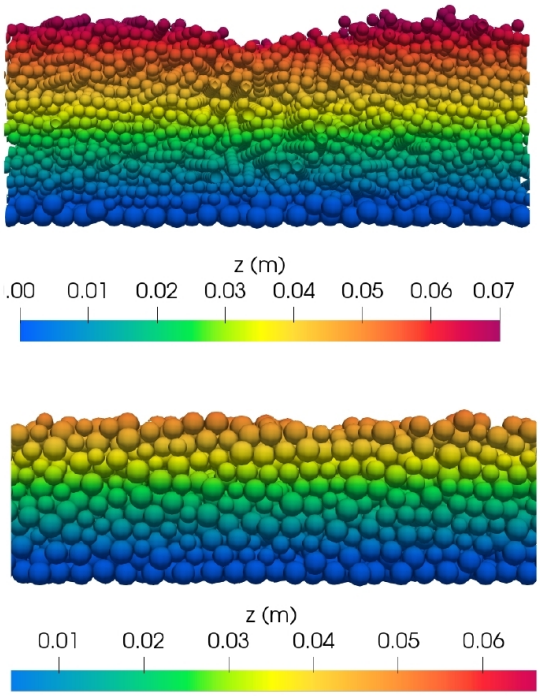
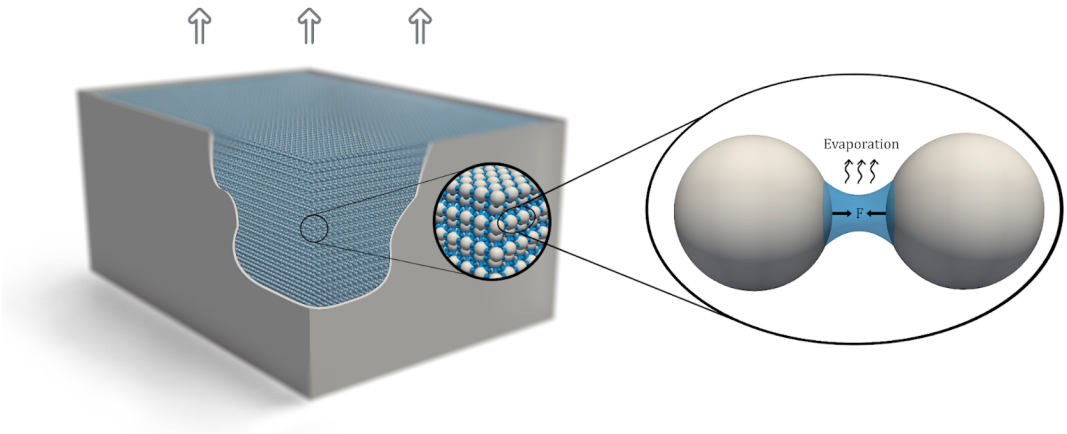
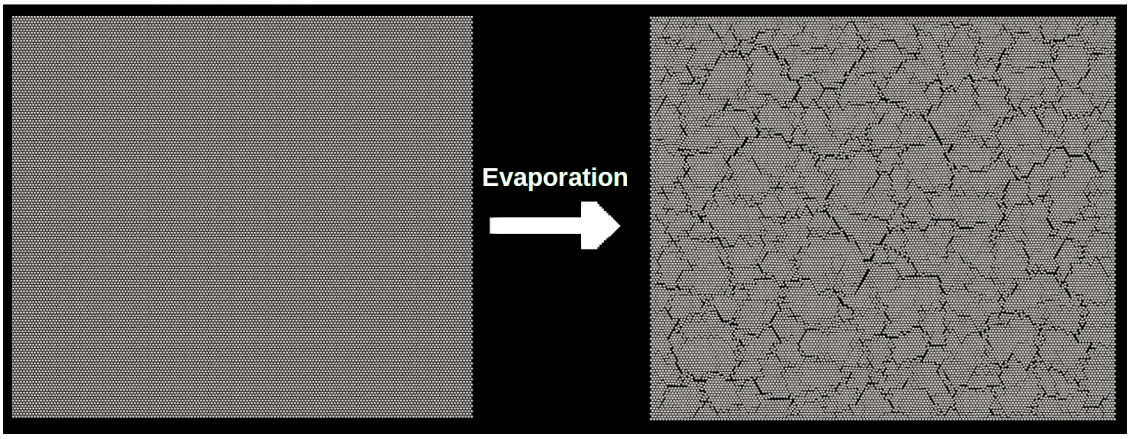


Figure: DEM simulation of wooden pegs. Top: Elongated particles show depth formation at the top of the shear band region. Bottom: In contrast, spherical particles exhibit a flat surface profile, lacking significant depth.

Meysam Bagheri, "Physics of drying suspensions"

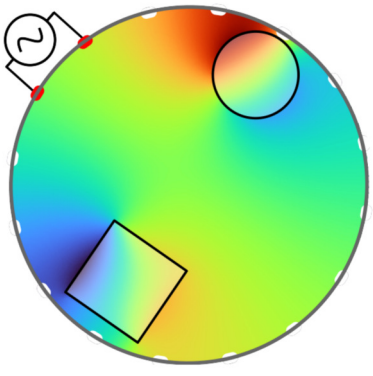
Drying suspensions display a fascinating network of cracks on drying. The cracks result from a number of complex interactions: The particles are concentrated into a close packed array due to the evaporation of the fluid. Further drying results in a network of particles which are interconnected by liquid 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.

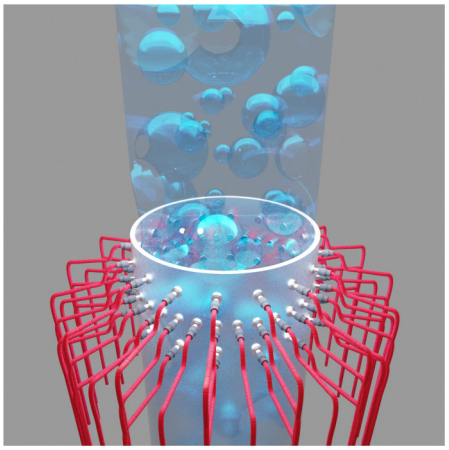




Nicolas Pechler, "Electrical Impedance Tomography for imaging in multiphase systems"

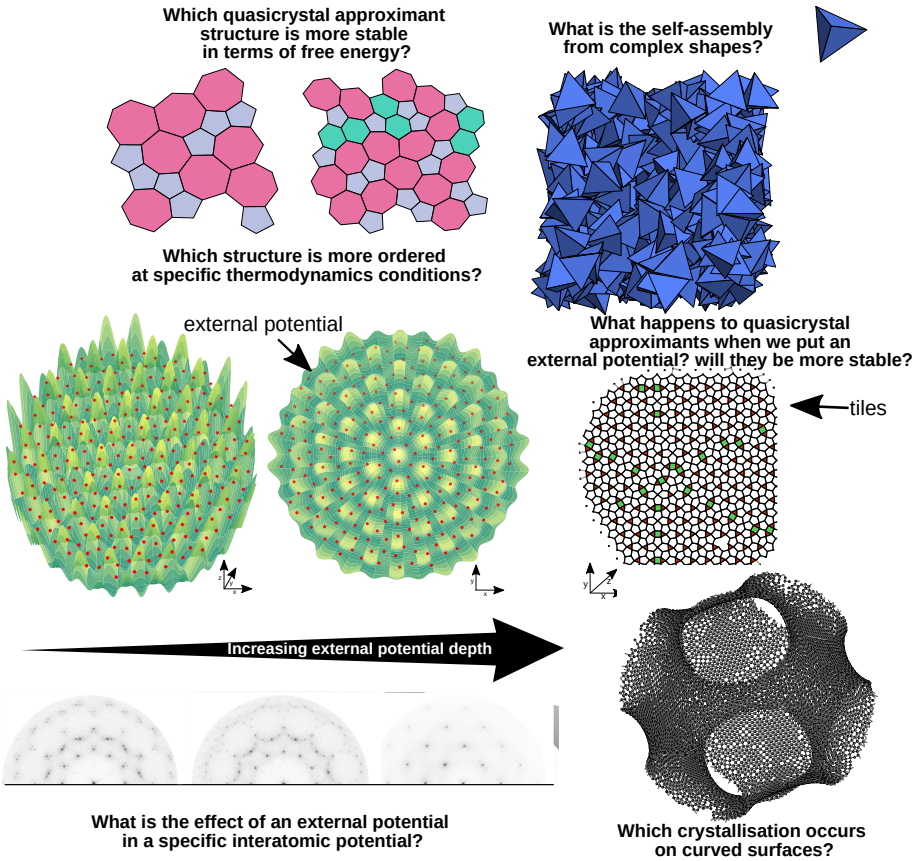
As part of the ROBIN project, aimed at developing a measurement and imaging method for high-resolution acquisition of thermal-hydraulic parameters in large-scale experimental facilities for nuclear safety research, we are developing a sensor based on electrical impedance tomography. This sensor is intended to enable non-intrusive monitoring of two-phase flows in large pipelines, allowing for the assessment of flow regimes, fluid velocity fields, and void fields.
Electrical Impedance Tomography (EIT) is a non-invasive imaging technique used to visualize and monitor the internal conductivity distribution of an object. This is done by placement of multiple electrodes on the sample's surface. Voltage is injected pairwise through two electrodes while the other ones are used for potential sensing. The application of voltage leads to a potential distribution which can be measured on the surface. With an internal change of conductivity the resulting equipotential lines shift, leading to a detection in measurement. For successful reconstruction measurement data of all injection electrode pairs is needed and then processed by a wide range of reconstruction algorithms.
However, one of the significant challenges associated with EIT is its inherently low spatial accuracy. The electrical potential distribution on the surface of the object exhibits only subtle differences, making precise measurements a demanding task. Therefore, the utilization of precise measurement equipment and techniques is of importance to overcome this limitation and enhance the overall accuracy of the imaging process.
Building upon the results of 2D preliminary experiments, where hollow bodies were placed within a bowl using a robotic arm to generate measurement data for training artificial intelligence, this project aims to extend the method to three dimensions (3D). Therefore, a bubble column is being built in order to automatically generate measurements from simulated phantoms to create a large dataset
In this context, an electronic excitation scheme is employed, utilizing a parallel application of frequency modulated alternating currents (frequency multiplexing), as opposed to traditional time multiplexing. Alongside determining an improved way of data evaluation for frequency multiplexed current EIT systems, the project also aims to optimize the electrode configuration, the geometric design, and the construction of the measurement apparatus.





Nydia Roxana Varela-Rosales, "Computational design and thermodynamic stability of aperiodic crystals and their approximants"

Aperiodic crystals, like quasicrystals, have emerged as groundbreaking structures in the field of crystallography in recent years. These structures exhibit a lack of periodicity and are found from elemental compositions like metallic alloys to biological structures like proteins. Despite significant progress in understanding these structures, their influence on physical properties remains unclear. Therefore, my research aimed to gain a comprehensive understanding of the thermodynamics and stability of aperiodic long-range order structures, particularly in the presence of external constraints (e. g. external potentials) and manifold constraints (e. g. surfaces). To achieve this, I employed particle local environments classification algorithms, both utilizing existing methods and developing new ones, to characterize the diverse symmetries observed in computational simulations of particles. These algorithms provided valuable insights into the arrangement and behavior of aperiodic structures under different conditions. Additionally, I utilized advanced free energy methods to analyze the stability of these structures, offering a deeper understanding of their energy landscapes and the factors that contribute to their stability. To expand the scope of my investigations on thermodynamic stability, I also employed hybrid sampling techniques to explore the formation of quasicrystal approximants. This approach allowed me to describe and analyze these approximants, which previously could only be achieved through quantum mechanical simulation methods. By bridging the gap between classical and quantum approaches. To provide an overview of the areas where my research has made valuable contributions, I present a comprehensive figure that addresses some general questions and highlights the insights gained from my investigations. This figure synthesizes the key findings and serves as a visual representation of the impact of my research on the understanding of aperiodic order and its physical properties.



Sarthak Jadhav, "Accurate melt pool volume calculations for LASER additive manufacturing"

Laser additive manufacturing (LAM) has emerged as a pivotal technology in material processing, necessitating precise control of the melt pool for ensuring part quality. Traditional computational models often simplify the melt pool dynamics by assuming a constant volume for the participating particles, which leads to discrepancies between simulated and actual behaviors. Addressing this gap, our research develops a sophisticated volumetric calculation model using a Temperature-Responsive Smoothed Particle Hydrodynamics (SPH) technique. This novel approach modifies the volume of SPH particles according to their thermal state, employing a set of experimentally-derived relationships that reflect the material's response to temperature variations encountered during LAM. Our model incorporates a heat transfer and fluid flow algorithm that dynamically updates particle volumes based on local temperatures, capturing the expansion and contraction effects as well as latent volume changes that are inherent to the melting and solidification processes. By integrating a temperature-volume coupling into the SPH framework, the model promises a more accurate representation of the melt pool geometry and thermodynamics.

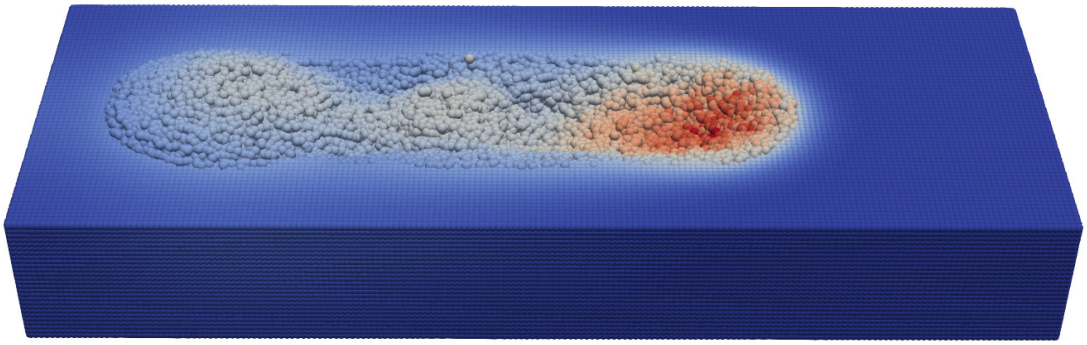


Figure: Temperature profile of metal block during laser melting.

Federico Tomazic, "Modelling particle aggregation and assembly into optimal structures"

Nanoparticles can be used as building blocs to assemble robust functionalized suprastructures, with a plethora of applications, including nanophotonics and chromatography. The interactions between nanoparticles that lead to the self-assembly into suprastructures are complex, since they depend on the interplay of particle shape and surface chemistry. In this project, we use computational techniques to relate the interactions between building blocs to the formation of a desired self-assembled suprastructure, in the frame of the Collaborative Research Centre Design of Particulate Products.

By modeling the crystallized polymeric ligand bundles on a nanoparticle as sphere-rod model, we show the effect of the particle shape on the self-assembly. By coarse-grained molecular dynamics simulations, we find that the dimension of the ligand bundle can control the shape of the self-assembled structures.

When constrained in a shrinking confinement by spray drying or double emulsion, spherical nanoparticles self-assemble into decahedral and icosahedral structures. The formation of ordered primary particles layers in proximity of the confinement constitutes an intermediate step in the crystallization process and causes the appearance of structural color. By event driven molecular dynamics simulations in a hard spherical confinement, we study the crystallization path of supraparticles, and in particular how the ordered layers on the surface of the confinement affect the final order in the supraparticles.

To model the interaction between anisotropic nanoparticles, we must 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 retrieving the precomputed potential to observe how different potentials affect the self-assembly.

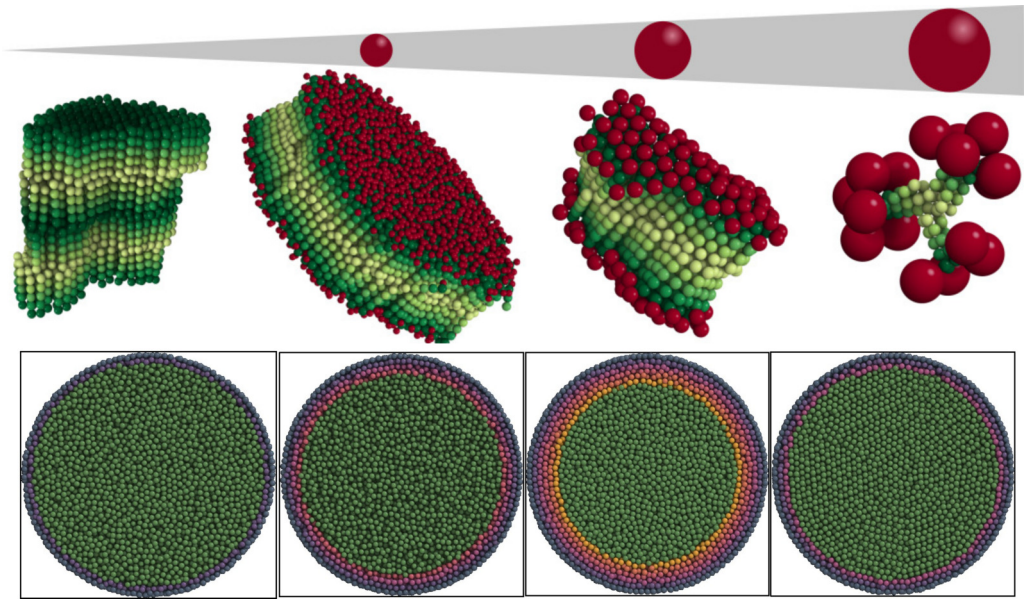


Figure: Self-assembly of nanoparticles into optimal structures. Top: Rigid polymer bundles. The ratio of the size of the bundle compared to the nanoparticle controls the shape of the self-assembled structure. Bottom: Evolution of layers formation for particle in spherical confinement.

Kaijie Zhao, "Strain field analysis of five-fold twinned gold nanoprisms"

Five-fold twinning on alternate coplanar twin planes in nano-particles creates unique morphology and symmetry . Such particles are composed of five equisized subunits, which join each other via twin planes along 111, enclosing an angle of 72° . Since two 111 planes in a relaxed fcc structure enclose an angle of 70.53°, the formation of five-fold twins inevitably introduces strain (by deformation or defects formation). Our collaborators in Rice University Houston have recently synthesized the five-fold twinned gold nanoprisms with own flat surfaces in 110. Based on 4D-STEM, they have observed deviation of strain distribution from theoretical computation. And our sim is to understand the inhomogeneous distribution between different subunits through simulation. We use HOOMD-blue to perform equilibration at various temperatures. Different features, such as imbalanced subunit size and defects are introduced to the perfect prism to evaluate their influence upon the strain distribution. So far we have validated the ideal strain distribution and bring up the assumption that such inhomogeneity arises mainly due to the presence of dislocations.

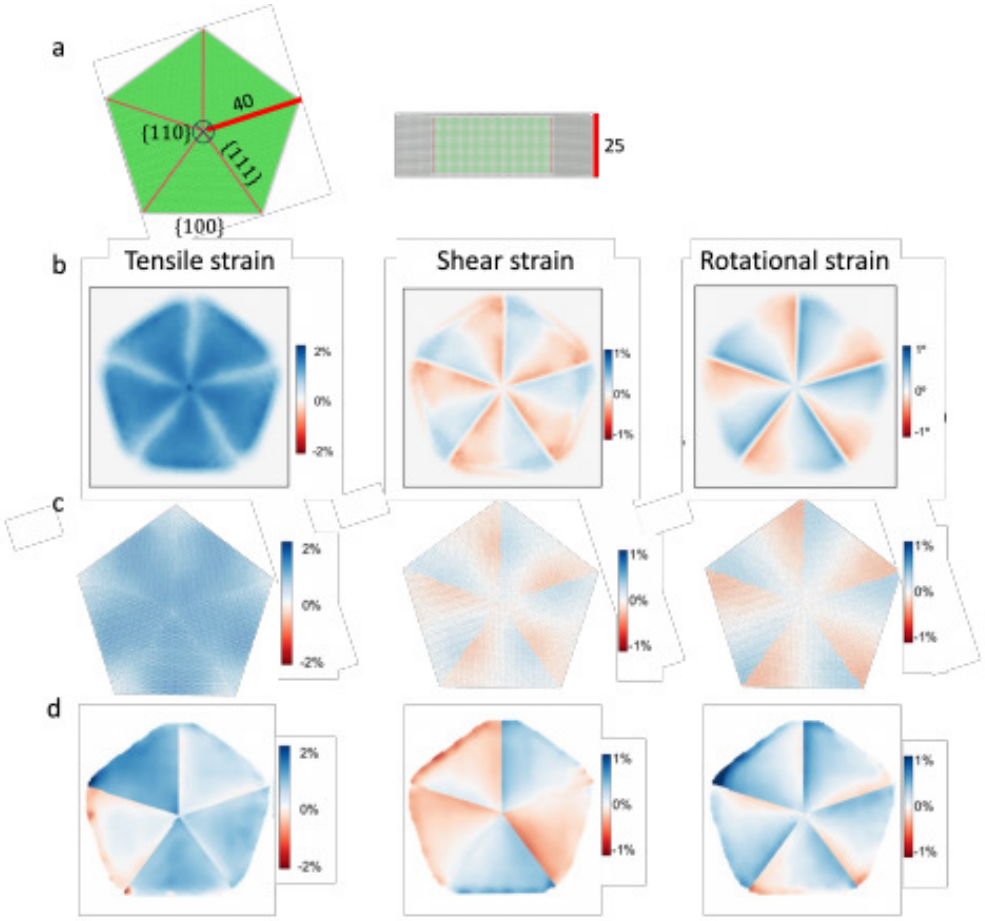


Figure: Structure and strain computation of five-fold twinned prisms. a) Projections of the single crystal prism and the corresponding lattice planes. Green: bulk FCC crystal; Red: twin grain boundaries. b) Ideal strain maps from experimental computation. c) Strain maps of perfect prism after relaxation from simulation. d) Strain maps for one synthesized crystal at room temperature.

