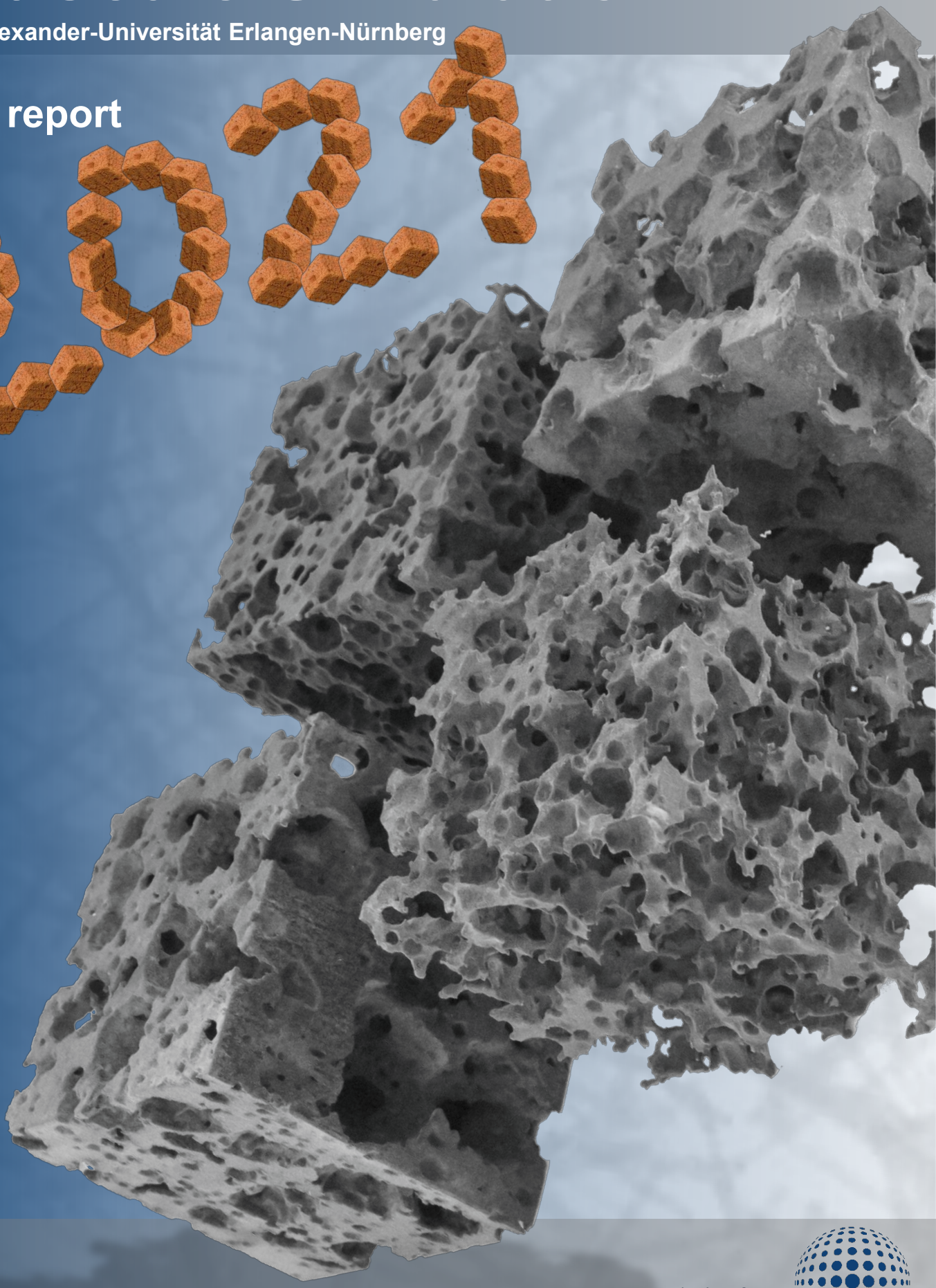
Institute for Multiscale Simulation

Prof. Thorsten Pöschel
Prof. Michael Engel

Friedrich-Alexander-Universität Erlangen-Nürnberg

annual report

2021



Friedrich-Alexander-Universität
Technische Fakultät

Institute for
Multiscale Simulation
MSS

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

Editor: Nydia Roxana Varela-Rosales

Titelpage: Artificial porous geometries for the simulation of heat and mass transport in ceramic foams by Patric Müller and Felix Buchele.

Institute for Multiscale Simulation

Annual Report 2021

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 2021.