Navid Panchi, "Efficient and acalable implementation of Debye scattering"

In materials development, the atomic-scale characterization plays a crucial role, and powder sample scattering emerges as a valuable tool due to its ability to provide precise statistical insights across a multitude of crystals. X-ray and neutron scattering data analysis involves modeling experimental powder diffractograms and pair distribution functions. Achieving high accuracy in these calculations is essential for capturing intricate features in material structures. Various mathematical formulations have been introduced, with the Debye scattering equation (DSE) gaining prominence in the past decade for its comprehensive atomistic materials description.

Despite the DSE's potential, its practical application is constrained by the quadratic increase in solution complexity with the number of atoms (N). While existing codes can efficiently solve the DSE for a single atomistic model in a reasonable time, the analysis of experimental data demands solving the DSE for thousands of models. There is a pressing need for a portable and efficient software application to facilitate materials research by handling the intricacies of powder scattering data.

The ongoing research project centers on the development of a efficient and scalable software solution for the Debye scattering equation (DSE). The primary objective is to create a tool that not only demonstrates robust performance but is also scalable, enabling its deployment on supercomputer clusters. A key aspect of the project involves optimizing the utilization of accelerator hardware, specifically GPUs, to enhance computational efficiency.

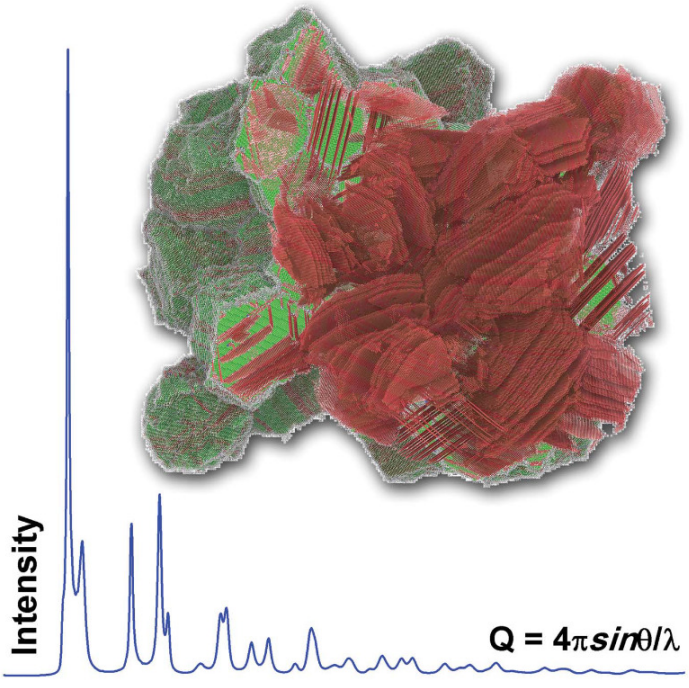
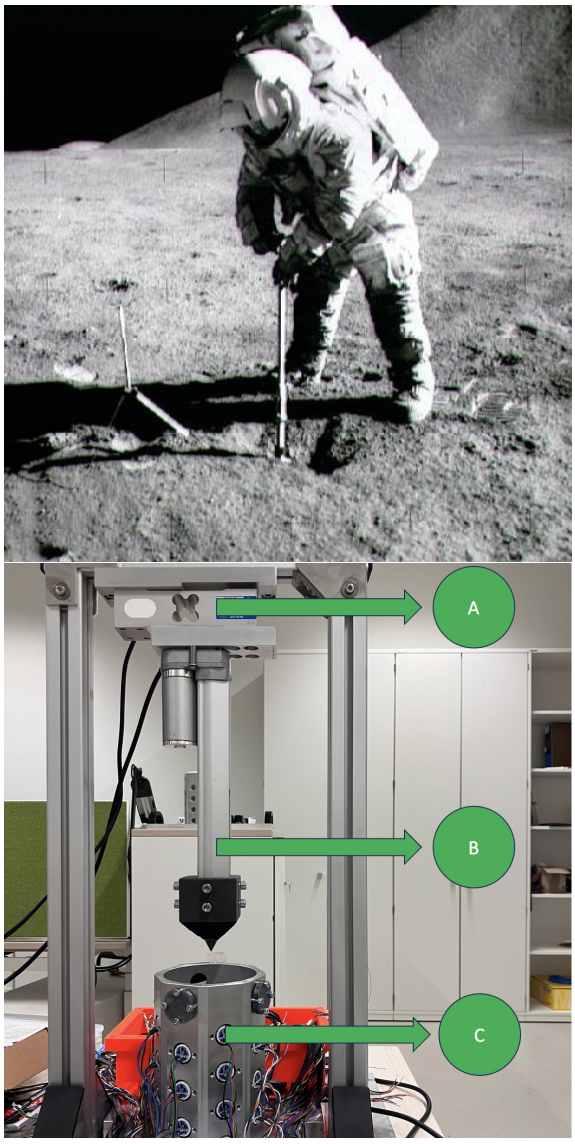


Figure: Simulated diffraction profile. A polycrystalline sample (top) with the corresponding diffraction pattern (bottom).

Geovane de Jesus Rodrigues, "Granular rheology in space"

With human returning to the Moon in the near future, it is important to understand the mechanics of Lunar soil, named regolith. In particular, we want to understand the effect of gravity on a typical test used to probe the geotechnical properties of a soil: penetration test. We reproduce a penetration test in a container filled with granular material. The pressure on the wall and at the bottom of the container, as well as the force experienced by the probe while penetrating the soil, are recorded. Two probes are tested to penetrate the soil: a stiff conical probe and a flexible linear probe. The experiment is conducted under hypergravity at the Large Diameter Centrifuge (LDC, ESA/ESTEC, Netherlands), and under low- and microgravity at the Bremen drop tower (ZARM, Germany).



Utku Canbolat, “Fractures in granular matter - Theory and large-scale simulations”

In the field of granular material fracture analysis, two primary particle-based approaches are recognized: the particle replacement method and the bond-breaking method, each with unique benefits and limitations in terms of computational efficiency and accuracy. Our research introduces a novel particle-breaking algorithm that aims to strike a balance between these factors. This algorithm incorporates both multisphere representation and image data (e.g. STL files) to enhance accuracy while reducing computational demands. When a fracture occurs, the algorithm splits the image data, allowing for the reconstruction of multispheres from the fragments. This method has several key advantages: it maintains the volume and mass of particles, retains their morphological information, and enables multiple fractures without sacrificing accuracy.
Our methodology is designed for scalability, capable of handling over 100,000 complex-shaped particles in various scientific and industrial scenarios within a reasonable timeframe. We chose YADE, an open-source discrete element method software, for our platform due to its adaptability and efficiency. For multisphere generation, we use PyCLUMP, which is the Python version of the CLUMP library, developed at the MSS. PyCLUMP library enables the multisphere creation in YADE. For simulating fractures, we employ the combined Mohr-Coulomb-Weibull criterion for its balance of computational efficiency and accuracy. The model calculates fracture probability by assessing the stress on each clump and deciding on splitting based on the Mohr-Coulomb curve threshold.
Testing on single and multi-particle systems has shown promising results, although some discrepancies in fragmentation methods were noted and are being addressed through ongoing modifications. Future enhancements include a refined mesh splitter and the inclusion of dynamical fracture features for applications like ball-milling processes. Additionally, we plan to integrate wear effects and heat transfer mechanisms (conduction and radiation) into the model, aiming to achieve a complete multiphysical model.

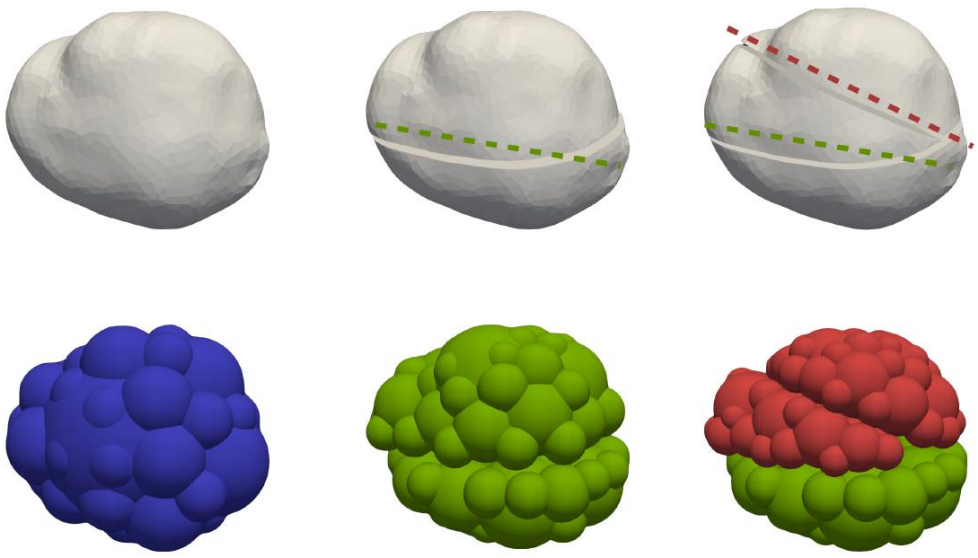
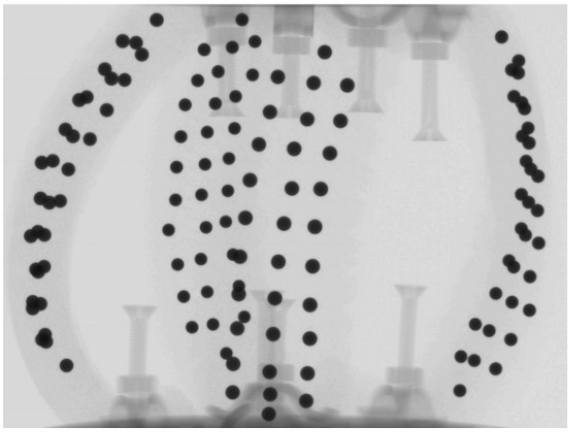


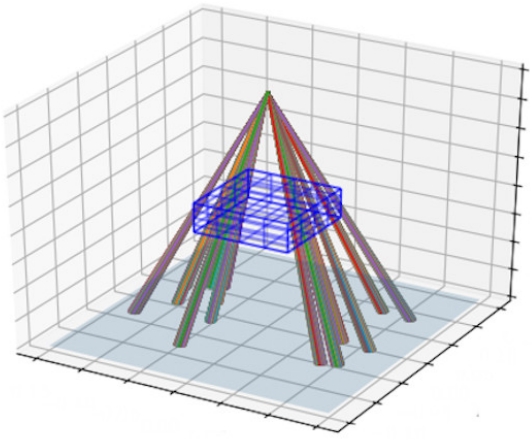
Figure: The upper images show the STL data, the the bottom images are their corresponding multisphere representation. The dashed lines indicate the fracture planes.

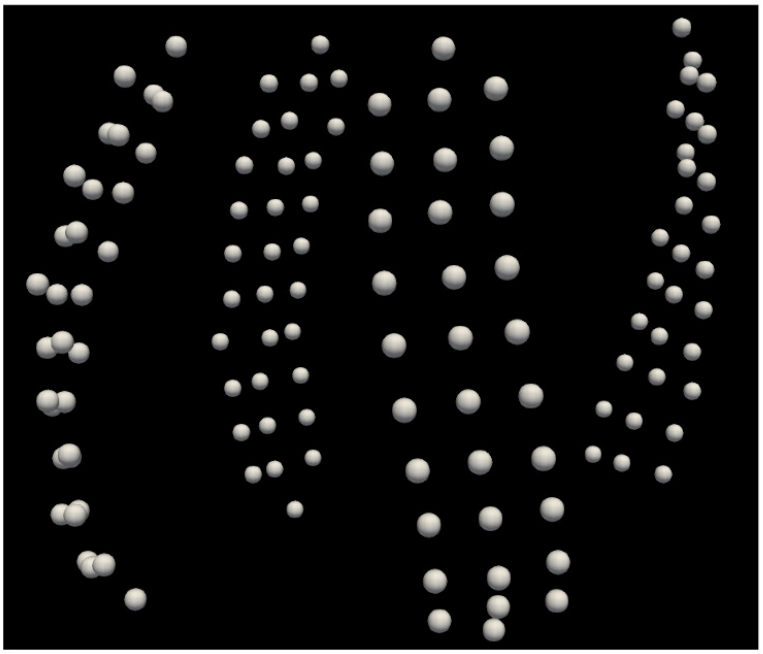
Atharva Pandit, "Multi-axial X-ray computed tomography"

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.







6. Teaching Activities

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- **Simulation Granularer und Molekularer Systeme**
  Lecturer (Prof. Thorsten Pöschel, Prof. Michael Engel)
  Lab session (Federico Tomazic)

- **Multiphase Flows**
  Lecturer (Prof. Thorsten Pöschel)

- **Multiscale Simulation Techniques**
  Lecturer (Prof. Thorsten Pöschel)

- **Granular Matter - MSS Seminar**
  Lecturer (Prof. Thorsten Pöschel)

- **Data Science for Engineers**
  Lecturer (Prof. Michael Engel)
  Exercise (Navid Panchi)

- **Pre-course on Linux and Python (Block Lecture)**
  Lecturer (Prof. Michael Engel, Dr. Carlos Lange Bassani)

- **Messtechnik 2 - Messmethoden und Analytik**
  Lecturer (Dr. Achim Sack)
  Exercise (Nicolas Pechler)

- **Digitale Bildverarbeitung**
  Lecturer (Dr. Achim Sack)

- **Self-Organization Processes**
  Lecturer (Dr. Carlos Lange Bassani, Dr. Giulia Magnabosco, Prof. Robin Klupp Taylor)

- **Basics in Computational Materials Science and Process Simulation 1**
  Lecturer (Prof. Michael Engel, Prof. Andreas Bück)

- **Discrete Element Simulations**
  Lecturer (Dr. Vasileios Angelidakis)

- **Granular Matter and Applications**
  Lecturer (Dr. Sudeshna Roy)

- **Scanning and Printing in 3D**
  Lecturer (Dr. Olfa D'Angelo, Dr. Patric Müller)
  Exercise (Dr. Patric Müller)
  Lab session (Dr. Olfa D'Angelo, Dr. Patric Müller, Felix Buchele)

- **Artificial Intelligence and Machine Learning in Engineering (Künstliche Intelligenz und maschinelles Lernen im Ingenieurwesen)**
  Lecturer (Dr. Patric Müller, Holger Götz)
  Exercise (Dr. Patric Müller, Holger Götz)
  Lab session (Dr. Patric Müller, Holger Götz)

- **Computeranwendungen in der Verfahrenstechnik I**
  Lecturer (Prof. Thorsten Pöschel)
  Exercise (Felix Buchele)

- **Scientific Computing in Engineering**
  Lecturer (Prof. Thorsten Pöschel)
  Exercise (Felix Buchele)

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

13.01.2023	Thorsten Pöschel	*Polydirectional stability of granular matter*
20.01.2023	Navid Panchi	*Bayesian optimization for diffraction profile modelling*
27.01.2023	Holger Götz	*Granular jamming beam: Influence of particle properties*
03.02.2023	Carlos Lange Bassani	*Simulation of nanocrystal growth with Kinetic Monte Carlo: I. Method and implications*
10.02.2023	Nicolas Pechler	*Calibration of multiaxis CT devices*
17.02.2023	Carlos Lange Bassani	*Simulation of nanocrystal growth with Kinetic Monte Carlo: II. Kinetic Wulff shapes*
24.02.2023	Michael Engel	*Self assembly of tetrahedra: 14 years of research*
03.03.2023	Sudeshna Roy	*Characterization of shear zone for mixtures of soft and hard granular materials*
10.03.2023	Aswathy Muttathukattil Narayanan	*Self-limiting assembly in systems of bipods: Role of geometrical frustration*
17.03.2023	Hongyi Xiao	*Jamming and free surface deformation enable reciprocal swimming in granular materials*
17.03.2023	Angel Santarossa	*Effect of particle size on the suction mechanism in granular grippers*
24.03.2023	Olfa D'Angelo	*Granular rheology in space: to the Moon—and back*
31.03.2023	Adriana Enriquez Florat	*Acoustic propulsion of active macroparticles*
14.04.2023	Vasileios Angelidakis	*Apparent cohesion of interlocked granular metamaterials with cohensionless particles*
21.04.2023	Meysam Bagheri	*From microscopic clues to macroscopic insights: Exploring a (potential) predictor and quantifier of crack onset in drying suspensions*
28.04.2023	Deniz Fakioglu	*Automation of an electrical impedance tomograph by using robotics and image processing*
05.05.2023	Chandrew Aseervatham	*The Dzhanibekov Effect*

12.05.2023	Atharva Pandit	*Reconstruction & velocimetry in muti-axial X-ray computer tomography*
19.05.2023	Yazan Alzaghah	*Electrode design and testing of an electrical impedance tomograph*
26.05.2023	Utku Canbolat	*Novel fracture model in DEM simulations with complex-shaped particles*
02.06.2023	Felix Buchele	*Towards a mesoscopic model for complex catalytic reactions*
09.06.2023	Carlos Andres	*A better algorithm for the stable integration of non-spherical particle rotations*
16.06.2023	Federico Tomazic	*Coarse-grained simulations of ligand-tethered nano-plates*
23.06.2023	Vasileios Angelidakis	*DEM simulation of the powder application in additive manufacturing*
30.06.2023	Sahib Abdullayev	*Handling imbalanced data in machine learning for process monitoring*
30.06.2023	Isabella Schneider	*Simulation of porous medium evolution of gas clathrate hydrates*
07.07.2023	Carlos Andres	*Development of a DEM-Based model for the simulation of fractures in brittle materials*
14.07.2023	MSS	*Presentations of video and image contributions to DEM9 conferance*
28.07.2023	Holger Götz	*Granular convection in zero gravity*
04.08.2023	Kaijie Zhao	*Prediction of physical parameters from simulated 2D dendritic morphology via machine learning*
29.09.2023	Laureano Ortellado	*Tomographic imaging-based finite element analysis of 3D mixed-mode crack front*
06.10.2023	Yasmin Gerlach	*Tomographische Analyse von Pigmentsuspensionen in porösen Strukturen für kosmetische Anwendungen" (Tomographic analysis of pigment suspensions in porous structures for cosmetic applications)*
13.10.2023	Sudeshna Roy	*Powder spreading of irregular particles with thermal properties*
20.10.2023	Diksha Kadre	*Identification of crystal polymorphs of natural gas hydrates using machine learning*
27.10.2023	Frederik Keil	*Random packing of Meissner tetrahedra*

03.11.2023	Carlos Lange Bassani	*Nanocrystal assemblies: Current advances and open problems*
10.11.2023	Geovane de Jesus Rodrigues	*Influence of Fe in a CoNi-based superalloy*
08.12.2023	Huzaif Rahim	*Granular Weissenberg Effect*
15.12.2023	Patric Müller	*Physics of Nuclear Magnetic Resonance*
22.12.2023	Meysam Bagheri	*Cascading cracks in drying suspensions*

7. 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.

- **Sahib Abdullayev, "Handling imbalanced data in machine learning for process monitoring"**

  I have carried out a collaborative Master Thesis project with MSS (FAU, Erlangen) and a specialty chemicals company Evonik (Essen). In this work, I have developed an algorithm to handle imbalanced data for chemical process monitoring. The developed algorithm

manipulates data distribution and allows the training of artificial neural network models without modifications to the training algorithm of the model.

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

  Granular materials are ubiquitous in our everyday life. Yet, some behaviors of granular media continue to surprise us, and a theory predicting granular flows from first principles is still missing. When the granular materials are compressed or sheared, they can change from a flowing fluid-like state to a rigid solid-like state. This change is called the jamming transition. The previous research shows that the granular packing fraction at the jamming point is lower in microgravity than on Earth. This small change in jamming packing fraction could influence the handling of granular materials in microgravity. To investigate this question, we probed the jamming point in microgravity, provided by drop tower Bremen. Additional discrete element method simulations were also performed to complement the practical experiments. Our experiments showed that the average jamming packing fraction in microgravity is 0.0212 lower than on Earth. Simulation results showed that, for a system with 0 friction coefficient, the average jamming packing fraction in microgravity and Earth gravitational acceleration are 0.6032 and 0.6142. For a system with a 0.5 friction coefficient, the average jamming packing fraction in microgravity and Earth's gravitational acceleration are 0.5336 and 0.5448.

- **Yasmin Gerlach, "Tomographic analysis of pigment suspensions in porous structures for cosmetic applications"**

  My thesis was a cooperation between MSS and Faber- Castell Cosmetics with the title: Tomographic analysis of pigment suspensions in porous structures for cosmetic applications Goal of this thesis was to investigate cosmetic pigment inks that cause problems with certain pigment combinations. The ink ist transportet inside of the pen with capillary forces. If certain pigment combinations or concentrations are used the ink cannot flow into the tip of the pen but yet the reason of this phenomenon is not known. Therefore CT-meassurements of different modified inks were made to see how the ink behaves inside of the structures and draw conclusions from the results.

- **Nadja Al Akkam, "Rheology of lunar regolith and its simulants"**

  We investigate the rheology of Lunar regolith simulant, a granular material produced to mimic the sand covering the Moon, known as regolith. Most information available about the flow-behavior of 39;real39; regolith, as found on the Moon, comes from NASA's Apollo missions (1963 - 1972). To study the slope stability, trench tests were conducted by astronauts. We propose an experiment, the vertical slope collapse experiment, which is based on the trench test conducted on the Moon. We conduct this experiment in air and in vacuum (20 mbar). As the Lunar environment is under high vacuum, devoid of air and gaseous water, we want to understand the effect of ambient air and water on the collapse and slope of regolith simulant. The experimental set-up consists of a box filled with granulate; the front wall is lowered progressively, uncovering a vertical slope of granular material, held by cohesion. Eventually, when a critical height is reached, the material fails and forms a slope. Repeated material failures are captured by two cameras, which provide a top and front view. By image analysis, we obtain the angle of repose versus slope height. We use the Mohr-Coulomb framework to analyze the results to obtain the parameters cohesion and internal friction angle from the vertical slope collapse height and angle of repose. Both parameters are used to describe the material and are compared with results collected for regolith on the Moon.

- **Prashanth Prakash Kamath, "Simulation of critical settling velocity of gas hydrate slurries"**

  This thesis addresses the significance of gas hydrates, particularly their role in causing plugging issues within offshore hydrocarbon production flowlines.Critical settling velocity models developed for materials with high solid-to-liquid density ratios do not correspond to gas hydrate scenarios. To bridge this research gap, this work introduces an Euler-Euler approach to simulate the stability of gas hydrate slurries.This research represents a significant step forward in enhancing the ability to predict and mitigate plugging risks associated with gas hydrates in hydrocarbon production, ultimately contributing to improved operational efficiency and safety in the industry.

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's tetrahedra are three-dimensional convex bodies of constant width, similar to spheres. This means that if clamped between two parallel planes touching the surface, the distance between them is always constant. But in contrast to spheres, Meissner tetrahedra have an orientation that stems from their construction. In this bachelor thesis a new algorithm was developed to describe the positions and orientations of the individual Meissner tetrahedra within a packing from tomographic data.

- **Valentin Hartinger, "Can you hear the temperature of water?"**

  My bachelor's thesis investigated the correlation between the sound of water and temperature through two experimental approaches. The initial experiment revealed distinctive patterns tied to bubble formation and cooking process status. The second experiment observed changes in sound intensity and frequency peaks with changing water temperatures. Through this, a connection between sound characteristics and water density was found.

- **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.

Programming Projects

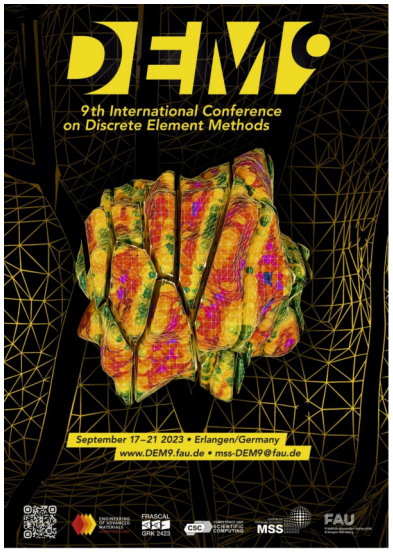
- **Navid Panchi, "Hybrid network simulation"**

  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.

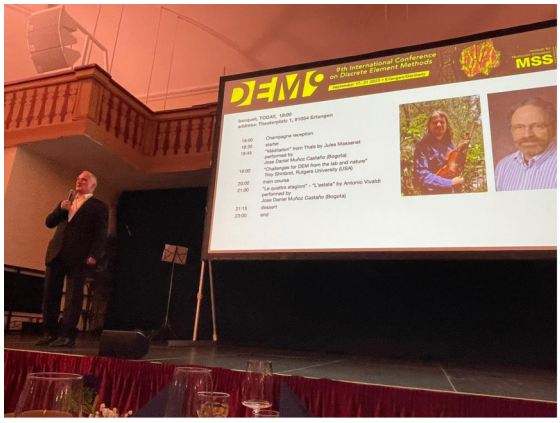
8. Service for the Scientific Community

MSS hosted the 9th International Conference on Discrete Element Methods

From September 17, 2023 to September 21, 2023, our institute proudly hosted the 9th International Conference on Discrete Element Methods (DEM9) in Erlangen. This prestigious event, a frontrunner in the realm of discrete element simulation, focused on the most recent developments in simulating particulate systems through discrete element methods. Topics of discussion included coupled simulations, the fragmentation of particles, the dynamics of non-spherical particles, and the intricacies of multiscale and multiphase systems. The DEM series, with a history spanning over three decades, is renowned in the field. Previous conferences were held in various locations worldwide.

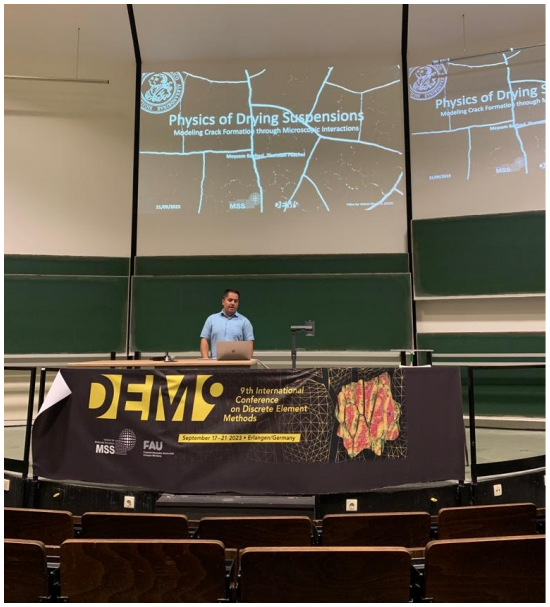


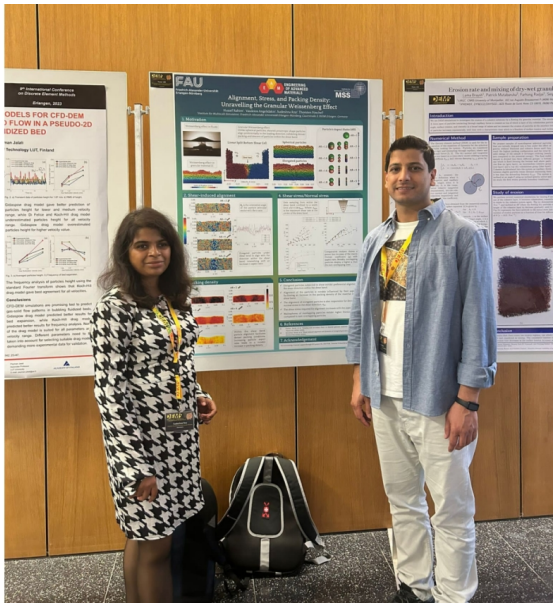
The conference began on September 18, attracting scientists from across the globe. The opening plenary session featured a talk by Mikio Sakai, who discussed the essential technologies in development of the DEM-based digital twin.



The conference dinner took place in the evening, followed by a talk by Troy Shinbrot on "Challenges for DEM from the Lab and Nature".

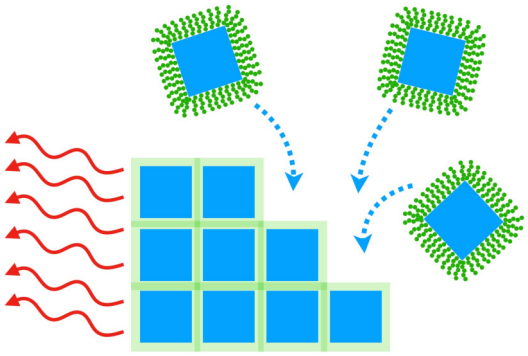
Spanning four days, the conference included 17 sessions. Additionally, it featured mini-symposiums and poster presentations, creating a vibrant arena for fruitful scientific discussions.

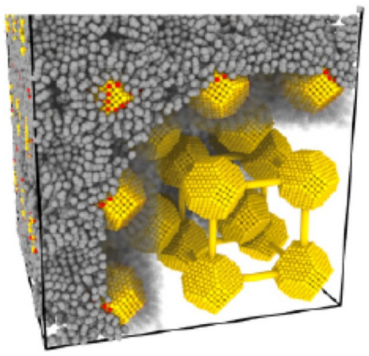




MSS researchers co-organized a conference and workshop at the Kavli Institute of Theoretical Physics

In the period Mar 27, 2023 — May 19, 2023, Alex Travesset (Iowa State University), Michael Engel (MSS), Eran Rabani (University of California Berkeley), Monica Olvera de la Cruz (Northwestern University), and Laura Na Liu (Universität Stuttgart) coordinated a scientific program at the Kavli Institute of Theoretical Physics (KITP), University of California, Santa Barbara on the topic of nanoparticle self-assembly. The program consisted of an eight-week workshop and culminated in a one-week conference. the workshop entitled "Nanoparticle Assemblies: A New Form of Matter with Classical Structure and Quantum Function", brought together more than sixty eminent scientists from diverse communities: physicists, chemists and material scientists in an effort to address the emerging fundamental questions and long-term prospects of this young field. It developed collaborative efforts in the areas of programmable assembly, structure prediction, inverse methods, electronic properties and new functional materials. The conference entitled "Structure Design and Emerging Phenomena in Nanoparticle Assemblies: What's next?" provided a coherent view of the current state of the field. The goal was to catalyze the development of new methods, both theoretical, computational and experimental, and define the basic science.





Materials whose elementary building blocks are nanoparticles with dimensions between a few and hundred nanometers, such as nanocrystals and colloids, instead of atoms or molecules, provide a new form of matter, with many properties, both in structure and function, that are not achievable with traditional materials. This raises a number of new fundamental questions that the conference aimed to address:

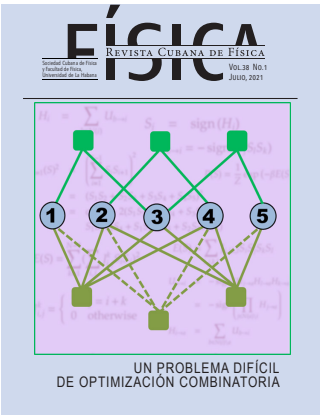
- What is the minimal physical description at the nanoscale?
- How to discover new assemblies?
- What are the effects or properties for these new materials and the characterization of equilibrium and metastability?

These questions underscore the innovative and exploratory nature of the conference, seeking to push the boundaries of current scientific understanding in nanoparticle self-assembly. The discussions and collaborative efforts initiated here aim to lay the groundwork for future breakthroughs in the field.

Editorial Boards

Revista Cubana de Física
Cuban Physical Society (SCF)

`www.revistacubanadefisica.org`



Prof. Thorsten Pöschel
Senior Editor since 2014

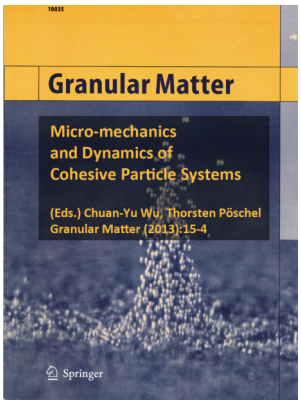
Computational Particle Mechanics
Springer/Nature

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

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

Granular Matter
Springer/Nature

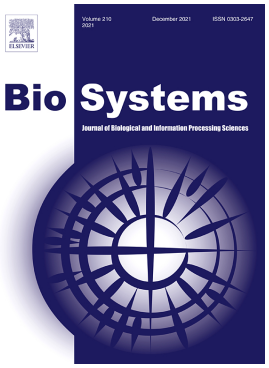
`www.springer.com/journal/10035`



Prof. Thorsten Pöschel
Editor since 2006

Biosystems
Elsevier

`www.journals.elsevier.com/`
`biosystems`



Prof. Thorsten Pöschel
Associate Editor since 2003

Guest Editor

Dr. Sudeshna Roy, a postdoctoral researcher at MSS, has been appointed as a guest editor for the journal Granular Matter. She will be an editor for the special issue focusing on the Simulation of Particle Processes in Additive Manufacturing.

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.

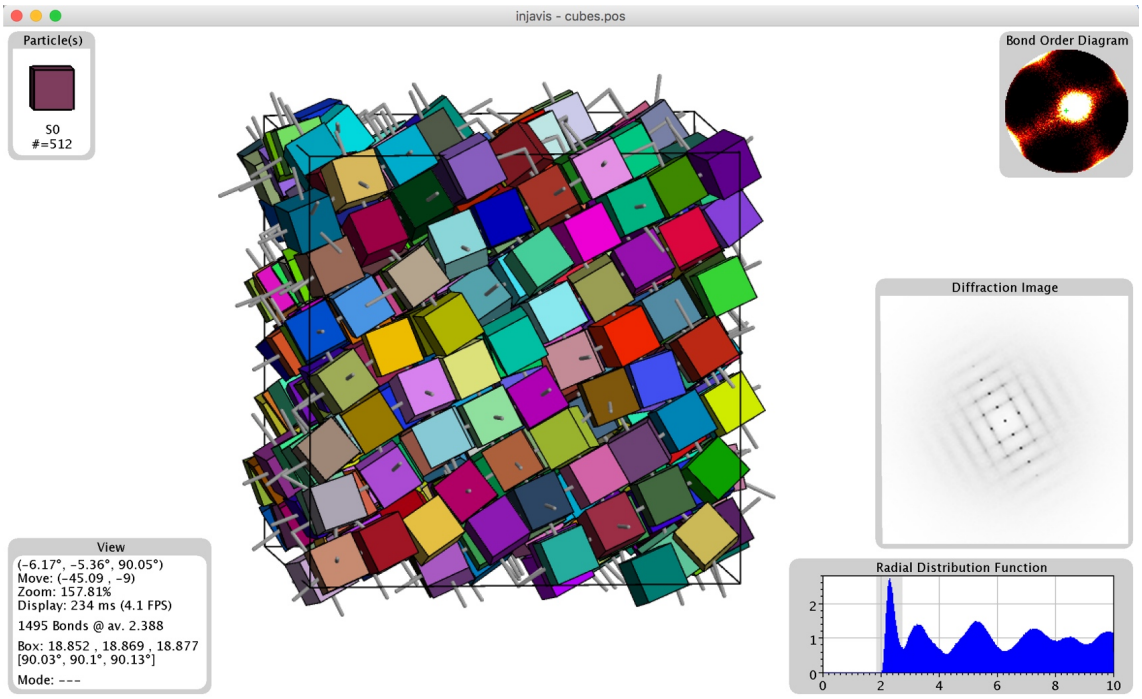


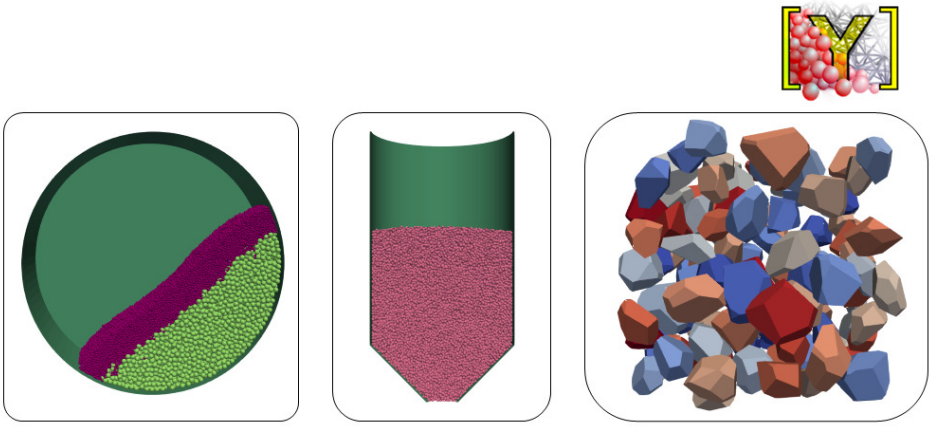
Figure: Screenshot of injavis showing a snapshot of a simulation of hard cubes. (top left) particle module; (top right) bonds module; (middle right) diffraction module; (bottom left) view module; (bottom right) RDF module

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.

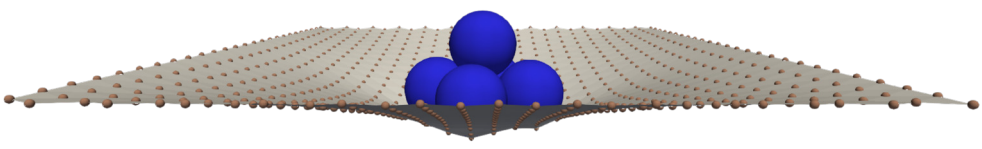
Yade comprises a wide range of contact laws, for dry and wet granular materials, along with various classes for non-spherical particles, including polyhedra, potential particles, flexible spheropolyhedra and flexible surface elements, concave non-spherical particles using the LS-DEM, just to name a few. 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.



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`



9. University Self-Administration

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
Interdisciplinary Center for Nanostructured Films, Cooperative Head	Prof. Thorsten Pöschel
Scientific Committee of the BayWISS Joint Academic Partnership Energy (Wissenschaftlicher Ausschuss des BayWISS Verbundkollegs Energie)	Prof. Thorsten Pöschel
Habilitation Committee of the Technical Faculty (Kommission für Habilitationen und wissenschaftlichen Nachwuchs)	Prof. Thorsten Pöschel
Council of the Department for Chemical and Biological Engineering	Prof. Thorsten Pöschel Dr. Patric Müller
Recognition Committee at the Government of Swabia according to the Regulation for the Regulation of Compensation Measures in Accordance with the Bavarian Engineering Act (Anerkennungsausschuss bei der Regierung von Schwaben nach der Verordnung zur Regelung von Ausgleichsmaßnahmen nach dem Bayerischen Ingenieurgesetz) (BayIngAMV)	Prof. Thorsten Pöschel

Council of the Faculty of Engineering (Fakultätrat)	Prof. Michael Engel
Study Grants Committee (Studienzuschusskommission)	Prof. Michael Engel
Executive Board Member and Focal Subject Head for Computational Materials Science and Process Simulation, Advanced Materials and Processes (MAP)	Prof. Michael Engel
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
Admission Committee for Master's Students in Clean Energy Process in the Department for Chemical and Biological Engineering	Dr. Sudeshna Roy
PR-Team of the Department for Chemical and Biological Engineering	Ulrike Hansl

10. Awards

MSS postdoctoral researcher won the best poster presentation award at International Conference on Gas Hydrates (ICGH10)

Dr. Carlos Lange Bassani received the best poster presenation award at International Conference on Gas Hydrates (ICGH10), held 9 to 14 of June 2023 in Singapore. The work is titled "A new approach for gas hydrate slurry flow based on a multiscale model for multiphase flow". Carlos is currently a postdoctoral fellow at the Institute for Multiscale Simulation.


ICGH10
9 - 14 July 2023 SINGAPORE

10th INTERNATIONAL CONFERENCE ON GAS HYDRATES (ICGH10)

9-14 JULY 2023
Singapore

NUS National University of Singapore

AIChE Singapore Local Section

BEST POSTER AWARD

Awarded to

Carlos L. Bassani, Rigoberto E. M. Morales, Ana Cameirão, Jean-Michel Herri, Amadeu K. Sum

For the Paper

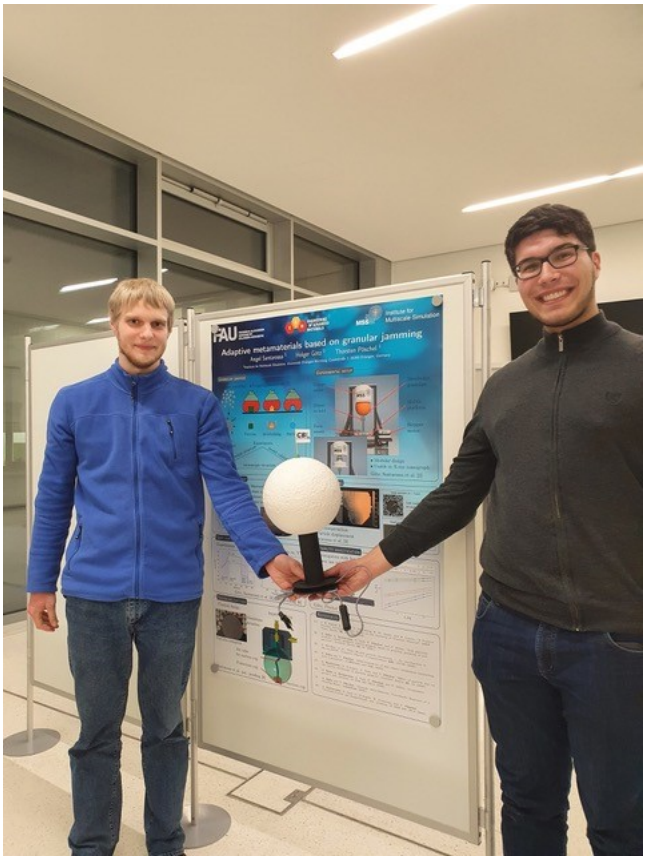
A New Approach for Gas Hydrate Slurry Flow based on a Multiscale Model for Multiphase Flow

PROF. PRAVEEN LINGA
NUS SINGAPORE
CHAIR, ICGH10

Issued on:
14/07/2023

PROF. I. A. KARIMI
NUS SINGAPORE
CO-CHAIR, ICGH10

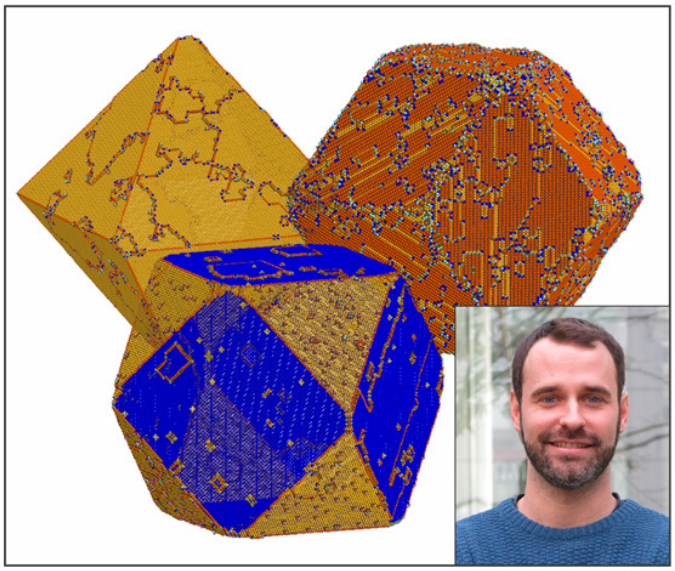
MSS doctoral researchers won the best poster award in CBI symposium
Angel Santarossa and Holger Götz received the best poster award among 50 scientists at the CBI symposium on February 2, 2023. The poster is titled "Adaptive metamaterials based on granular jamming".