Erlangen, December 2021
Thorsten Pöschel, Michael Engel

1. Staff Members

Professors

Prof. Dr.
Thorsten Pöschel

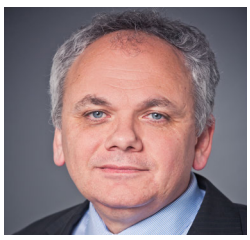
Prof. Dr.
Michael Engel

Visiting Professors

Prof. Dr.
Leopoldo Gómez

Prof. Dr.
José Daniel
Muñoz Castaño

Assistant Professor (Privatdozent) and Habilitation Candidates



Priv.-Doz. Dr. habil.
Igor Goychuk

Dr. phil.
Alberto Leonardi

Dr. rer. nat.
Patric Müller

Postdoctoral Researchers

Dr.-Ing.
Olfa D'Angelo

Dr. Zhiyuan Cui

Dr. Aswathy
Muttathukattil
Narayanan

Dr.-Ing.
Sudeshna Roy

Dr. rer. nat.
Achim Sack

Doctoral Candidates

M. Sc.
Ayman Ameen

M. Sc.
Meysam Bagheri

M. Sc.
Michael Blank

M. Eng.
Felix Buchele

Dr.-Ing.
Fru Mbah Chrameh

M. Sc.
Holger Götz

M. Sc.
Sarthak Jadhav

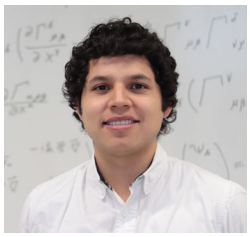
Dr. rer. nat.
Marco Klement

M. Sc.
Valentina Marzulli

M. Sc.
Atharva Pandit

M. Sc.
Angel Santarossa

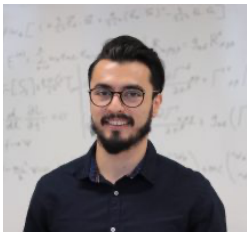
M. Sc.
Federico Tomazic



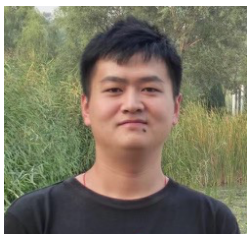
M. Sc.
Luis Torres Cisneros

Dr.-Ing.
Harol Torres Menéndez

M. Sc.
Nydia Roxana
Varela-Rosales



M. Sc.
Ali Mauricio
Velasco Sabogal



M. Sc.
Song Zhiyu

Master, Bachelor and Mini-project students

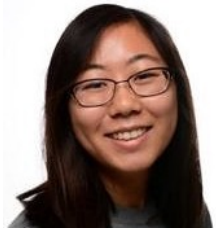
Abeer Al-Ani
Master student

Alice Bellettini
Master student

Kamilia Gabaidullina
Master student

Lan-Tien Hsu
Miniproject

Tengda Huang
Miniproject



Natalie Lam
Miniproject

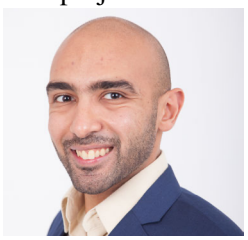
Khaled Mansour
Miniproject

Jonathan Martín
Miniproject

Navid Panchi
Programming Project

Theresa Rogge
Master student

Kilian Tscharke
Miniproject



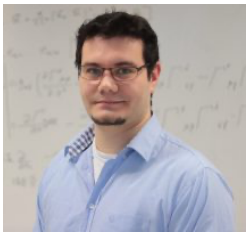
Omar Zeair
Miniproject

Technical and Administrative Staff

Dipl.-Pol.
Roland Haberkorn
Systems Admin.

Ulrike Hansl
Secretary

Dr. Michael Heckel
Technician



Meister
Walter Pucheanu
Technician

Student Assistants

Nicole Illinger

Verena Merten

Navid Panchi

Nicolas Pechler

Sebastian Weigelt

2. MSS Seminar

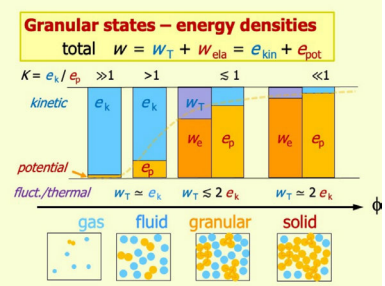
138. **Prof. Stefan Luding**
Institute for Multi Scale Mechanics, University of Twente
"From particle simulations towards a universal continuum theory about jamming, un-jamming transitions"
October 7, 2021
139. **Dr. Paolo Malgaretti**
Helmholtz-Institute Erlangen-Nürnberg
"Coarse-grained colloidal dynamics: confinement, free energy and information"
October 13, 2021
140. **Prof. José-Daniel Muñoz**
National University of Columbia
"Lattice Boltzmann beyond Fluid Mechanics"
October 20, 2021
141. **Dr. Sudeshna Roy**
School of Engineering and Physical Sciences, Heriot-Watt University, UK
"Hydrodynamics of wet granular materials"
October 27, 2021
142. **Prof. Thorsten Pöschel**
FAU Erlangen-Nürnberg, Institute for Multiscale Simulation
"History and Structure of Granular Sediments"
November 3, 2021
143. **Prof. Robin Klupp-Taylor**
Institute of Particle Technology, University of Erlangen-Nuremberg
"Crystal growth on spherical substrates: Inspiration from experiments"
November 10, 2021
144. **Prof. Matthias Möbius**
School of Physics, Trinity College Dublin
"Properties of lightweight fibrous structures made by a foam forming technique"
November 17, 2021

138th MSS-Seminar
Thursday, October 7th,
16:30 hrs, Room KS 1,
Cauerstraße 4, Erlangen.

From particle simulations towards a universal continuum theory about jamming, un-jamming transitions

Prof. Dr. Stefan Luding,
Chair for Multi Scale Mechanics, University of Twente

The dynamic and static behavior of particulate and granular matter is special:
they can behave both solid-like and fluid-like. The ultimate goal is a continuum theory that can deal with all states from gas- or fluid-like, or solid-like, as well as all transitions between the states, including jamming and un-jamming. Such a "universal granular rheology" combines the worlds of fluid- and solid-mechanics, eventually allowing to solve real world, large-scale application problems.

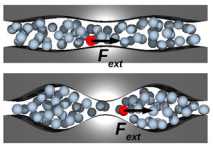


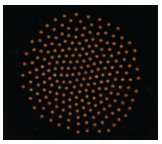
139th MSS-Seminar
Wednesday, October 13th,
15:30 hrs, H5,
Cauerstr. 7/9, Erlangen.

Coarse-grained colloidal dynamics: confinement, free energy and information

Dr. Paolo Malgaretti
Helmholtz Institute Erlangen-Nürnberg

Within this seminar I describe three scenarios in which, by means of coarse-graining, insight into the dynamics of diverse systems can be obtained. First, I will introduce simple analytical models that capture the stationary flux of diverse systems such as electrolytes and colloids across porous media. Second, I will show that these model can be used to extract the equilibrium free energy profile and the (inhomogeneous) transport coefficient from non-equilibrium steady state simulations. Finally, I will show that the non-equilibrium patterns formed by spinning disks at fluid interfaces are well captured by the entropy associated to the nearest-neighbor probability distribution.



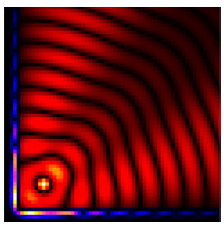


140th MSS-Seminar
Wednesday, October 20th,
15:30 hrs, H3,
Egerlandstr. 3, Erlangen.

Lattice Boltzmann beyond Fluid Mechanics

Prof. José-Daniel Muñoz
National University of Columbia

Lattice-Boltzmann methods (LBM) are usually saw as mesoscopic representations of a discrete fluid, where particle densities travel from cell to cell and collide on each other preserving mass, momentum and energy. But they can also be seen as a more general computational scheme: information travels from cell to cell and collide at each one driven by a Boltzmann transport equation, representing systems that evolve with other conservation laws. In this talk we will show how LBM can be used to represent Electrodynamics, Acoustics and Advection-Diffusion phenomena. In addition, we will show for the last two cases how to formulate them on generalized curvilinear grids (for instance, to simulate the acoustic waves inside the human cochlea or to increase resolution in some regions), so that the main advantage of LBM – that is, that each cell evolves without asking information to the neighboring cells – is almost preserved.

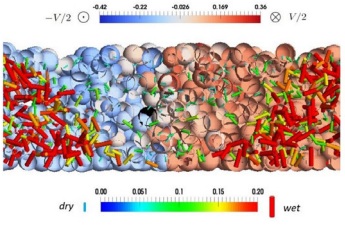


141st MSS-Seminar
Wednesday, October 27th,
15:30 hrs, H3,
Egerlandstr. 3, Erlangen.