Sudeshna Roy has been awarded the FFL Habilitation Fellowship
Dr. Sudeshna Roy, a postdoctoral researcher at our institute, has been awarded Förderung von Frauen in Forschung und Lehre (FFL) Scholarship as part of the Bavarian Equal Opportunities Sponsorship program. This scholarship is dedicated to outstanding female doctoral candidates in the final stages of their doctoral degree and young female researchers who aspire to pursue an academic career.

Carlos Lange Bassani was awarded the EAM Starting Grant 2023

Dr. Carlos Lange Bassani was awarded the EAM Starting Grant 2023 with the project entitled "Kinetic Pathways of Lower Symmetry Nanocrystal Habits". The EAM Starting Grant supports scientific independence of postdoctoral researchers and junior group leaders, and promotes applications to larger funding projects at the German and European levels, such as the DFG Emmy Noether Programm and the ERC Starting Grant.



Awards at DEM9

At the 9th International Conference on Discrete Element Methods (DEM9), Meysam Bagheri, Nicolas Pechler and Carlos Andres del Valle were honored with the "Best Image", "Best Movie" and "Best Poster" awards, respectively.

From left to right, Meysam Bagheri, Nicolas Pechler, and Carlos Andres del Valle.

Meysam Bagheri's artwork in 2024 EAM Calendar
The artwork submitted by Meysam Bagheri for the DEM9 art contest has been selected for inclusion in the 2024 Engineering of Advanced Materials (EAM) calendar. This piece will be highlighted as the image for the month of March in the calendar.

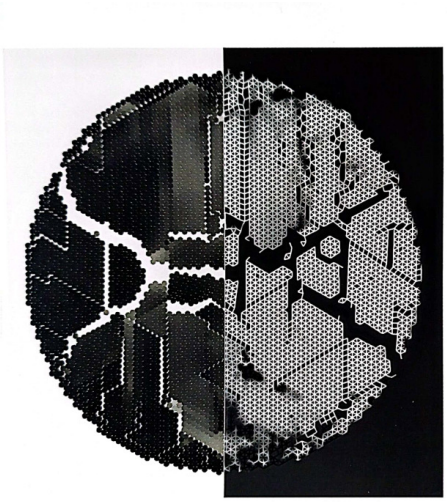
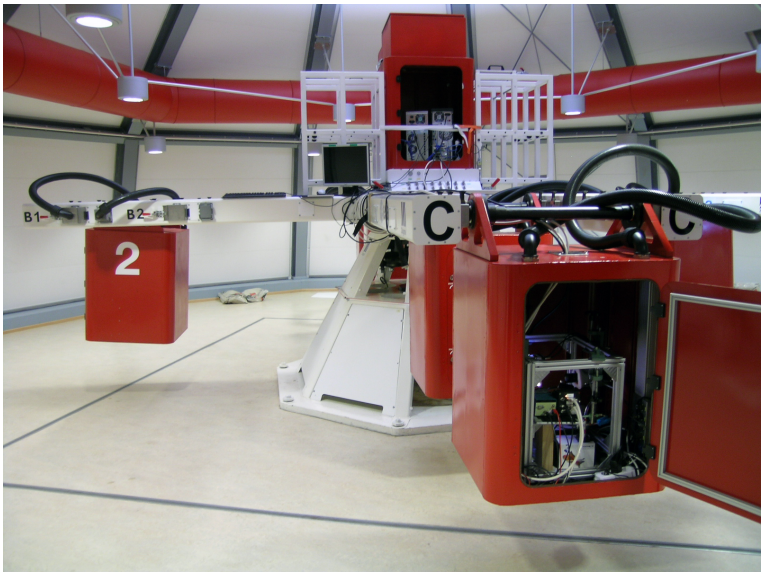


Illustration of crack pattern emerging as a suspension dries. DEM9 art contest.
(Meysam Bagheri, Multiscale Simulation)

March
2024

Mo	Tu	We	Th	Fr	Sa	Su
26	27	28	29	1	2	3
4	5	6	7	8	9	10
11	12	13	14	15	16	17
18	19	20	21	22	23	24
25	26	27	28	29	30	31

Nadja Al Akkam and Dr. Olfa D'Angelo were awarded the International Visiting Scholarship
Nadja Al Akkam and Olfa D'Angelo were awarded the International Visiting Scholarship for their project on the rheology of Lunar regolith. Nadja Al Akkam is doing her Master's project under the supervision of Olfa D'Angelo; both will be going to the European Space Agency's Large Diameter Centrifuge at ESTEC in the Netherlands.



Cover image of Soft Matter journal
The journal Soft Matter chose our submission to be featured as the cover image. This particular image is associated with the paper titled "Macroscopic analogue to entangled polymers," authored by Leopoldo Gómez, Nicolas García, and Thorsten Pöschel.

Michael Engel among top 2% most widely cited scientists
Michael Engel, professor at MSS, is among the 2% most cited scientists worldwide in 2022. The study by a team of researchers from Stanford University is based on data extracted from Scopus: `https://doi.org/10.17632/btchxktzyw.6` See also: `https://www.fau.eu/2023/10/19/news/more-than-200-researchers-from-fau-are-cited-particularly-often/#tf`

11. 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)

- "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)
  Applicants: **Prof. Thorsten Pöschel**, Prof. Uwe Hampel, Prof. Antonio Hurtado, Jun.-Prof. Juliana Panchenko

- "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)

- "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)

- "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: **Dr. 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**

- "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**

- "Morphological and Mechanical Characterisation of Granular Metamaterials with Non-spherical Particles"
  Emerging Talents Initiative (ETI)
  Applicant: **Dr. Vasileios Angelidakis**

- " Framework for gas hydrate agglomeration under multiphase flow"
  Emerging Talents Initiative (ETI)
  Applicant: **Dr. Carlos Lange Bassani**

- "Kinetic Pathways towards Lower-Symmetry Nanocrystal Habits"
  EAM Starting Grant 2023/2024 Funded by: FAU Competence Center Engineering of Advanced
  Applicant: **Dr. Carlos Lange Bassani**

- "Granular Rheology in Space (GRIS) "
  German Aerospace Center (DLR) - DLR50WM2342A
  Applicant: **Dr. Olfa D'Angelo**

- “LADA: LASER-Draht-Auftragsschweißen in Schwerelosigkeit”
  German Aerospace Center (DLR) - DLR50WM2357/Laser
  Applicant: **Prof. Thorsten Pöschel**

Cooperations with Industry (Funding)

- “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**

12. Publications

Scientific Papers Published by the MSS in Peer-Reviewed Journals in 2023

1. L. R. Gómez, N. A. García, T. Pöschel, Macroscopic analogue to entangled polymers. *Soft Matter* **19**, 3538–3542, DOI 10.1039/d3sm00148b (2023).
2. H. Götz, T. Pöschel, Granular meta-material: response of a bending beam. *Granular Matter* **25**, DOI 10.1007/s10035-023-01336-9 (2023).
3. H. Götz, T. Pöschel, DEM-simulation of thin elastic membranes interacting with a granulate. *Granular Matter* **25**, DOI 10.1007/s10035-023-01344-9 (2023).
4. A. R. Thornton, T. Plath, I. Ostanin, H. Götz, J.-W. Bisschop, M. Hassan, R. Roeplal, X. Wang, S. Pourandi, T. Weinhart, Recent advances in MercuryDPM. *Mathematics in Computer Science* **17**, DOI 10.1007/s11786-023-00562-x (2023).
5. A. Nabiyan, A. Muttathukattil, F. Tomazic, D. Pretzel, U. S. Schubert, M. Engel, F. H. Schacher, Self-assembly of core–shell hybrid nanoparticles by directional crystallization of grafted polymers. *ACS Nano* **17**, 21216–21226, DOI 10.1021/acsnano.3c05461 (2023).
6. C. F. Mbah, J. Wang, S. Englisch, P. Bommineni, N. R. Varela-Rosales, E. Spiecker, N. Vogel, M. Engel, Early-stage bifurcation of crystallization in a sphere. *Nature Communications* **14**, DOI 10.1038/s41467-023-41001-6 (2023).
7. Y. Wang, J. Chen, R. Li, A. Götz, D. Drobek, T. Przybilla, S. Hübner, P. Pelz, L. Yang, B. Apeleo Zubiri, E. Spiecker, M. Engel, X. Ye, Controlled self-assembly of gold nanotetrahedra into quasicrystals and complex periodic supracrystals. *Journal of the American Chemical Society* **145**, 17902–17911, DOI 10.1021/jacs.3c05299 (2023).
8. N. R. Varela-Rosales, A. Santarossa, M. Engel, T. Pöschel, Granular binary mixtures improve energy dissipation efficiency of granular dampers. *Granular Matter* **25**, DOI 10.1007/s10035-023-01337-8 (2023).
9. A. Bruns, A. A. Spiesberger, A. Triantafyllopoulos, P. Müller, B. W. Schuller, presented at the Proceedings of the 5th Workshop on analySis, Understanding and proMotion of heritAge Contents, DOI 10.1145/3607542.3617351.

10. I. Ostanin, V. Angelidakis, T. Plath, S. Pourandi, A. Thornton, T. Weinhart, Rigid clumps in the MercuryDPM particle dynamics code. *Computer Physics Communications* **296**, 109034, DOI 10.1016/j.cpc.2023.109034 (2024).

11. C. A. del Valle, V. Angelidakis, S. Roy, J. D. Muñoz, T. Pöschel, SPIRAL: An efficient algorithm for the integration of the equation of rotational motion. *Computer Physics Communications*, 109077, DOI 10.1016/j.cpc.2023.109077 (2024).

12. M. Dosta, D. Andre, V. Angelidakis, R. Caulk, M. Celigueta, B. Chareyre, J.-F. Dietiker, J. Girardot, N. Govender, C. Hubert, R. Kobyłka, A. Moura, V. Skorych, D. Weatherley, T. Weinhart, Comparing open-source DEM frameworks for simulations of common bulk processes. *Computer Physics Communications* **296**, 109066, DOI 10.1016/j.cpc.2023.109066 (2024).

13. S. Roy, M. Y. Shaheen, T. Pöschel, Effect of cohesion on structure of powder layers in additive manufacturing. *Granular Matter* **25**, DOI 10.1007/s10035-023-01349-4 (2023).

14. J. Heieis, J. Böcker, O. D'Angelo, U. Mittag, K. Albracht, E. Schönau, A. Meyer, T. Voigtmann, J. Rittweger, Curvature of gastrocnemius muscle fascicles as function of muscle–tendon complex length and contraction in humans. *Physiological Reports* **11**, DOI 10.14814/phy2.15739 (2023).

15. A. Santarossa, L. Ortellado, A. Sack, L. R. Gómez, T. Pöschel, A device for studying fluid-induced cracks under mixed-mode loading conditions using x-ray tomography. *Review of Scientific Instruments* **94**, DOI 10.1063/5.0145709 (2023).

16. A. Santarossa, O. D'Angelo, A. Sack, T. Pöschel, Effect of particle size on the suction mechanism in granular grippers. *Granular Matter* **25**, DOI 10.1007/s10035-022-01306-7 (2023).

17. P. Raczyński, K. Górny, P. Bełdowski, B. Marciniak, T. Pöschel, Z. Dendzik, Influence of silicon nanocone on cell membrane self-sealing capabilities for targeted drug delivery—Computer simulation study. *Archives of Biochemistry and Biophysics* **749**, 109802, DOI 10.1016/j.abb.2023.109802 (2023).

18. 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).

19. H. Götz, T. Pöschel, O. D'Angelo, Structural features of jammed-granulate metamaterials. *Physical Review Research* **6**, DOI 10.1103/physrevresearch.6.013061 (2024).

20. L. R. Gómez, N. A. García, J. C. Fernández Márquez, T. Pöschel, Ring-linear mixtures of semiflexible rubber bands. *New Journal of Physics* **25**, 083004, DOI 10.1088/1367-2630/ace844 (2023).

Book and book chapters published by MSS in 2023

21. M. Blank, T. Pöschel, in *Proceedings of CASICAM 2022, Temperature gradients as a source of balling and humping in laser processing of titanium,* (Springer Nature Switzerland, 2023), pp. 161–172, ISBN: 9783031329272, DOI 10.1007/978-3-031-32927-2_15.

22. V. Angelidakis, M. Blank, E. J. R. Parteli, S. Roy, D. S. Nasato, H. Xiao, T. Pöschel, *DEM simulation of the powder application in powder bed fusion*, 2023, DOI 10.48550/ARXIV.2310.14031.

23. S. Roy, H. Xiao, M. Y. Shaheen, T. Pöschel, in *Proceedings of CASICAM 2022, Local structural anisotropy in particle simulations of powder spreading in additive manufacturing* (Springer Nature Switzerland, 2023), pp. 139–149, ISBN: 9783031329272, DOI 10.1007/978-3-031-32927-2_13.

Other publications published by MSS in 2023 and submitted manuscripts

24. M. Blank, P. Nair, T. Pöschel, *Surface tension and wetting at free surfaces in Smoothed Particle Hydrodynamics*, 2023, DOI 10.48550/ARXIV.2311.09640.

25. M. Bagheri, S. Roy, T. Pöschel, *Approximate expressions for the capillary force and the surface area of a liquid bridge between identical spheres*, 2023, DOI 10.48550/ARXIV.2310.11485.

26. S. Roy, H. Xiao, V. Angelidakis, T. Pöschel, *Structural fluctuations in thin cohesive particle layers in powder-based additive manufacturing*, 2023, DOI 10.48550/ARXIV.2310.14013.

27. A. P. Singh, V. Angelidakis, T. Pöschel, S. Roy, *Shear zones in granular mixtures of hard and soft particles with high and low friction*, 2023, DOI 10.48550/ARXIV.2311.02875.

28. C. L. Bassani, M. Engel, *Nanocrystal Assemblies: Current advances and open problems, Submitted to ACS Nano on October 18, 2023*.

29. D. E. Wolf, T. Pöschel, *Fractal packing of nanomaterials*, 2023, DOI 10.48550/ARXIV.2312.03117.

30. A. Ameen, A. Sack, T. Pöschel, *TSS-ConvNet for electrical impedance tomography image reconstruction (submitted)*, 2023.

31. A. Madanchi, H. Rahbari, J. Yu, W. B. Leeand, M. R. Rahimi Tabar, T. Pöschel, *Heterogeneity of viscosity in bulk-metallic glasses by active microrheology (submitted)*, 2023.

Patent Application

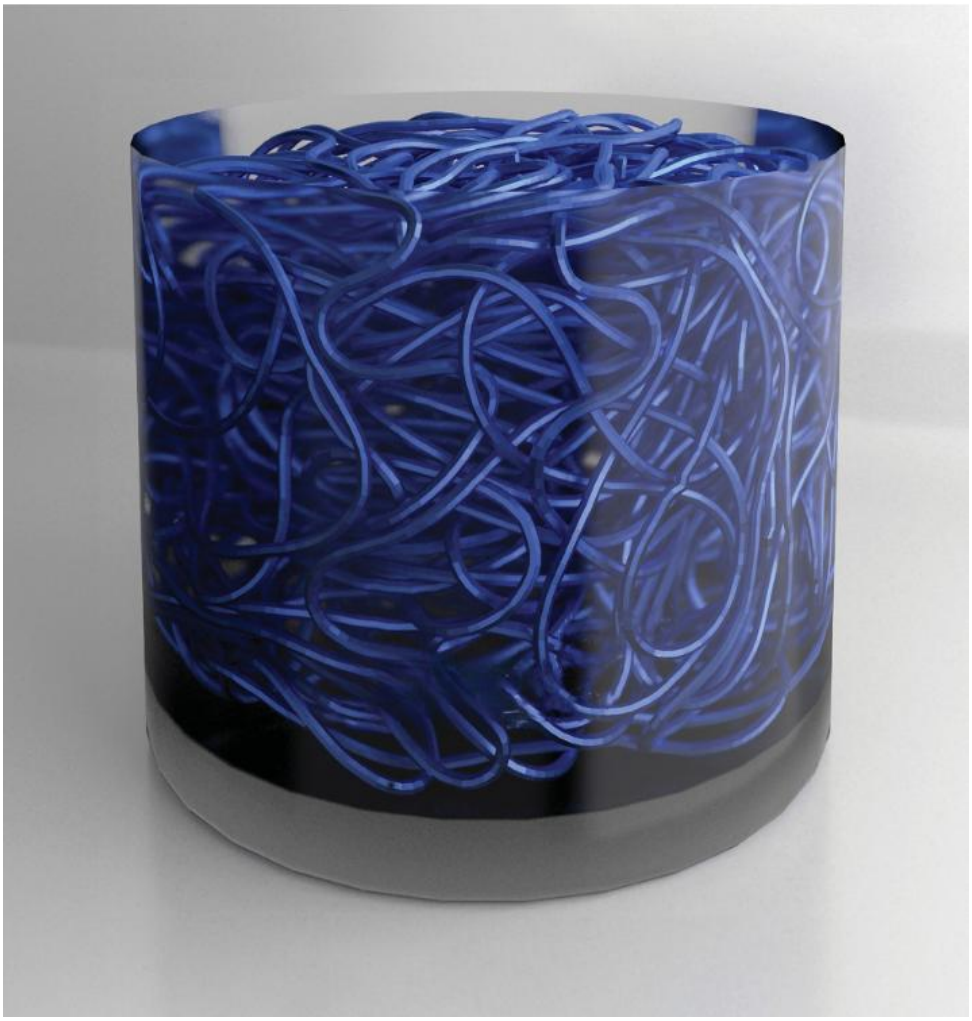
32. O. D'Angelo, A. Sack, T. Pöschel, *Resilient deployable structure with programmable mechanical properties*, German Patent Application: DE 10 2023 130 608.1, 2023.

Macroscopic analogue to entangled polymers

Leopoldo R. Gomez, Nicolas A. Garcia, and ***Thorsten Pöschel***

Abstract:

The entangled structure of polymeric materials is often described as resembling a bowl of spaghetti, swarms of earthworms, or snakes. These analogies not only illustrate the concept, but form the foundation of polymer physics. However, the similarity between these macroscopic, athermal systems and polymers in terms of topology remains uncertain. To better understand this relationship, we conducted an experiment using X-ray tomography to study the structure of arrays of linear rubber bands. We found that, similar to linear polymers, the average number of entanglements increases linearly with the length of the ribbons. Additionally, we observed that entanglements are less frequent near the surface of the con- tainer, where there are also more ends, similar to what has been seen in trapped polymers. These findings provide the first experi- mental evidence supporting the visualization of polymer structures using macroscopic, athermal analogues, confirming the initial intui- tive insights of the pioneers of polymer physics.

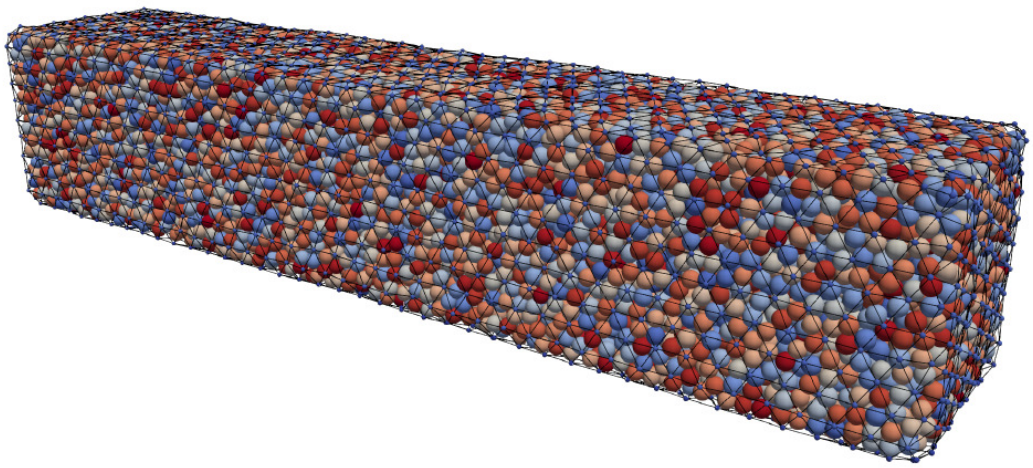


1. L. R. Gómez, N. A. García, T. Pöschel, Macroscopic analogue to entangled polymers. *Soft Matter* **19**, 3538–3542, DOI 10.1039/d3sm00148b (2023).

Granular meta-material: response of a bending beam

Holger Götz** and **Thorsten Pöschel

Abstract:
Jammed granular matter can be considered a meta-material that behaves viscoelastic for small deformations. We characterize the elastic properties of the meta-material through the response of a simply supported bending beam consisting of jammed granular matter under weak load and quasistatic deformation.