Hydrodynamics of wet granular materials

PhD Sudeshna Roy
Institute for Multiscale Simulation

Most studies in granular physics focus on dry granular materials and their flow rheology. However, wet granular materials are ubiquitous in geology and many real world applications where interstitial liquid is present between the grains. The main focus areas of my research are (i) the formulation of suitable constitutive equations for the hydrodynamic density-stress-strain relations, (ii) the deduction of the constitutive equations from discrete element simulations, specifically for wet granular materials, and (iii) their validation with theoretical and experimental results. My research proposes a modified generalized flow rule for granular materials to close the fundamental conservation laws for mass and momentum. Another aspect of studying unsaturated granular media is the movement of interstitial liquid due to the rupture of existing and formation of new liquid bridges. Shearing of the system causes re-distribution and transport of the interstitial liquid. We study both the phenomenon (i) re-distribution of liquid which is limited to smaller shear scales and (ii) liquid transport that is predominant at larger shear scales.



142nd MSS-Seminar
Wednesday, November 3rd,
15:30 hrs, H3,
Egerlandstr. 3, Erlangen.

MSS

History and Structure of Granular Sediments

Prof. Thorsten Pöschel

Institute for Multiscale Simulation

We consider the sedimentation of monodisperse granular particles under the influence of gravity. The history of the process is described by the surface of the sediment as a function of time. We show that the resulting structure of the sediment, characterized by the field of contact number is intimately related to the process of sedimentation such that the history of the process can be deduced from the time-independent field of contact number of the sediment.

143rd MSS-Seminar
Wednesday, November 10th,
15:30 hrs, Waebersaal,
Schottkystr. 10, Erlangen.

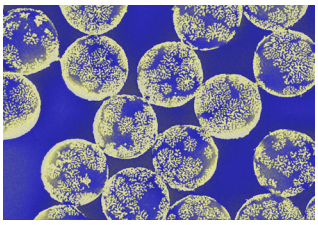
MSS

Crystal growth on spherical substrates: Inspiration from experiments

Prof. Robin Klupp Taylor

Chair of Particle Technology, University of Erlangen-Nuremberg

In this seminar I will introduce a simple and scalable method developed in my group to produce a new class of complex functional nanomaterial. The approach is based around the heterogeneous nucleation and growth of thin noble metal coatings on spherical core particles. Depending on the conditions used, these coatings can be dense or fractal in nature. The system presents both opportunities and challenges. I will give details of our attempts to understand the formation mechanism of the coatings and also show how the optical properties strongly depend on the morphology. The latter support the in situ analysis of the coating formation and, in future could enable autonomous production of particles with targeted function.



144th MSS-Seminar
Wednesday, November 17th,
15:30 hrs, H3,
Egerlandstr. 3, Erlangen.

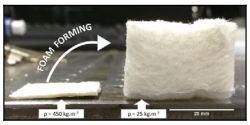
MSS

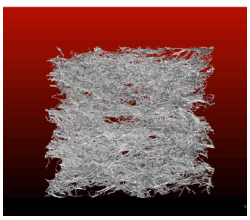
Properties of lightweight fibrous structures made by a foam forming technique

Prof. Matthias Möbius

School of Physics, Trinity College Dublin

The use of foam provides an attractive alternative method to produce lightweight, non-woven fibrous structures that can be used for thermal insulation or packaging. It not only reduces the usage of water compared to the traditional slurry-based methods, but also enables the processing of larger natural fibres such as peat that would sediment otherwise. Here we explore the influence of cellulose fibre concentration and liquid content of a foam-fibre dispersion on the mechanical properties of the fibrous samples that are produced from this dispersion. We find that the elastic modulus increases by a factor of up to seven just by changing the liquid content of the dispersion with no change in sample density. We investigate the microstructure of the fibrous material using µCT to obtain insight into the mechanical properties. We find that the liquid content of the foam fibre dispersion plays a major role in the orientation of fibres which determines the strength and anisotropy of the elastic response of the fibrous material.





3. Conference Presentations

- Michael Engel:
  Local point group symmetry analysis in particle simulation data (oral presentation)
  CECAM Workshop: Local Structure Meets Machine Learning in Soft Matter Systems
  28 June - 1 July, Lausanne, Switzerland
- Michael Engel:
  Newtonian Event-Chain Monte Carlo with Spheres and Polyhedra (oral presentation)
  Workshop ECMC
  May 11, 2021, online
- Aswathy Muttathukattil:
  Self-assembly of silica nanoparticles guided by directional crystallization of grafted polymers (oral presentation)
  DPG spring meeting (BPCPPDYSOE21)
  March, 2021, online
- Michael Engel:
  Building Block Design for Complex Structure and Chirality (oral presentation)
  Materials Research Meeting 2021
  13-17 Dec, 2021, Pacifico Yokohama North, Japan
- Michael Engel:
  Beyond the constraints of chemistry: Crystal structure discovery in particle simulation data (poster presentation)
  IRN-APERIODIC
  3-8 October, Carry-le-Rouet, France
- Michael Engel:
  Beyond the constraints of chemistry: Crystal structure discovery in particle simulation data (oral presentation)
  Twenty-Fifth Congress and General Assembly of the International Union of Crystallography
  14-22 August, Prague, Czech Republic
- Michael Engel:

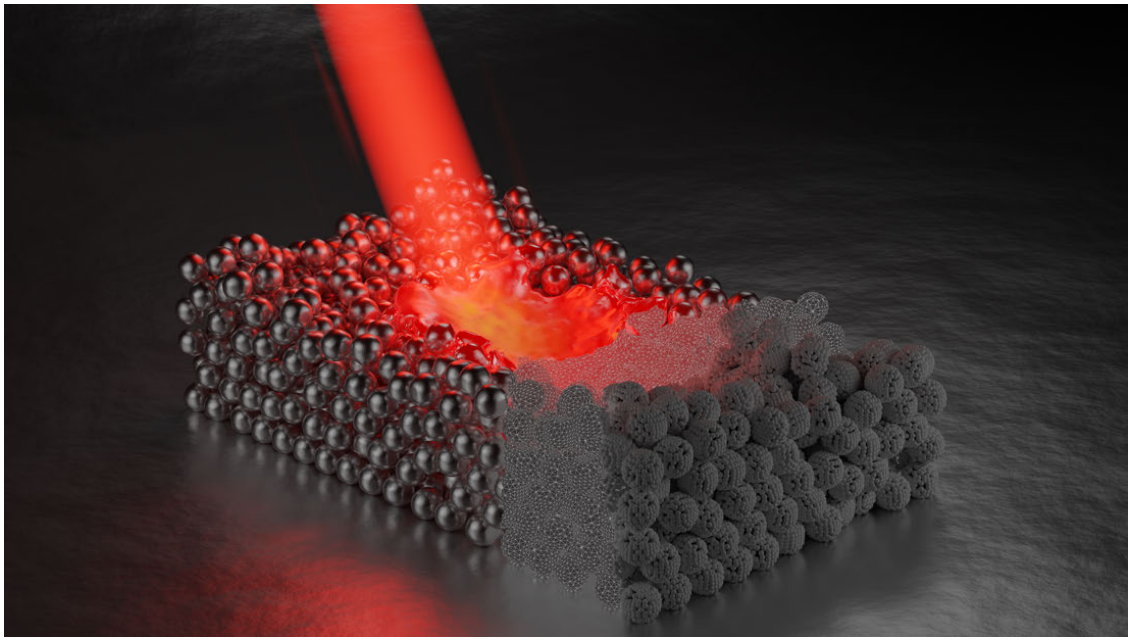
Free-energy calculation of partially ordered clusters (oral presentation)
SIAM Conference on Mathematical Aspects of Materials Science
18-22 May, 2021, online

- Federico Tomazic:
Coarse-Grained Simulation of Tripod Nanocrystal Assembly (poster presentation)
13th European Congress of Chemical Engineering and 6th European Congress of Applied Biotechnology
20-23 September, 2021, online
- Felix Buchele:
Numerics of Discrete Element Simulations in Milli-g Environments: Problems and Solutions (oral presentation)
Particles
4-5 October, 2021, Hamburg, Germany
- Valentina Marzulli:
Modeling Grain Fracture within DEM Simulations (oral presentation)
5th FRASCAL RTG-Seminar
23 April, 2021, online
- Michael Blank:
Simulation of the Selective Laser Melting (SLM) process of Titanium powder (poster presentation)
ProcessNet-Fachgruppensitzung MPH and CFD
9-10 March, 2021, online
- Alberto Leonardi:
Anisotropy of Thermal Disorder in Nanocrystals (oral presentation)
70th Denver X-Ray Conference
2-6 August, 2021, online
- Alberto Leonardi:
Thermal Disorder and Mechanical Anisotropy in Nanocrystals (oral presentation)
Shape and lattice deformation contributions to powder scattering (poster presentation)
25th IUCr Conference
13-22 August, 2021, online
- Federico Tomazic:
Effect of Steric Hindrance on the Self-Assembly of Crystallized Polymer Bundles (poster presentation)
Bunsen-Tagung
10-12 May, 2021, online
- Ali Mauricio Velasco Sabogal:
Modelling Grain Fracture within DEM Simulations (poster presentation)
5th FRASCAL RTG Seminar
23 April, 2021, online
- Nydia Roxana Varela-Rosales, Michael Engel:
Free energy calculations of 2D and 3D model quasicrystals (oral presentation)
International Research Network Open space between aperiodic order and physics
3-7 October 2021, Carry-le-Rouet, France
- Nydia Roxana Varela-Rosales:
Point group crystal structure analysis with machine learning (poster presentation)
CECAM Workshop: Local Structure Meets Machine Learning in Soft Matter Systems
Lausanne, Switzerland (28 Jun-1 Jul)
- Nydia Roxana Varela-Rosales:
Tiling simulations of oxide quasicrystal layers under external potential (oral presentation)
International Research Network Aperiodic meeting
21, May 2021, online