2. H. Götz, T. Pöschel, Granular meta-material: response of a bending beam. *Granular Matter* **25**, DOI 10.1007/s10035-023-01336-9 (2023).

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 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 in computation efficiency. The simulation method is demonstrated and benchmarked for a triaxial test.

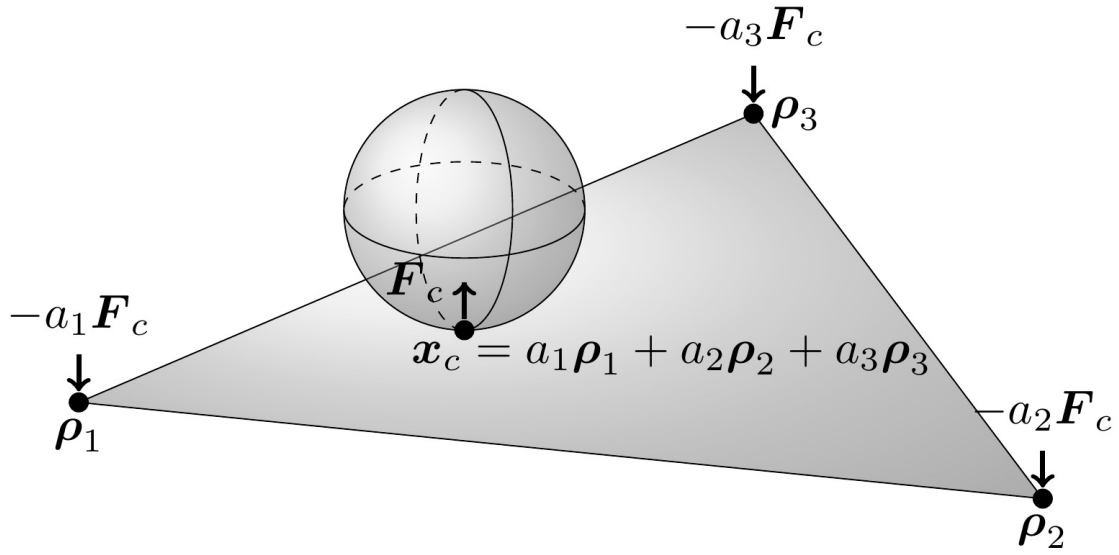


Figure: Sketch of the interaction between a granular particle and a surface patch.

3. H. Götz, T. Pöschel, DEM-simulation of thin elastic membranes interacting with a granulate. *Granular Matter* **25**, DOI 10.1007/s10035-023-01344-9 (2023).

Recent advances in MercuryDPM

*Anthony R. Thornton, Timo Plath, Igor Ostanin , **Holger Götz** , Jan-Willem Bisschop, Mohamed Hassan , Raïsa Roeplal, Xiuqi Wang, Sahar Pourandi, and Thomas Weinhart*

Abstract:

In this paper we introduce the open-source code MercuryDPM: a code for simulating dis- crete particles. The paper discusses software and management issues that may be interesting for the developers of other open-source codes. Then we review the new features that have been added since the last publication: an improved Hertz-Mindlin model; a new liquid bridge model of Lian and Seville; a droplet-spray model; better support for re-creating complex, measured particle size distributions; a new implementation of rigid clumps; an implementa- tion of elastic membranes; a wear model for walls; a soft-kill feature and a cloud-deployment interface for AWS.

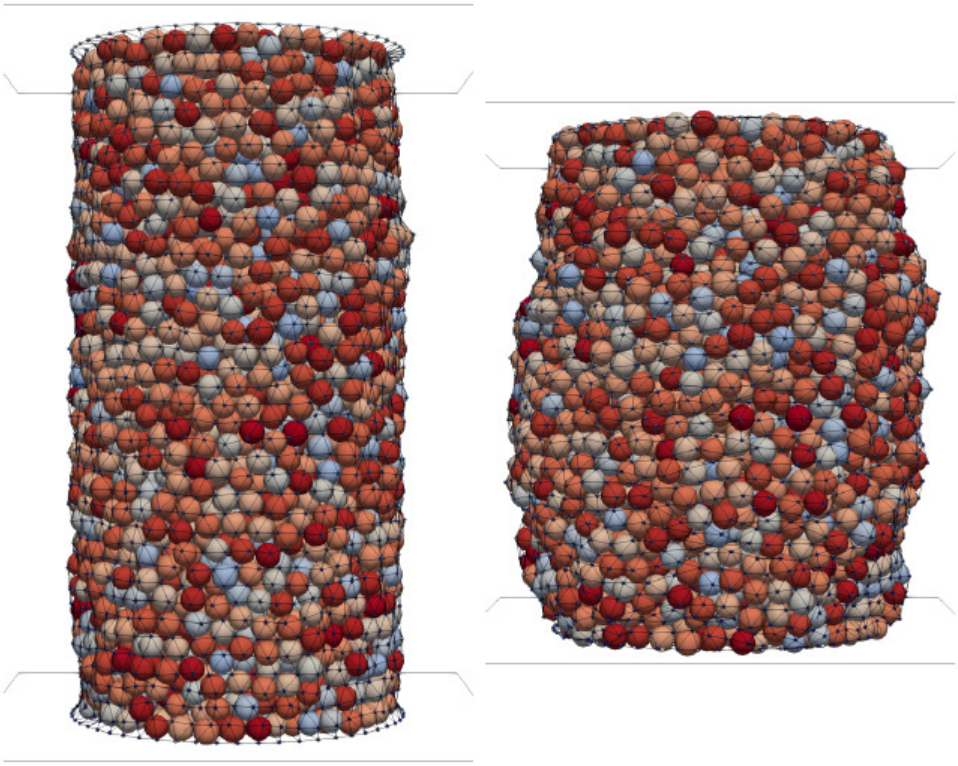


Figure: A triaxial test cell in its initial and final state simulated with the implementation of elastic membranes.

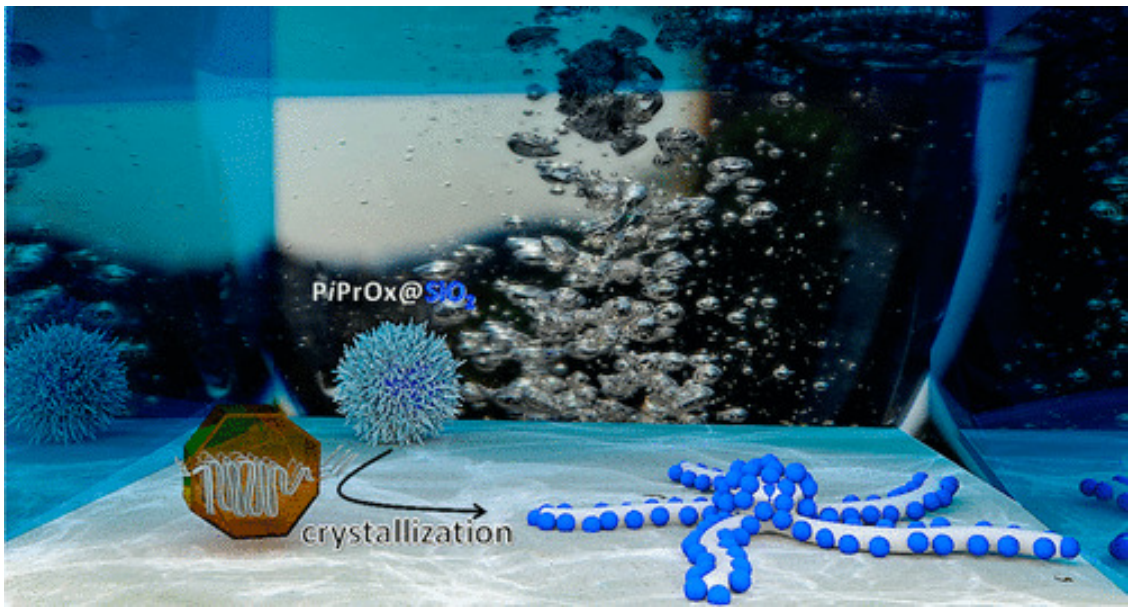
4. A. R. Thornton, T. Plath, I. Ostanin, H. Götz, J.-W. Bisschop, M. Hassan, R. Roeplal, X. Wang, S. Pourandi, T. Weinhart, Recent advances in MercuryDPM. *Mathematics in Computer Science* **17**, DOI 10.1007/s11786-023-00562-x (2023).

Self-assembly of core–shell hybrid nanoparticles by directional crystallization of grafted polymers

Afshin Nabiyan, ***Aswathy Muttathukattil****,* ***Federico Tomazic****, David Pretzel, Ulrich S. Schubert,* ***Michael Engel****, and Felix H. Schacher*

Abstract:

Nanoparticle self-assembly is an efficient bottom-up strategy for the creation of nanostructures. In a typical approach, ligands are grafted onto the surfaces of nanoparticles to improve the dispersion stability and control interparticle interactions. Ligands then remain secondary and usually are not expected to order significantly during superstructure formation. Here, we investigate how ligands can play a more decisive role in the formation of anisotropic inorganic–organic hybrid materials. We graft poly(2-iso-propyl-2-oxazoline) (PiPrOx) as a crystallizable shell onto SiO2 nanoparticles. By varying the PiPrOx grafting density, both solution stability and nanoparticle aggregation behavior can be controlled. Upon prolonged heating, anisotropic nanostructures form in conjunction with the crystallization of the ligands. Self-assembly of hybrid PiPrOx@SiO2 (shell@core) nanoparticles proceeds in two steps: First, the rapid formation of amorphous aggregates occurs via gelation, mediated by the interaction between nanoparticles through grafted polymer chains. As a second step, slow radial growth of fibers was observed via directional crystallization, governed by the incorporation of crystalline ribbons formed from free polymeric ligands in combination with crystallization of the covalently attached ligand shell. Our work reveals how crystallization-driven self-assembly of ligands can create intricate hybrid nanostructures.



5. A. Nabiyan, A. Muttathukattil, F. Tomazic, D. Pretzel, U. S. Schubert, M. Engel, F. H. Schacher, Self-assembly of core–shell hybrid nanoparticles by directional crystallization of grafted polymers. *ACS Nano* **17**, 21216–21226, DOI 10.1021/acsnano.3c05461 (2023).

Early-stage bifurcation of crystallization in a sphere

Chrameh Fru Mbah, Junwei Wang, Silvan Englisch, Praveen Bommineni, ***Nydia Roxana Varela-Rosales****, Erdmann Spiecker, Nicolas Vogel, and* ***Michael Engel***

Abstract:

Bifurcations in kinetic pathways decide the evolution of a system. An example is crystallization, in which the thermodynamically stable polymorph may not form due to kinetic hindrance. Here, we use confined self-assembly to investigate the interplay of thermodynamics and kinetics in the crystallization pathways of finite clusters. We report the observation of decahedral clusters from colloidal particles in emulsion droplets and show that these decahedral clusters can be thermodynamically stable, just like icosahedral clusters. Our hard sphere simulations reveal how the development of the early nucleus shape passes through a bifurcation that decides the cluster symmetry. A geometric argument explains why decahedral clusters are kinetically hindered and why icosahedral clusters can be dominant even if they are not in the thermodynamic ground state.

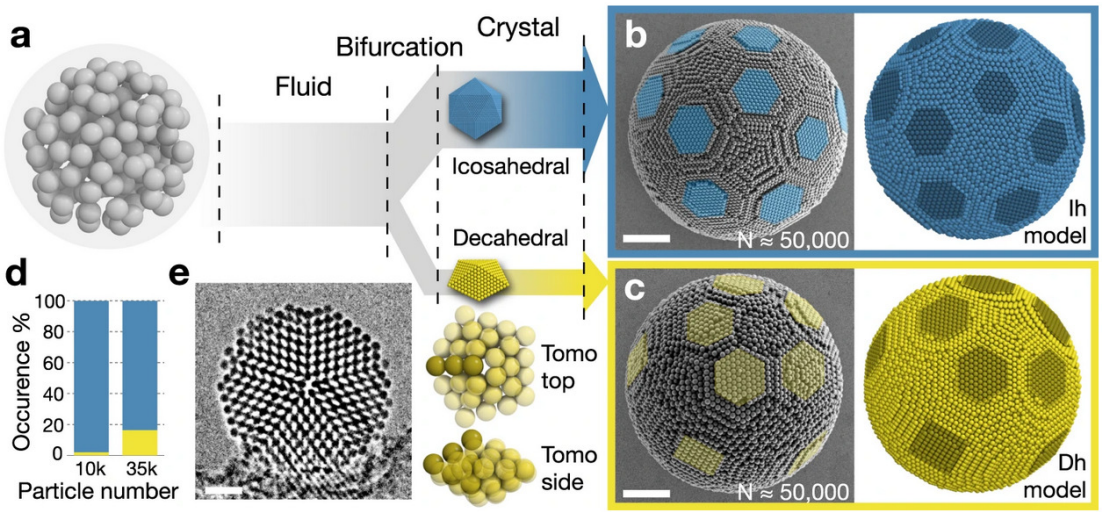


Figure: a Colloidal particles in spherical confinement crystallize into clusters with icosahedral and decahedral symmetry. b Icosahedral clusters (Ih) are characterized by the presence of multiple fivefold symmetry axes. c Decahedral clusters (Dh) are characterized by only one fivefold symmetry axis at their surface. Scanning electron microscopy observations (left in b, c) are compared to ideal structure models (right in b, c). d The occurrence of decahedral clusters is significantly lower than the occurrence of icosahedral clusters. A total number of 100 (68) clusters, among them 2 (11) decahedral clusters (yellow color), were analyzed for clusters with particle number 10k (35k). e Transmission X-ray image along the fivefold axis and segmented central region of tomographic reconstruction (Tomo, Supplementary Fig. S5) confirm the presence of decahedral symmetry by revealing particles columns (dark contrast) and their fcc arrangement with slight deformation in five twinned grains. Due to positive Zernike phase contrast, particle columns appear dark while the empty interstices appear bright. All scalebars, 2 μm.

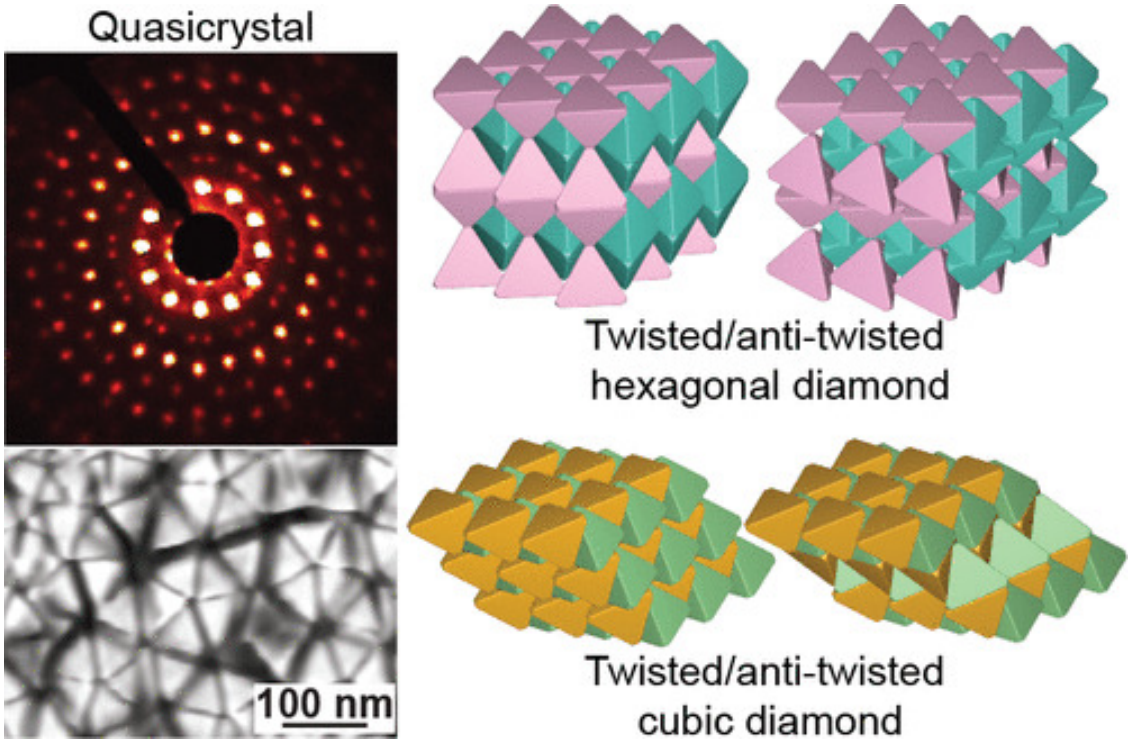
6. C. F. Mbah, J. Wang, S. Englisch, P. Bommineni, N. R. Varela-Rosales, E. Spiecker, N. Vogel, M. Engel, Early-stage bifurcation of crystallization in a sphere. *Nature Communications* **14**, DOI 10.1038/s41467-023-41001-6 (2023).

Controlled self-assembly of gold nanotetrahedra into quasicrystals and complex periodic supracrystals

Yi Wang, Jun Chen, Ruipeng Li, Alexander Götz, Dominik Drobek, Thomas Przybilla, Sabine Hübner, Philipp Pelz, Lin Yang, Benjamin Apeleo Zubiri, Erdmann Spiecker, ***Michael Engel****, and Xingchen Ye*

Abstract:

The self-assembly of shape-anisotropic nanocrystals into large-scale structures is a versatile and scalable approach to creating multifunctional materials. The tetrahedral geometry is ubiquitous in natural and manmade materials, yet regular tetrahedra present a formidable challenge in understanding their self-assembly behavior as they do not tile space. Here, we report diverse supracrystals from gold nanotetrahedra including the quasicrystal (QC) and the dimer packing predicted more than a decade ago and hitherto unknown phases. We solve the complex three-dimensional (3D) structure of the QC by a combination of electron microscopy, tomography, and synchrotron X-ray scattering. Nanotetrahedron vertex sharpness, surface ligands, and assembly conditions work in concert to regulate supracrystal structure. We also discover that the surface curvature of supracrystals can induce structural changes of the QC tiling and eventually, for small supracrystals with high curvature, stabilize a hexagonal approximant. Our findings bridge the gap between computational design and experimental realization of soft matter assemblies and demonstrate the importance of accurate control over nanocrystal attributes and the assembly conditions to realize increasingly complex nanopolyhedron supracrystals.



7. Y. Wang, J. Chen, R. Li, A. Götz, D. Drobek, T. Przybilla, S. Hübner, P. Pelz, L. Yang, B. Apeleo Zubiri, E. Spiecker, M. Engel, X. Ye, Controlled self-assembly of gold nanotetrahedra into quasicrystals and complex periodic supracrystals. *Journal of the American Chemical Society* **145**, 17902–17911, DOI 10.1021/jacs.3c05299 (2023).

Granular binary mixtures improve energy dissipation efficiency of granular dampers

Nydia Roxana Varela-Rosales, Angel Santarossa, Michael Engel, and Thorsten Pöschel

Abstract:
Granular dampers are systems used to attenuate undesired vibrations produced by mechanical devices. They consist of cavities filled by granular particles. In this work, we consider a granular damper filled with a binary mixture of frictionless spherical particles of the same material but different size using numerical discrete element method simulations. We show that the damping efficiency is largely influenced by the composition of the binary mixture.

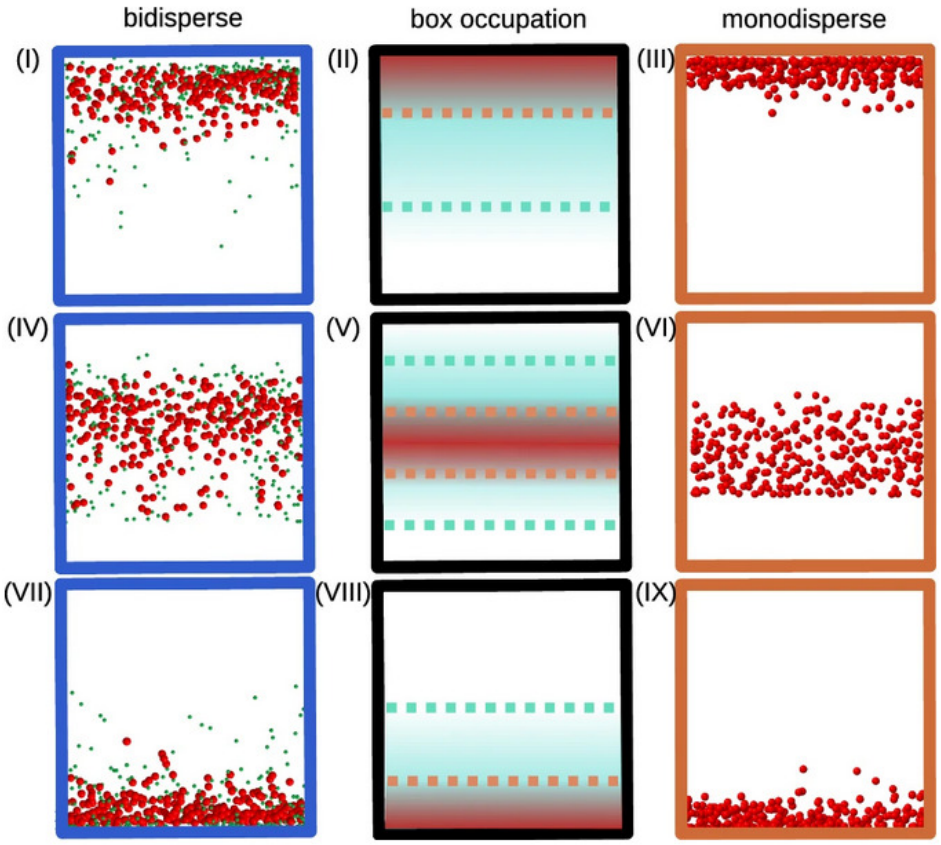


Figure: Class (a): Snapshots of the monodisperse reference system (red boxes) at the times of minimal (III, IX) and maximal (VI) velocity and the same for a bidisperse granulate (blue boxes) with $\sigma = 0.1$ (I, IV, VII). Red circles show particles with radius $R = R_{\mathrm{ref}}$, green circles show small particles, $R = \sigma R_{\mathrm{ref}}$. In (II, VIII), we show the particle probability density at minimal velocity for monodisperse spheres (red shaded area) and for the binary mixture (blue shaded area). Dotted lines in (II, V, VIII) indicate the outer limits of these probabilities.