4. Ongoing PhD Projects

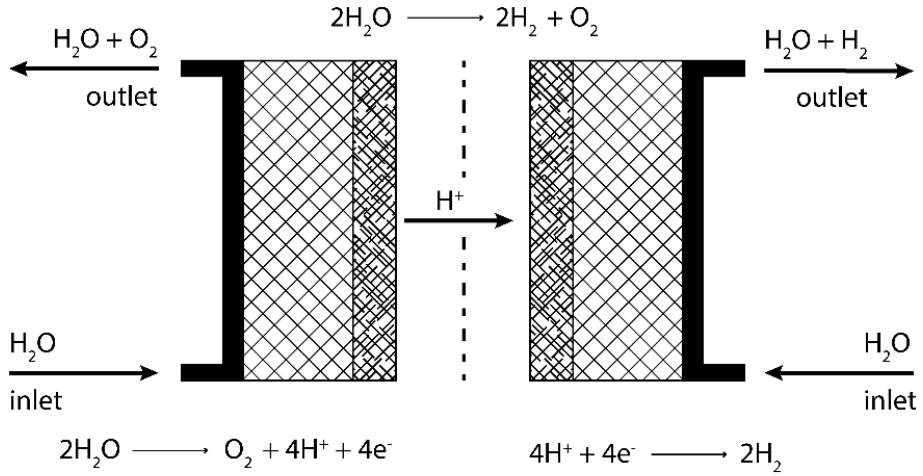
Michael Blank, "Simulation of the selective laser melting process"

We propose a numerical model based on the Smoothed Particle Hydrodynamics method that is capable to accurately model the energy transfer of a laser beam with an arbitrary energy distribution into a material with complex surface morphology as well as the melt pool dynamics. We employ a free-surface formulation where the gas phase is modeled using boundary conditions. We investigate the heat transfer into porous structures, the influence of the capillary forces and the thermocapillary motion under rapid heating and evaporation of the melt pool geometry. The formation of defects are observed and consequently minimized by adjusting the processing parameters.



Felix Buchele, "Reactive Flow in Porous Media"

With regard to the decarbonization required to stop the course of global warming, new technologies for energy storage and processing are required. One key technology that might help in the transition to a carbon neutral economy is hydrogen production by means of electrolyzers and its subsequent conversion to electricity by fuel cells. In particular electrolyzers are not yet market-ready and still require a substantial amount of research. This PhD thesis will address one of the most urgent problems regarding polymer electrolyte membrane (PEM) electrolyzers: gaining insight on the influence of porous catalyst and gas diffusion layer on the overall cell performance. Thereby it should be possible to reduce the amount of noble catalyst materials (Pt, Ir) thus reducing the cell and stack costs which are the main hindering factor for a widespread use of electrolyzers.



$$
\begin{aligned}
2\,H_2O &\xrightarrow{\Delta G_1} OH_{(ad)} + H^+ + e^- + H_2O \\
OH_{(ad)} + H^+ + e^- + H_2O &\xrightarrow{\Delta G_2} O_{(ad)} + 2\,H^+ + 2\,e^- + H_2O \\
O_{(ad)} + 2\,H^+ + 2\,e^- + H_20 &\xrightarrow{\Delta G_3} OOH_{(ad)} + 3\,H^+ + 3\,e^- \\
OOH_{(ad)} + 3\,H^+ + 3\,e^- &\xrightarrow{\Delta G_4} O_2 + 4\,H^+ + 4\,e^-
\end{aligned}
$$

$$
\begin{aligned}
2\,H^+ + 2\,e^- &\xrightarrow{\Delta G_1} 2\,H_{(ad)} && (\textit{Volmer-reaction}) \\
H_{(ad)} + H_{(ad)} &\xrightarrow{\Delta G_2} H_2 && (\textit{Tafel-reaction})
\end{aligned}
$$

$$
\begin{aligned}
H^+ + e^- &\xrightarrow{\Delta G_1} H_{(ad)} && (\textit{Volmer-reaction}) \\
H_{(ad)} + H^+ + e^- &\xrightarrow{\Delta G_2} H_2 && (\textit{Heyrovsky-reaction})
\end{aligned}
$$

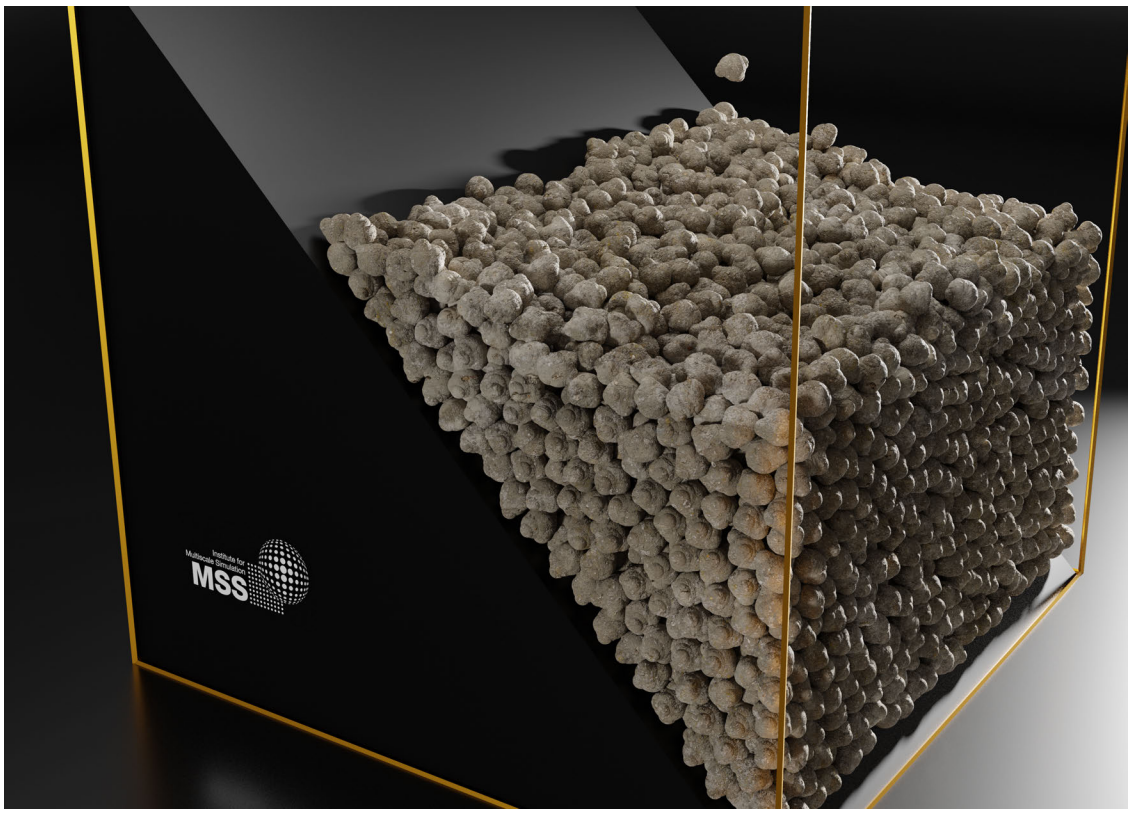
Angel Santarossa, “Mechanics of granular grippers”

Robotic granular grippers, which exploit the process of granular jamming to manipulate a vast range of diverse objects, represent a hugely promising nascent technology with potential applicability spanning almost all industrial sectors. While these soft-robotic grippers carry the potential to prove transformative to the modern manufacturing process, current-generation systems remain unoptimised and unreliable, and their microscopic dynamics and structures almost entirely unresearched.

The goal of this project is to start from the current gripper and improve its design while at the same time investigating its interior and gaining information about the ongoing microscopic processes. This is achieved by a close combination of experimental and computational method. In the experimental part we have developed a modular gripper setup that has specifically been designed to fit within an X-ray machine. Combined with an advanced image analysis technique, we are able to investigate the performance of the gripper as well as the internal granular structure experimentally. This setup is complemented by a newly implemented computational method that enables us to accurately simulate a robotic gripper.