8. N. R. Varela-Rosales, A. Santarossa, M. Engel, T. Pöschel, Granular binary mixtures improve energy dissipation efficiency of granular dampers. *Granular Matter* **25**, DOI 10.1007/s10035-023-01337-8 (2023).

"Do touch!" - 3D scanning and printing technologies for the haptic representation of cultural assets: a study with blind target users

Arne Bruns, Anika A. Spiesberger, Andreas Triantafyllopoulos, ***Patric Müller****, and Björn W. Schuller*

Abstract:

Visiting museums can be challenging for visually impaired people, as many objects are hidden behind glass walls and information is limited to descriptions. One of the best ways to increase accessibility and inclusion in museums and other cultural heritage institutions is through the use of 3D-printed replicas. However, there are several different scanning and printing processes that not only differ in terms of effort and cost but can also produce very different results. This paper evaluates two different scanning techniques and four different printing processes in terms of these aspects and includes feedback from a group of blind and partially sighted users on the aesthetic quality and fidelity of the printed objects. We found differences between the scanning methods mainly regarding their ease of use. Of the printing methods tested, stereolithography was preferred by the majority of participants for use in the museum. Additionally, we include user comments which touch on the general aspects of presenting museum artefacts using haptic devices. Our study thus provides valuable insights into the preferences of the target users, which can be used to inform decisions about more inclusive museum experiences.

Figure: Density waves in gravity driven granular pipeflow.

9. A. Bruns, A. A. Spiesberger, A. Triantafyllopoulos, P. Müller, B. W. Schuller, presented at the Proceedings of the 5th Workshop on analySis, Understanding and proMotion of heritAge Contents, DOI 10.1145/3607542.3617351.

Rigid clumps in the MercuryDPM particle dynamics code

Igor Ostanin, ***Vasileios Angelidakis****, Timo Plath, Sahar Pourandi, Anthony Thornton, and Thomas Weinhart*

Abstract:

Discrete particle simulations have become the standard in science and industrial applications exploring the properties of particulate systems. Most of such simulations rely on the concept of interacting spherical particles to describe the properties of particulates, although, the correct representation of the nonspherical particle shape is crucial for a number of applications. In this work we describe the implementation of clumps, i.e. assemblies of rigidly connected spherical particles, which can approximate given nonspherical shapes, within the MercuryDPM particle dynamics code. MercuryDPM contact detection algorithm is particularly efficient for polydisperse particle systems, which is essential for multilevel clumps approximating complex surfaces. We employ the existing open-source CLUMP library to generate clump particles. We detail the pre-processing tools providing necessary initial data, as well as the necessary adjustments of the algorithms of contact detection, collision/migration and numerical time integration. The capabilities of our implementation are illustrated for a variety of examples.

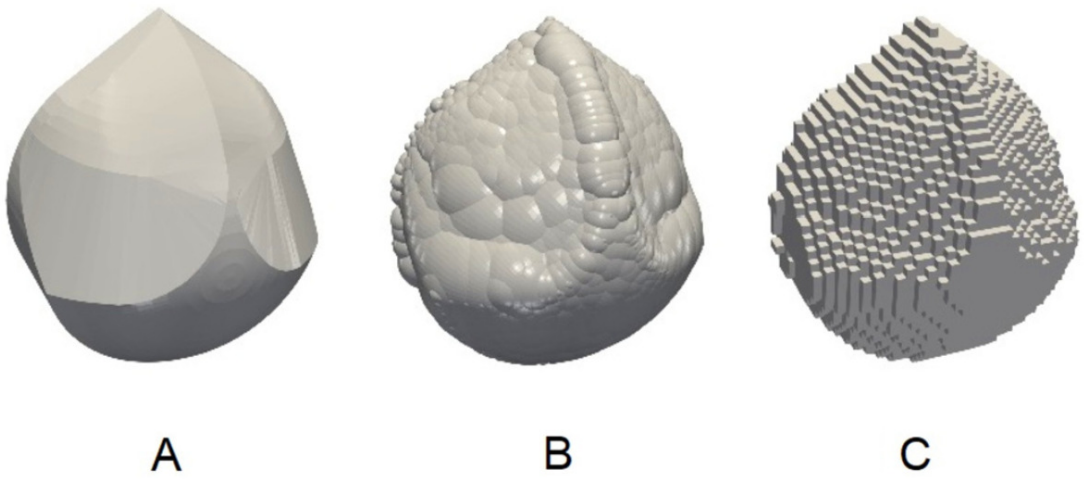


Figure: Representation of a non-spherical shape as (A) triangulated surface, (B) rigid clump of spherical particles, (C) 3D array of voxels.

10. I. Ostanin, V. Angelidakis, T. Plath, S. Pourandi, A. Thornton, T. Weinhart, Rigid clumps in the MercuryDPM particle dynamics code. *Computer Physics Communications* **296**, 109034, DOI 10.1016/j.cpc.2023.109034 (2024).

SPIRAL: An efficient algorithm for the integration of the equation of rotational motion

Carlos Andres del Valle**, **Vasileios Angelidakis**, **Sudeshna Roy**, José Daniel Muñoz, and **Thorsten Pöschel

Abstract:

SPIRAL: An Efficient Algorithm for the Integration of the Equation of Rotational Motion
We introduce Spiral, a third-order integration algorithm for the rotational motion of ex- tended bodies. It requires only one force calculation per time step, does not require quater- nion normalization at each time step, and can be formulated for both leapfrog and syn- chronous integration schemes, making it compatible with many particle simulation codes. The stability and precision of Spiral exceed those of state-of-the-art algorithms currently used in popular DEM codes such as Yade, MercuryDPM, LIGGGHTS, PFC, and more, at only slightly higher computational cost. Also, beyond DEM, we see potential applications in all numerical simulations that involve the 3D rotation of extended bodies.

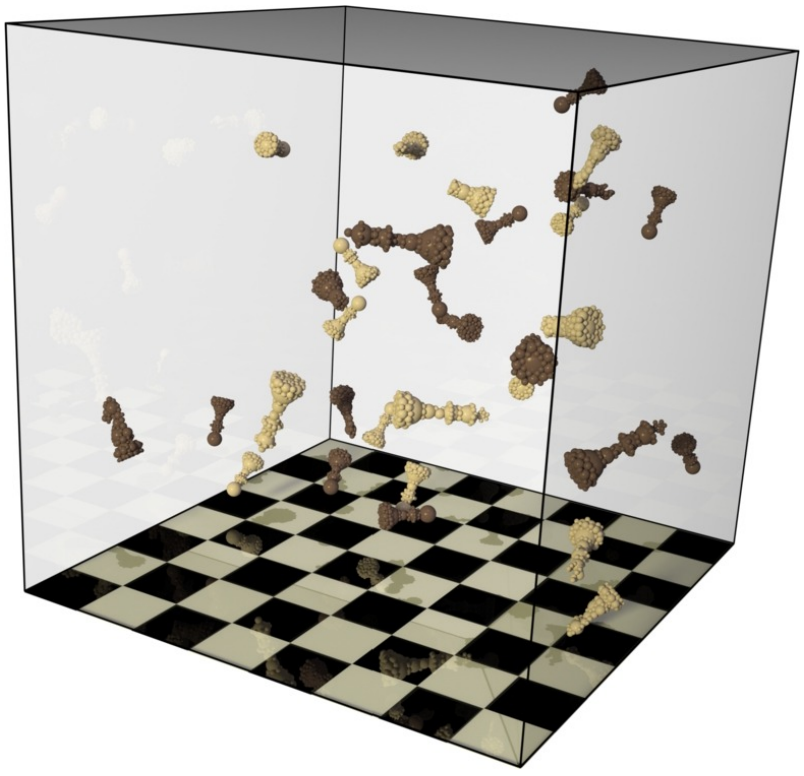


Figure: Snapshot of a simulation of non-spherical particles (chess pieces modeled as multi-spheres) bouncing in a box. The elastic Hertz contact force describes particle-particle and particle-wall collisions.

11. C. A. del Valle, V. Angelidakis, S. Roy, J. D. Muñoz, T. Pöschel, SPIRAL: An efficient algorithm for the integration of the equation of rotational motion. *Computer Physics Communications*, 109077, DOI 10.1016/j.cpc.2023.109077 (2024).

Comparing open-source DEM frameworks for simulations of common bulk processes

*M. Dosta, D. Andre, **V. Angelidakis**, R.A. Caulk, M.A. Celigueta, B. Chareyre, J.-F. Dietiker, J. Girardot, N. Govender, C. Hubert, R. Kobyłka, A.F. Moura, V. Skorych, D.K. Weatherley, and T. Weinhart*

Abstract:

Multiple software frameworks based on the Discrete Element Method (DEM) are available for simulating granular materials. All of them employ the same principles of explicit time integration, with each time step consisting of three main steps: contact detection, calculation of interactions, and integration of the equations of motion. However, there exist significant algorithmic differences, such as the choice of contact models, particle and wall shapes, and data analysis methods. Further differences can be observed in the practical implementation, including data structures, architecture, parallelization and domain decomposition techniques, user interaction, and the documentation of resources. This study compares, verifies, and benchmarks nine widely-used software frameworks. Only open-source packages were considered, as these are freely available and their underlying algorithms can be reviewed, edited, and tested. The benchmark consists of three common bulk processes: silo emptying, drum mixing, and particle impact. To keep it simple and comparable, only standard features were used, such as spherical particles and the Hertz-Mindlin model for dry contacts. Scripts for running the benchmarks in each software are provided as a dataset.

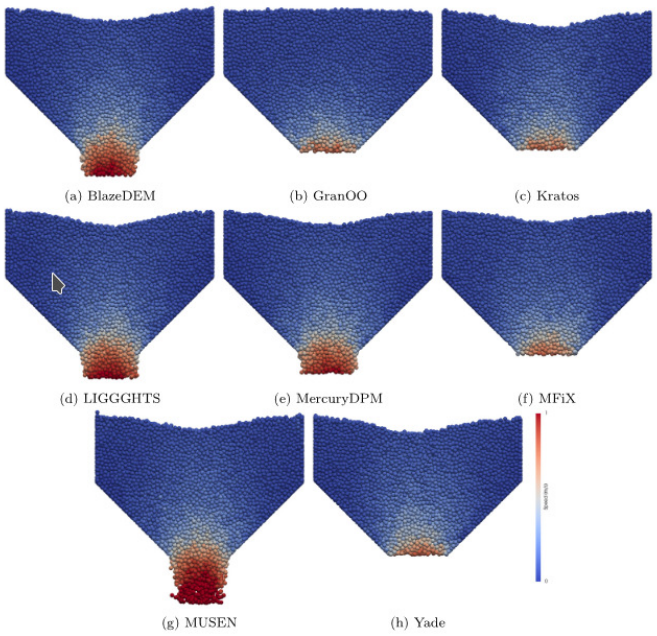


Figure: Simulations snapshots of the large-orifice silo with M1 particles at = 2 s, coloured by particle speed. Only particles located within 1 cm of the silo axis in depth direction are shown, thus the selection represents a cross-section through the centre of the silo.

12. M. Dosta, D. Andre, V. Angelidakis, R. Caulk, M. Celigueta, B. Chareyre, J.-F. Dietiker, J. Girardot, N. Govender, C. Hubert, R. Kobyłka, A. Moura, V. Skorych, D. Weatherley, T. Weinhart, Comparing open-source DEM frameworks for simulations of common bulk processes. *Computer Physics Communications* **296**, 109066, DOI 10.1016/j.cpc.2023.109066 (2024).

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. The effect of particle cohesion on the quality of powder layers 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.

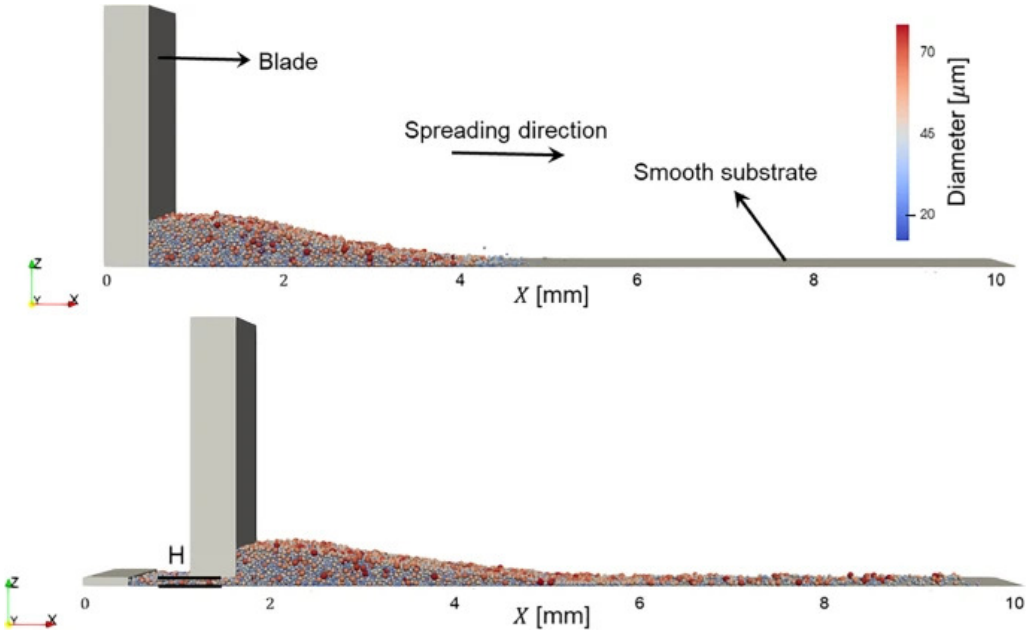


Figure: Numerical setup for powder spreading on a smooth substrate before and during spreading.

13. S. Roy, M. Y. Shaheen, T. Pöschel, Effect of cohesion on structure of powder layers in additive manufacturing. *Granular Matter* **25**, DOI 10.1007/s10035-023-01349-4 (2023).

Curvature of gastrocnemius muscle fascicles as function of muscle-tendon complex length and contraction in humans

Jule Heieis, Jonas Böcker, ***Olfa D'Angelo****, Uwe Mittag, Kirsten Albracht, Eckhard Schönau, Andreas Meyer, Thomas Voigtmann, and Jörn Rittweger*

Abstract:

It has been shown that muscle fascicle curvature increases with increasing contraction level and decreasing muscle-tendon complex length. The analyses were done with limited examination windows concerning contraction level, muscle-tendon complex length, and/or intramuscular position of ultrasound imaging. With this study we aimed to investigate the correlation between fascicle arching and contraction, muscle-tendon complex length and their associated architectural parameters in gastrocnemius muscles to develop hypotheses concerning the fundamental mechanism of fascicle curving. Twelve participants were tested in five different positions (90°/105°*, 90°/90°*, 135°/90°*, 170°/90°*, and 170°/75°*; *knee/ankle angle). They performed isometric contractions at four different contraction levels (5%, 25%, 50%, and 75% of maximum voluntary contraction) in each position. Panoramic ultrasound images of gastrocnemius muscles were collected at rest and during constant contraction. Aponeuroses and fascicles were tracked in all ultrasound images and the parameters fascicle curvature, muscle-tendon complex strain, contraction level, pennation angle, fascicle length, fascicle strain, intramuscular position, sex and age group were analyzed by linear mixed effect models. Mean fascicle curvature of the medial gastrocnemius increased with contraction level ($+5\ \mathrm{m}^{-1}$ from 0% to 100%; $p = 0.006$). Muscle-tendon complex length had no significant impact on mean fascicle curvature. Mean pennation angle ($2.2\ \mathrm{m}^{-1}$ per 10°; $p < 0.001$), inverse mean fascicle length ($20\ \mathrm{m}^{-1}$ per cm^{-1}; $p = 0.003$), and mean curvature strain ($-0.07\ \mathrm{m}^{-1}$ per +10%; $p = 0.004$) correlated with mean fascicle curvature. Evidence has also been found for intermuscular, intramuscular, and sex-specific intramuscular differences of fascicle curving. Pennation angle and the inverse fascicle length show the highest predictive capacities for fascicle curving. Due to the strong correlations between pennation angle and fascicle curvature and the intramuscular pattern of curving we suggest for future studies to examine correlations between fascicle curvature and intramuscular fluid pressure.

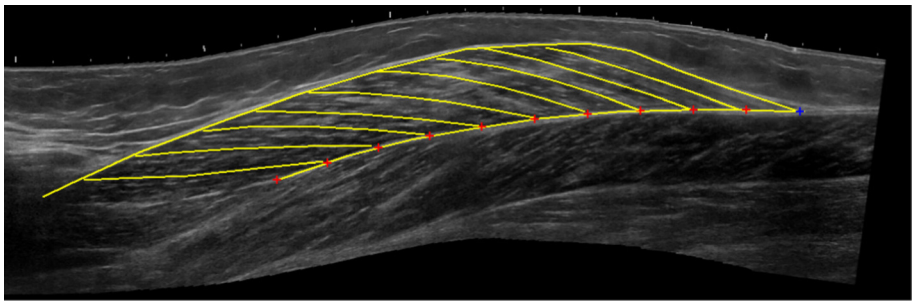


Figure: Processed panoramic ultrasound image of medial gastrocnemius with manually labeled superficial and deep aponeuroses and nine fascicles.

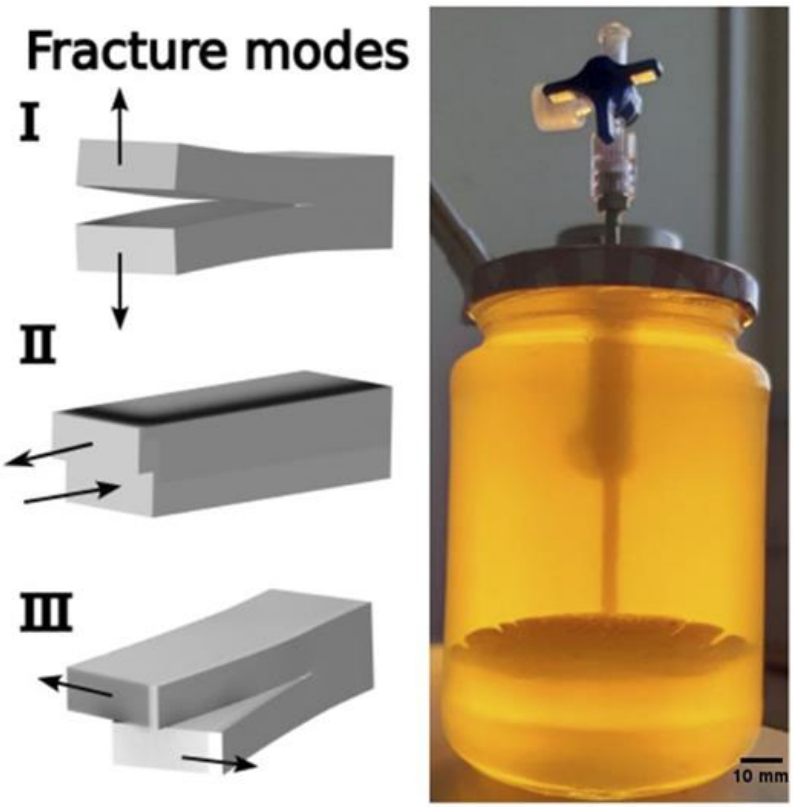
14. J. Heieis, J. Böcker, O. D'Angelo, U. Mittag, K. Albracht, E. Schönau, A. Meyer, T. Voigtmann, J. Rittweger, Curvature of gastrocnemius muscle fascicles as function of muscle–tendon complex length and contraction in humans. *Physiological Reports* **11**, DOI 10.14814/phy2.15739 (2023).

A device for studying fluid-induced cracks under mixed-mode loading conditions using x-ray tomography

Angel Santarossa**, Laureano Ortellado, **Achim Sack**, Leopoldo R. Gomez, and **Thorsten Pöschel

Abstract:

We introduce an innovative instrument designed to investigate fluid-induced fractures under mixed loading conditions, including uniaxial tension and shear stress, in gels and similar soft materials. Equipped with sensors for measuring force, torque, and fluid pressure, the device is tailored for compatibility with x-ray tomography scanners, enabling non-invasive 3D analysis of crack geometries. To showcase its capabilities, we conducted a study examining crack-front segmentation in a hydrogel subjected to air pressure and a combination of tension and shear stress.



15. A. Santarossa, L. Ortellado, A. Sack, L. R. Gómez, T. Pöschel, A device for studying fluid-induced cracks under mixed-mode loading conditions using x-ray tomography. *Review of Scientific Instruments* **94**, DOI 10.1063/5.0145709 (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 work, 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=120m) achieve higher conformation around the object than larger particles (d4mm), thus allowing the formation of air-tight seals. 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.

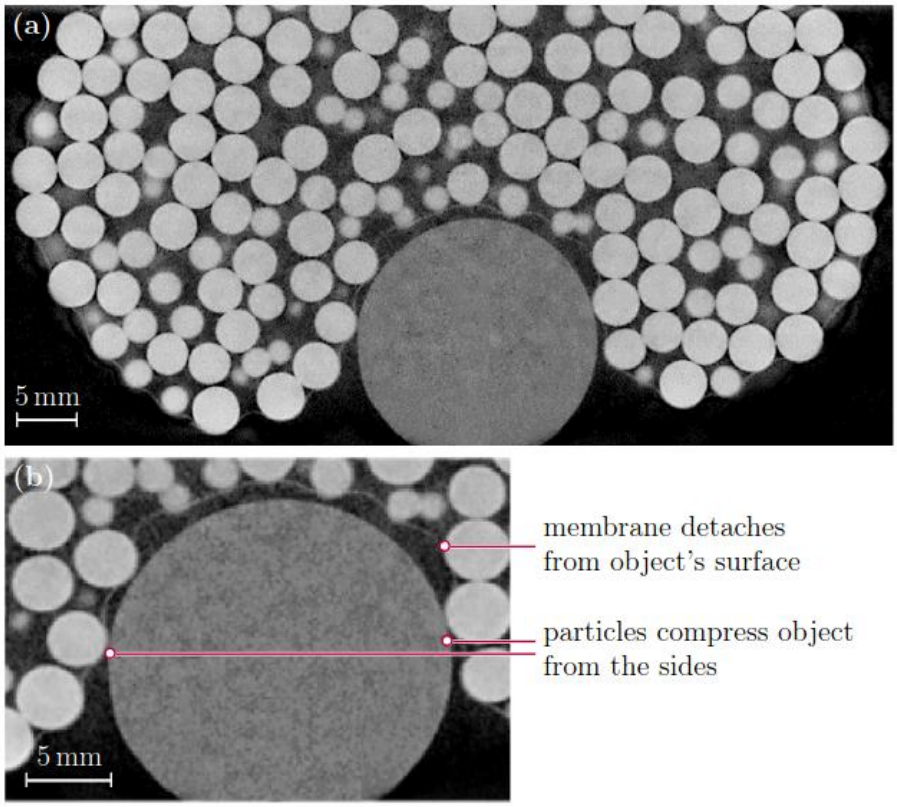


Figure: X-ray tomogram slice for large particles, after evacuation of the air from the gripper: original snapshot (a) and magnification in the region around the object (b)

16. A. Santarossa, O. D'Angelo, A. Sack, T. Pöschel, Effect of particle size on the suction mechanism in granular grippers. *Granular Matter* **25**, DOI 10.1007/s10035-022-01306-7 (2023).

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

Przemylaw Raczynski, Krzysztof Gorny, Piotr Beldowski, Beata Marciniak, ***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 nanocone 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.

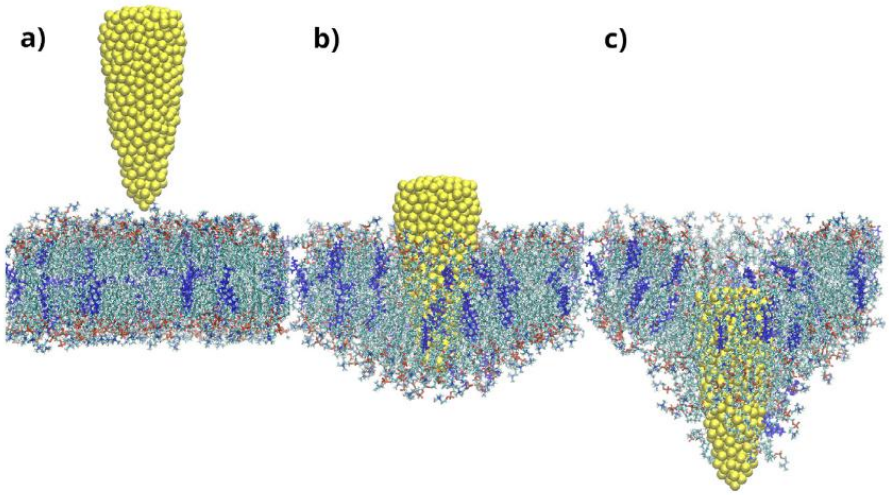


Figure: The snapshots of the instantaneous indentation phases: (a) initial configuration, (b) nanocone travels the distance of approximately 63 , (c) nanocone travels the distance of approximately 105 . The cholesterols in the membrane are colored blue.

17. P. Raczyński, K. Górny, P. Bełdowski, B. Marciniak, T. Pöschel, Z. Dendzik, Influence of silicon nanocone on cell membrane self-sealing capabilities for targeted drug delivery—Computer simulation study. *Archives of Biochemistry and Biophysics* **749**, 109802, DOI 10.1016/j.abb.2023.109802 (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. Our model does not rely on fitting parameters and can be applied to different variants of SPH. We demonstrate its robustness and accuracy by simulating several notoriously difficult three-dimensional free surface flow problems driven by surface tension.

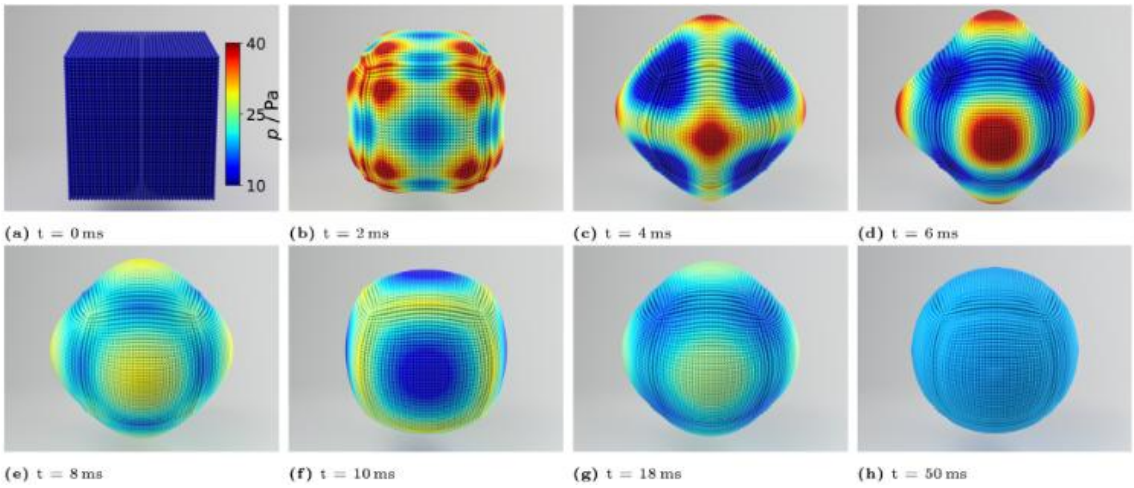


Figure: Relaxation of an initially cubic droplet. The figures show snapshots of the droplet at increasing time, colored by pressure.

18. 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).

Structural features of jammed-granulate metamaterials

Holger Götz, Thorsten Pöschel**, and **Olfa D'Angelo

Abstract:
Granular media near jamming exhibit fascinating properties, which can be harnessed to create jammed- granulate metamaterials: materials whose characteristics arise not only from the shape and material properties of the particles at the microscale but also from the geometric features of the packing. For the case of a bending beam made from jammed-granulate metamaterial, we study the impact of the particles' properties on the metamaterial's macroscopic mechanical characteristics. We find that the metamaterial's stiffness emerges from its volume fraction, in turn originating from its creation protocol; its ultimate strength corresponds to yielding of the force network. In contrast to many traditional materials, we find that macroscopic deformation occurs mostly through affine motion within the packing, aided by stress relief through local plastic events, surprisingly homogeneously spread and persistent throughout bending.

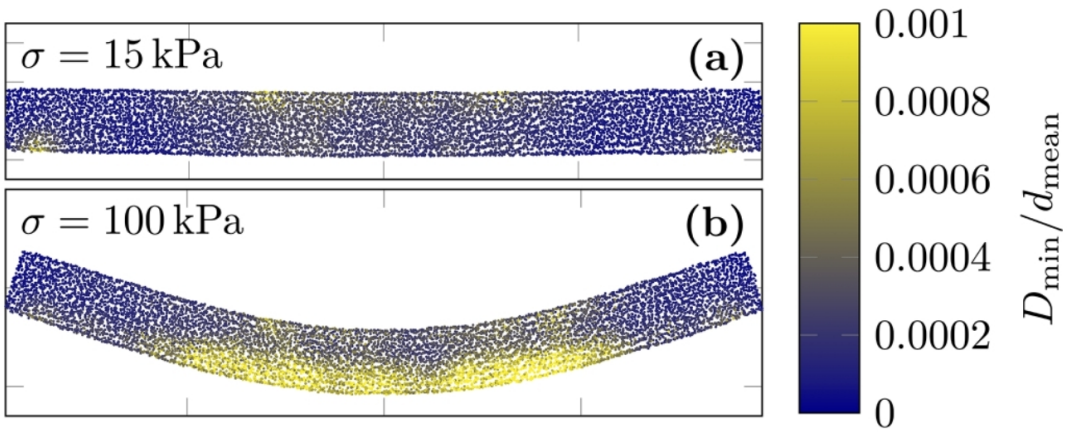


Figure: $D_{\mathrm{min}}/d_{\mathrm{mean}}$ of the beam. Examples are displayed for systems with the particles' stiffness $E_p = 100$ MPa and friction coefficient $\mu_p = 0.3$ and external stress values of (a) $\sigma = 15$ kPa and (b) $\sigma = 100$ kPa.

19. H. Götz, T. Pöschel, O. D'Angelo, Structural features of jammed-granulate metamaterials. *Physical Review Research* **6**, DOI 10.1103/physrevresearch.6.013061 (2024).

Ring-linear mixtures of semiflexible rubber bands

Leopoldo R. Gomez*, Nicolas A. Garcia, Juan Cruz Fernandez Marquez, and* ***Thorsten Pöschel***

Abstract:
During the synthesis of ring polymers, it is quite common to obtain mixtures containing both ring and linear molecules. Recent studies, including experiments and simulations, have shown that even small quantities of linear molecules can significantly influence the shape of ring polymers, ultimately altering their rheological response. To further explore this phenomenon, we investigated blends of semiflexible linear and ring filaments by using disordered assemblies of open and closed rubber bands. We employed x-ray tomography to analyze the structure of these mixtures, focusing on how the length and composition of linear bands influenced the overall mixture. In contrast to the behavior observed in fully-flexible polymers, our findings revealed that increasing the concentration of linear bands could actually decrease the average size of rings within a semiflexible ring-linear mixture. This outcome is attributable to a reduction in inter-ring threading, which naturally occurs as the proportion of rings diminishes. To validate our findings, we conducted molecular dynamics simulations on semiflexible ring-linear polymer mixtures in bulk. These simulations confirmed that our results stem from the semiflexibility of the bands or chains rather than confinement or athermal conditions.

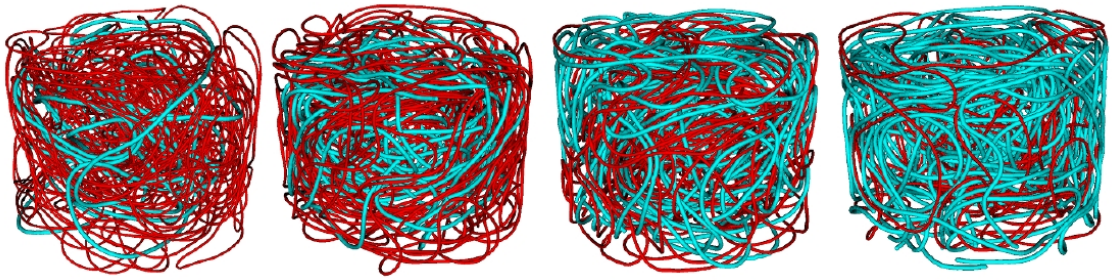


Figure: Visualizing the impact of linear contaminants on rubber band mixtures: reconstructions from x-ray tomography. This figure showcases typical reconstructions of rubber band mixtures comprising of ring (red) and linear (light-blue) bands. The concentrations of linear contaminants increase from left to right, with values of $phi = 0.16, 0.32, 0.66, 0.82$.

20. L. R. Gómez, N. A. García, J. C. Fernández Márquez, T. Pöschel, Ring-linear mixtures of semiflexible rubber bands. *New Journal of Physics* **25**, 083004, DOI 10.1088/1367-2630/ace844 (2023).

Temperature 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.

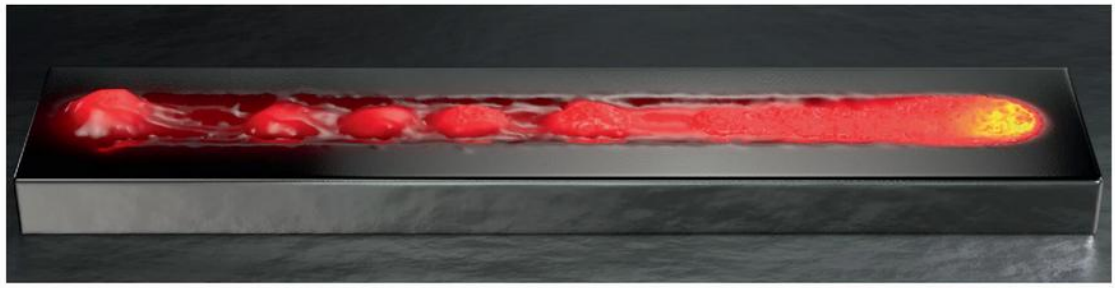


Figure: Simulation snapshot of the laser welding process of titanium using parameter set 4 exhibiting humping

21. M. Blank, T. Pöschel, in *Proceedings of CASICAM 2022, Temperature gradients as a source of balling and humping in laser processing of titanium,* (Springer Nature Switzerland, 2023), pp. 161–172, ISBN: 9783031329272, DOI 10.1007/978-3-031-32927-2_15.

DEM simulation of the powder application in powder bed fusion

Vasileios Angelidakis**, **Michael Blank**, Eric J. R. Parteli, **Sudeshna Roy**, Daniel Schiochet Nasato, **Hongyi Xiao**, and **Thorsten Pöschel

Abstract:

The packing behavior of powders is significantly influenced by various types of inter-particle attractive forces, including adhesion and non-bonded van der Waals forces. Alongside particle size and shape distributions, the inter-particle interactions, in particular frictional and adhesive forces, play a crucial role in determining the flow behavior and consequently the packing density of the powder layer. The impact of various types of attractive forces on the packing density of powders with different materials and particle size distributions remains largely unexplored and requires further investigation. Accurately comprehending these effects through experiments while considering specific particle size distributions and material properties poses significant challenges. To address these challenges, we employ Discrete Element Method (DEM) simulations to characterize the packing behavior of fine powders. We can demonstrate quantitative agreement with experimental results by incorporating the appropriate particle size distribution and using an adequate model of attractive particle interactions. Furthermore, our findings indicate that both adhesion, which is modeled using the Johnson-Kendall-Roberts (JKR) model, and van der Waals interactions are crucial factors that must be taken into account in DEM simulations.

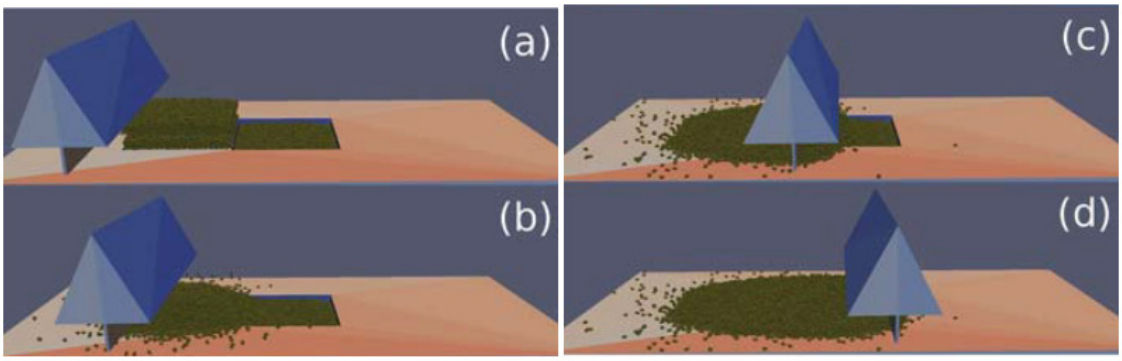


Figure: Snapshots of a simulation of particles with complex geometric shapes. Particles constructed with the multisphere method are inserted into the system with dynamic boundary conditions that mimic the device used in additive manufacturing

22. V. Angelidakis, M. Blank, E. J. R. Parteli, S. Roy, D. S. Nasato, H. Xiao, T. Pöschel, *DEM simulation of the powder application in powder bed fusion*, 2023, DOI 10.48550/ARXIV.2310.14031.

Local structural anisotropy in particlesimulations of powder spreadingin 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 manufac- turing. 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 pow- der layer from homogeneous to heterogeneous for cohesive materials at Bo = 10. Including an idealized temperature-dependence of the normal contact force does not influence the structure of the deposited layer in powder spreading.

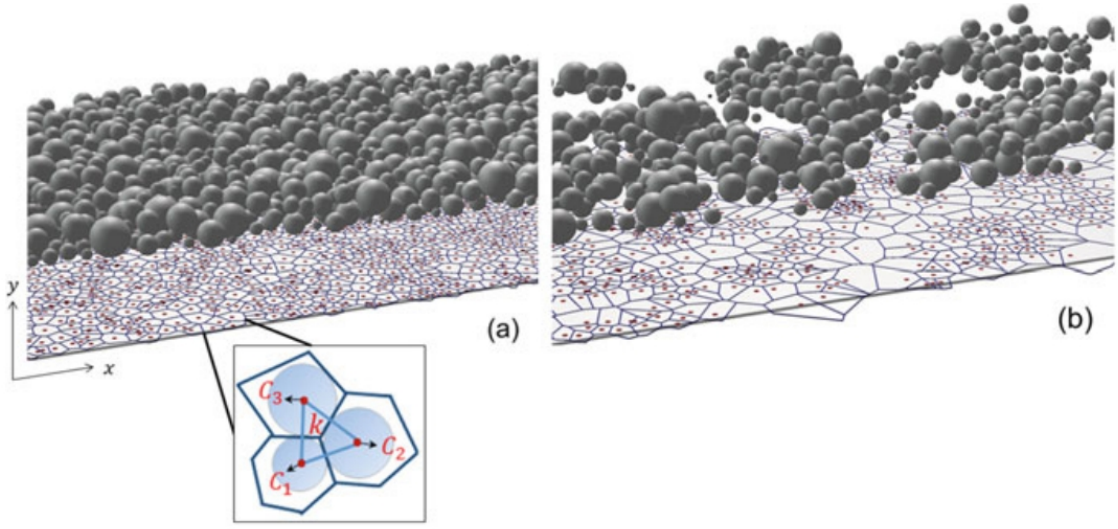


Figure: a Granular packing of powder layer for thermal particles. The particles are colored according to their temperature with color scale varying from 330 K (black) to 380 K (yellow). b Probability density of the normalized divergence of center-to-centroid vectors for quasi-2D packing of powder deposited for athermal particles (blue squares) and thermal particles (yellow circles)

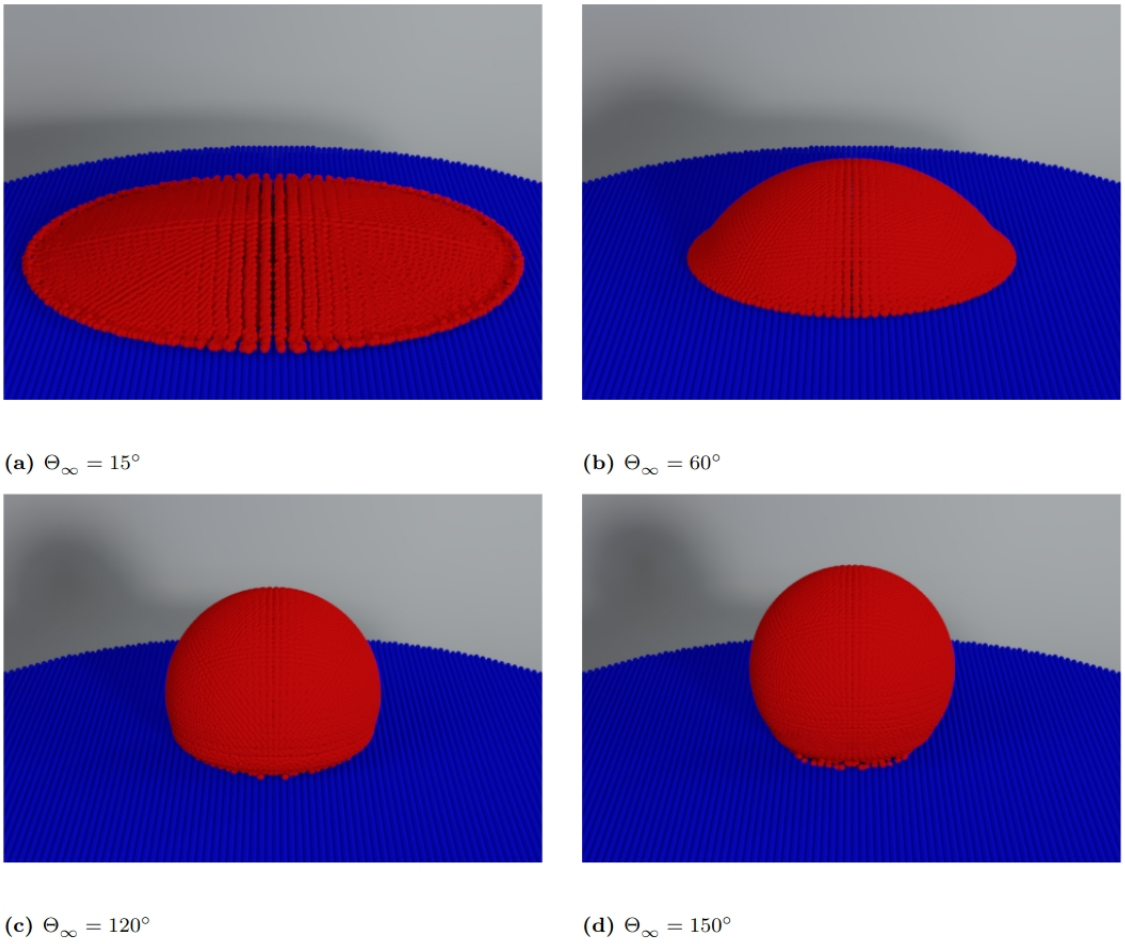
23. S. Roy, H. Xiao, M. Y. Shaheen, T. Pöschel, in *Proceedings of CASICAM 2022, Local structural anisotropy in particle simulations of powder spreading in additive manufacturing* (Springer Nature Switzerland, 2023), pp. 139–149, ISBN: 9783031329272, DOI 10.1007/978-3-031-32927-2_13.

Surface tension and wetting at free surfaces in Smoothed Particle Hydrodynamics

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

Abstract:

Surface tension and wetting are dominating physical effects in micro and nanoscale flows. We present an efficient and reliable model of surface tension and equilibrium contact angles in Smoothed Particle Hydrodynamics for free-surface problems. We demonstrate its robustness and accuracy by simulating several notoriously difficult three-dimensional free surface flow problems driven by interfacial tension.



(a) $\Theta_\infty = 15°$ **(b)** $\Theta_\infty = 60°$

(c) $\Theta_\infty = 120°$ **(d)** $\Theta_\infty = 150°$

Figure: At large time, $t = 1$ s, the drops have assumed their equilibrium shape. Liquid SPH particles are shown in red, and solid particles are shown in blue. For $\Theta_{\text{inf}\in\{120°,150°\}}$, some particles near the three-phase contact line disintegrated from the body of the liquid phase.

24. M. Blank, P. Nair, T. Pöschel, *Surface tension and wetting at free surfaces in Smoothed Particle Hydrodynamics*, 2023, DOI 10.48550/ARXIV.2311.09640.

Approximate expressions for the capillary force and the surface area of a liquid bridge between identical spheres

Meysam Bagheri, Sudeshna Roy, and Thorsten Pöschel

Abstract:

We consider a liquid bridge between identical spheres and present approximate expressions for the capillary force and the surface area. Prior studies focused on the capillary force, but our research fills the gap by providing new expressions for the surface area of the liquid bridge. These expressions are crucial for efficient numerical simulations, such as molecular dynamics or discrete element methods, and our results represent the first of their kind in this domain.

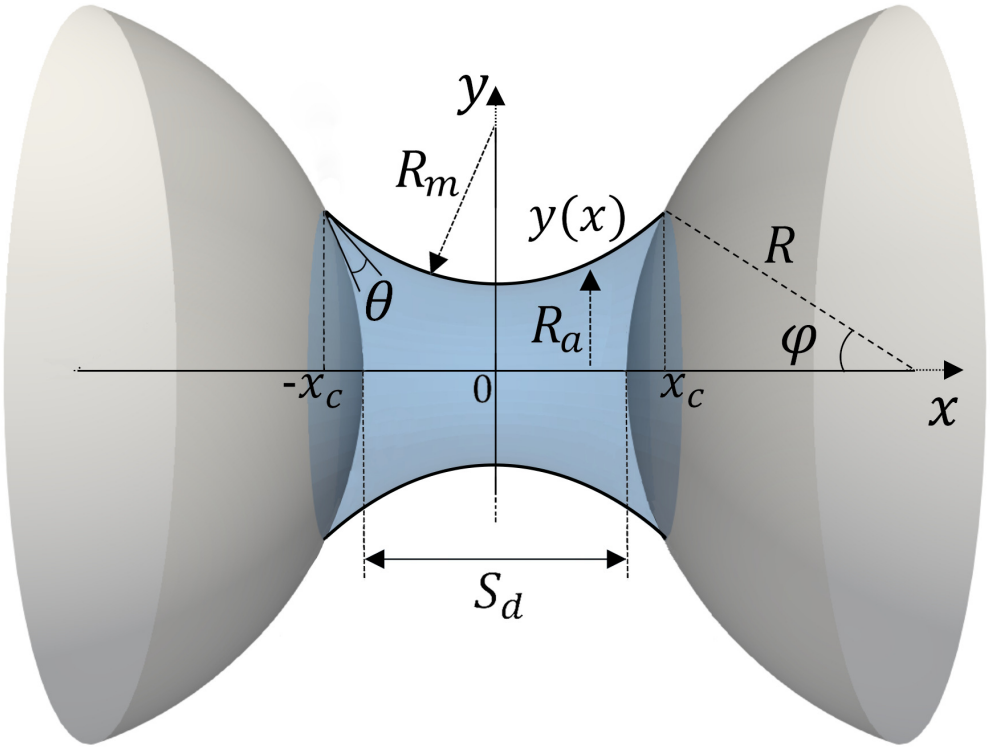


Figure: The shape of a liquid bridge between two identical spheres of radius R and distance S_d is a solution of the Young-Laplace equation with the solid-liquid contact angle, θ, the half-filling angle, ϕ, the surface tension coefficient, γ. R_m and R_a are meridian and azimuth radii, respectively.

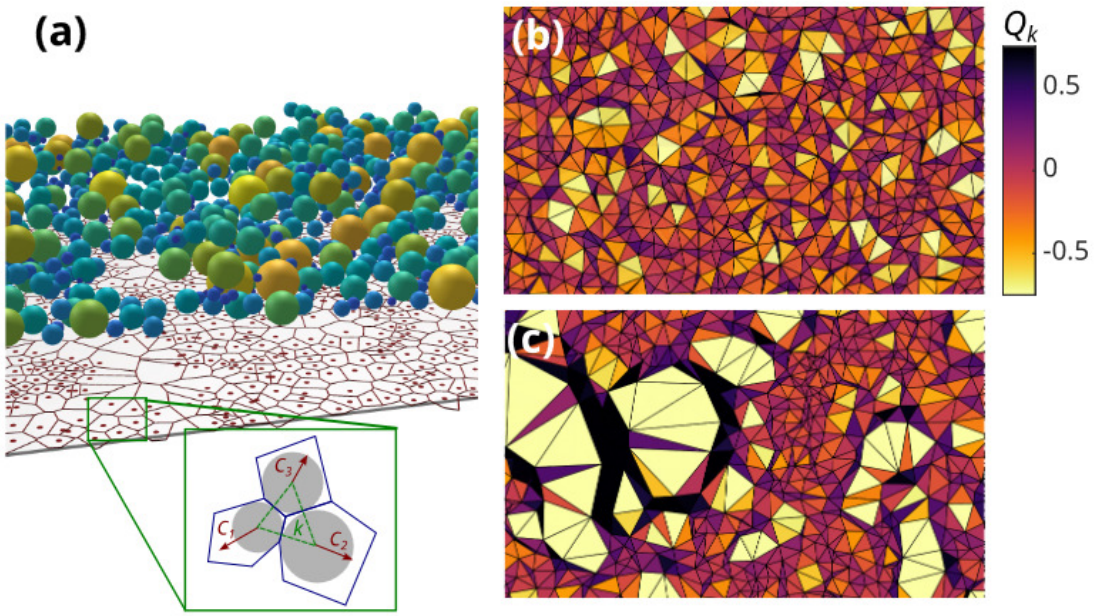
25. M. Bagheri, S. Roy, T. Pöschel, *Approximate expressions for the capillary force and the surface area of a liquid bridge between identical spheres*, 2023, DOI 10.48550/ARXIV.2310.11485.

Structural fluctuations in thin cohesive particle layers in powder-based additive manufacturing

Sudeshna Roy**, **Hongyi Xiao**, **Vasileios Angelidakis**, and **Thorsten Pöschel

Abstract:

Producing dense and homogeneous powder layers with smooth free surface is challenging in additive manufacturing, as interparticle cohesion can strongly affect the powder packing structure and therefore influence the quality of the end product. We use the Discrete Element Method to simulate the spreading process of spherical powders and examine how cohesion influences the characteristics of the packing structure with a focus on the fluctuation of the local morphology. As cohesion increases, the overall packing density decreases, and the free surface roughness increases, which is calculated from digitized surface height distributions. Local structural fluctuations for both quantities are examined through the local packing anisotropy on the particle scale, obtained from Voronoi tessellation. The distributions of these particle-level metrics quantify the increasingly heterogeneous packing structure with clustering and changing surface morphology.



26. S. Roy, H. Xiao, V. Angelidakis, T. Pöschel, *Structural fluctuations in thin cohesive particle layers in powder-based additive manufacturing*, 2023, DOI 10.48550/ARXIV.2310.14013.

Shear zones in granular mixtures of hard and soft particles with high and low friction

Aditya Pratap Singh, ***Vasileios Angelidakis****,* ***Thorsten Pöschel****, and* ***Sudeshna Roy***

Abstract:

Granular materials show inhomogeneous flows characterized by strain localization. When strain is localized in a sheared granular material, rigid regions of a nearly undeformed state are separated by shear bands, where the material yields and flows. The characteristics of the shear bands are determined by the geometry of the system, the micromechanical material properties, and the kinematics at the particle level. For a split-bottom shear cell, recent experimental work has shown that mixtures of hard, frictional and soft, nearly frictionless particles exhibit wider shear zones than samples with only one of the two components. To explain this finding, we investigate the shear zone properties and the stress response of granular mixtures using discrete element simulations. We show that both interparticle friction and elastic modulus determine the shear-band properties of granular mixtures of various mixing ratios, but their stress response depends strongly on the interparticle friction. Our study provides a fundamental understanding of the micromechanics of shear band formation in granular mixtures.

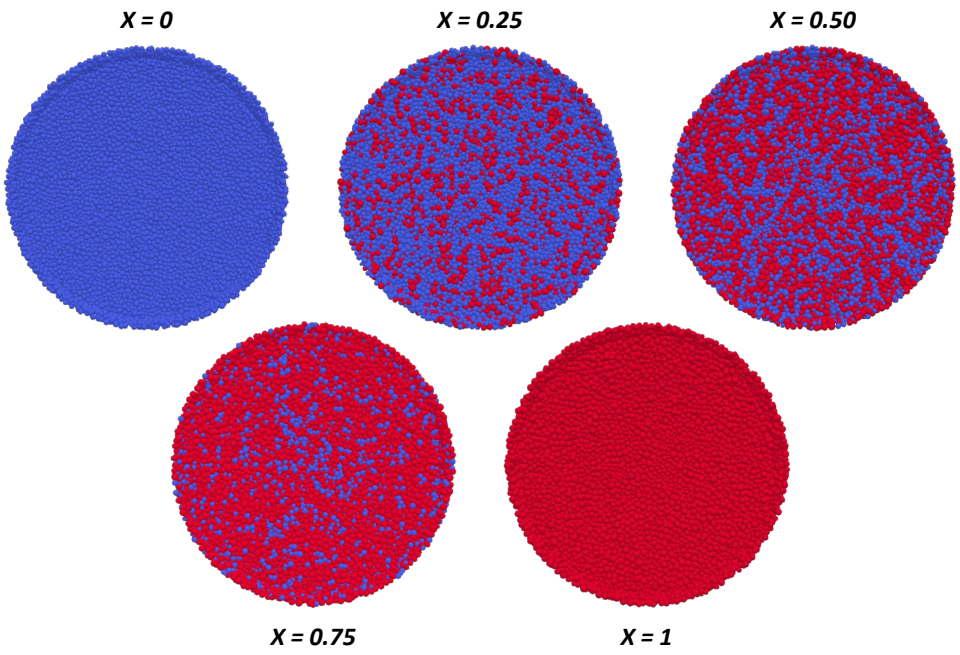


Figure: Top view of the shear cell for granular mixtures of different percentages of hard particles X, where the blue and red particles represent species A (soft) and B (hard), respectively.

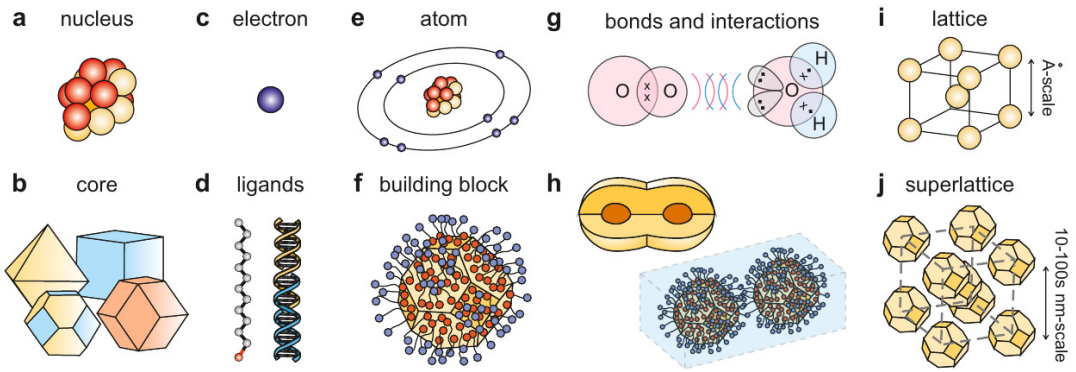
27. A. P. Singh, V. Angelidakis, T. Pöschel, S. Roy, *Shear zones in granular mixtures of hard and soft particles with high and low friction*, 2023, DOI 10.48550/ARXIV.2311.02875.

Nanocrystal assemblies: current advances and open problems

Carlos L. Bassani, *Greg van Anders, Uri Banin, Dmitry Baranov, Qian Chen, Mar- jolein Dijkstra, Michael S. Dimitriyev, Efi Efrati, Jordi Faraudo, Oleg Gang, Nicola Gaston, Ramin Golestanian, G. Ivan Guerrero-Garcia, Michael Gruenwald, Amir Haji-Akbari, Maria Ibanez, Matthias Karg, Tobias Kraus, Byeongdu Lee, Reid C. Van Lehn, Robert J. Macfarlane, Bortolo M. Mognetti, Arash Nikoubashman, Saeed Osat, Oleg V. Prezhdo, Grant M. Rotskoff, Leonor Saiz, An-Chang Shi, Sara Skrabalak, Ivan I. Smalyukh, Mario Tagliazucchi, Dmitri V. Talapin, Alexei V. Tkachenko, Sergei Tretiak, David Vaknin, Asaph Widmer-Cooper, Gerard C. L. Wong, Xingchen Ye, Shan Zhou, Eran Rabani,* ***Michael Engel****, and Alex Travesset*

Abstract:

We explore the potential of nanocrystals (term used equivalently to nanoparticles) as building blocks for new materials, and the opportunities that this presents for fundamental science developments and applications. Nanocrystal assemblies are inherently multiscale, and the possibility of generating revolutionary material properties requires a precise understanding of the relationship between structure and function, the former being determined by classical effects and the latter often by quantum effects. With an emphasis on theory and computation, we discuss challenges that ham- per current assembly strategies, and to what extent nanocrystal assemblies represent thermodynamic equilibrium or kinetically trapped metastable states. We also examine dynamic effects and optimization of assembly protocols. Finally, we discuss promising material functions and concrete examples of their realization with nanocrystal assemblies.



28. C. L. Bassani, M. Engel, *Nanocrystal Assemblies: Current advances and open problems, Submitted to ACS Nano on October 18, 2023*.

Fractal packing of nanomaterials

Dietrich E. Wolf and ***Thorsten Pöschel***

Abstract:
Cohesive particles form agglomerates that are usually very porous. Their geometry, particularly their fractal dimension, depends on the agglomeration process (diffusion-limited or ballistic growth by adding single particles or cluster-cluster aggregation). However, in practice, the packing structure depends not only on the initial formation but also on the mechanical processing of the agglomerate after it has grown. Surprisingly, the packing converges to a statistically invariant structure under certain process conditions, independent of the initial growth process. We consider the repeated fragmentation on a given length scale, followed by ballistic agglomeration. Examples of fragmentation are sieving with a given mesh size or dispersion in a turbulent fluid. We model the agglomeration by gravitational sedimentation. The asymptotic structure is fractal up to the fragmentation length scale, and the fragments have a power-law size distribution. A scaling relation connects the power law and the fractal dimension.

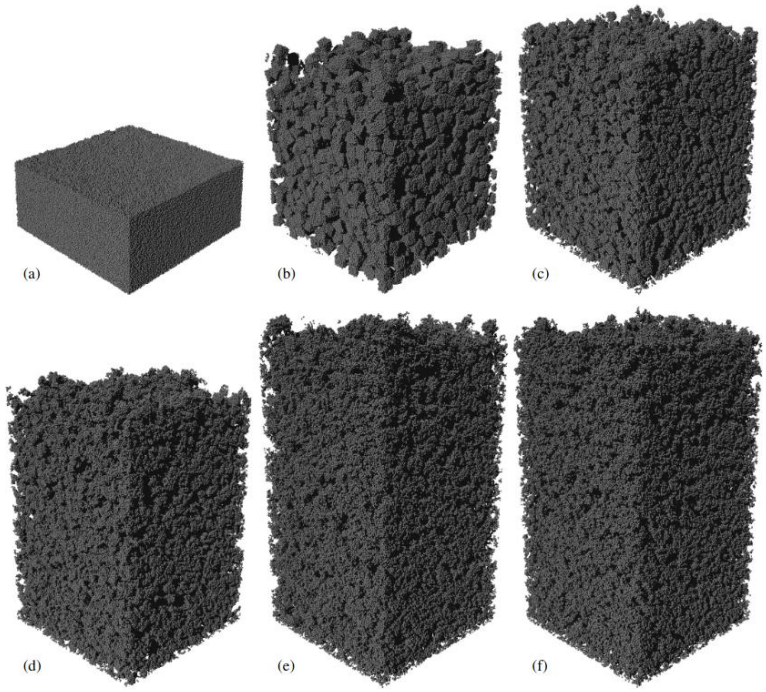


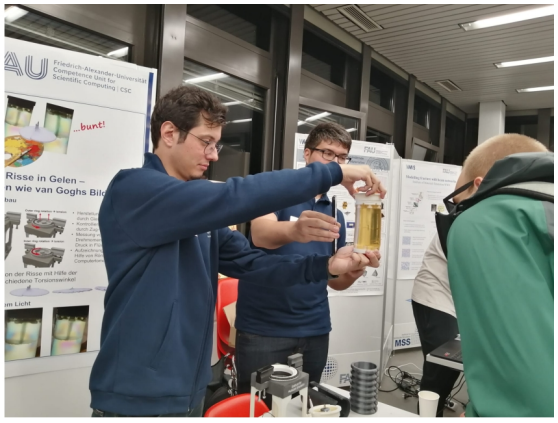
Figure: Snapshots of the packing containing $N = 10^6$ particles after t cycles of fragmentation with $l = 8d$ and subsequent sedimentation. The width of the system is $L = 128d$. (a) Initial packing, $t = 0$. (b) $t = 1$: Sedimented fragments of the initial packing. (c) $t = 2$: Sedimented fragments of packing (b). (d) $t = 3$. Between the 50th iteration (e) and the 100th iteration (f), the structure hardly changes anymore.

29. D. E. Wolf, T. Pöschel, *Fractal packing of nanomaterials*, 2023, DOI 10.48550/ARXIV.2312.03117.

13. Public Attention and Public Outreach

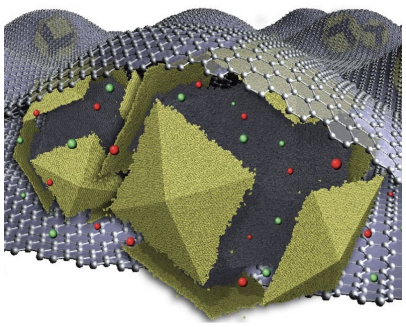
MSS participated in the Long Night of Science, "Lange Nacht der Wissenschaften"

The "Long Night of Science" took place on Saturday, October 21, 2023. The experiment showcasing hydrogel fracture, a creation of Angel Santarossa from MSS, garnered significant interest. This setup allows for the visualization of stress patterns within hydrogel materials, which appear as various colors when observed under polarized light.



From left to right: Utku Canbolat, Angel Santarossa

The researchers from Engel's group also showcased simulation packages and demonstrated interactive demonstrations highlighting how we study atoms and nanoparticles in computer simulation and theory. Visitors could learn about the function of simulations and conduct own simulations at computers, tables or in the browser of with their own smart phone



MSS goes Girl's day

Girls' Day offers a fantastic chance for girls in grades 5 to 11 to explore predominantly technical careers. Similar to previous years, MSS organized a two-hour tour titled "Licht ins Dunkel bringen" ("Shedding Light in the Dark?"), led by Achim Sack. During the session, participants delved into the process of generating a Computed Tomography scan, starting from the inception and characteristics of X-rays, progressing through the creation of a radiograph, culminating in a complete 3D reconstruction of a Kinder-Surprise egg.
We extend our gratitude to all attendees for their participation and their enthusiasm for science and technology.

Participants of the Girl's Day 2023.

14. Social Activities

MSS Resturant Invitations

This year, MSS organized multiple dinner events to celebrate the guest speakers of the MSS seminars.

From left to right: Michael Engel, Vasileios Angelidakis, Olfa D'Angelo, Carlos del Valle, Holger Götz, Huzaif Rahim, Utku Canbolat, Meysam Bagheri, Thorsten Pöschel, Catherine O'Sullivan, Hongy Xiao.