Mauricio Velasco, "Fragmentation in large scale DEM simulations"

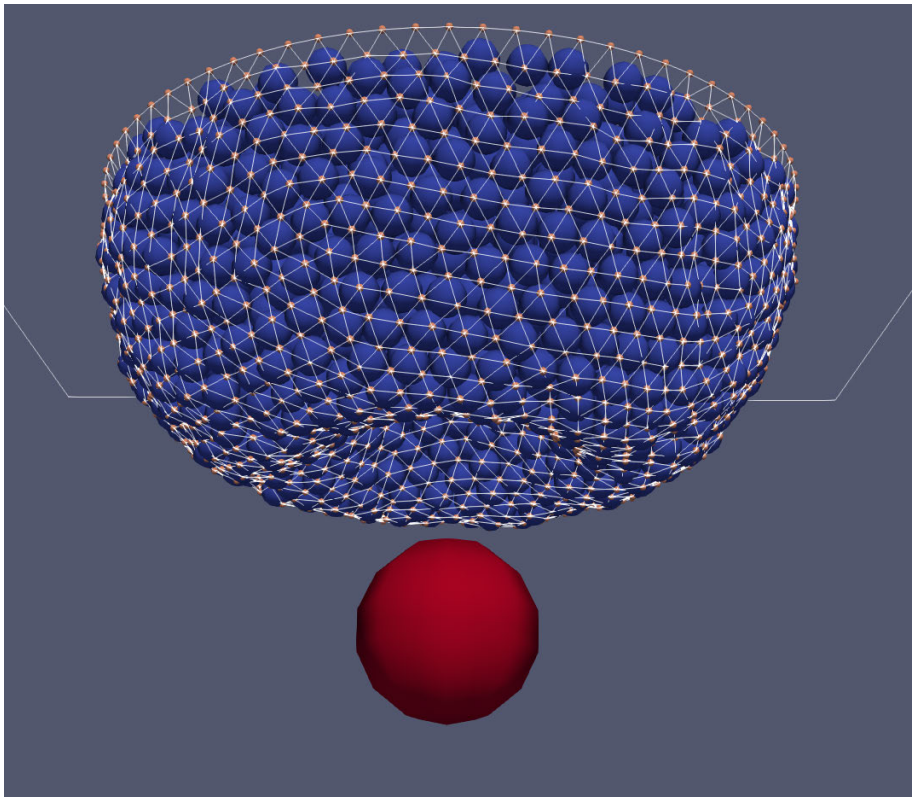
Grain and bulk fragmentation is a very important phenomena in the dynamics of granular media. In the field of cominution, the study of fragment shape and size distribution is of great relevance for industrial applications like milling and soils transporting. The aim of this project is to build an accurate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



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

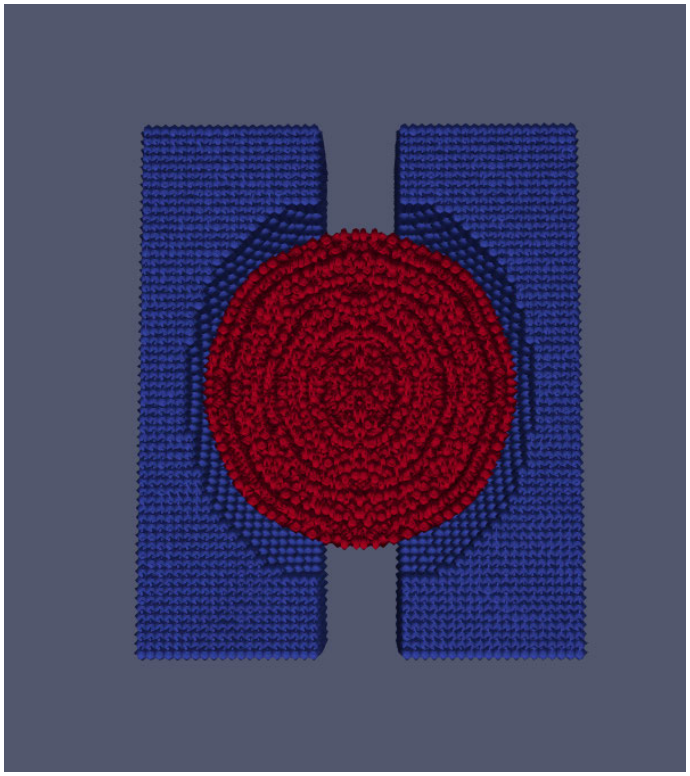
Within my PhD, I am focusing on the granular gripper. The granular gripper is a robotic end effector, that consists of particles enclosed by a flexible membrane. Such grippers exploit the process of granular jamming to manipulate a vast range of diverse objects and represent a hugely promising nascent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

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



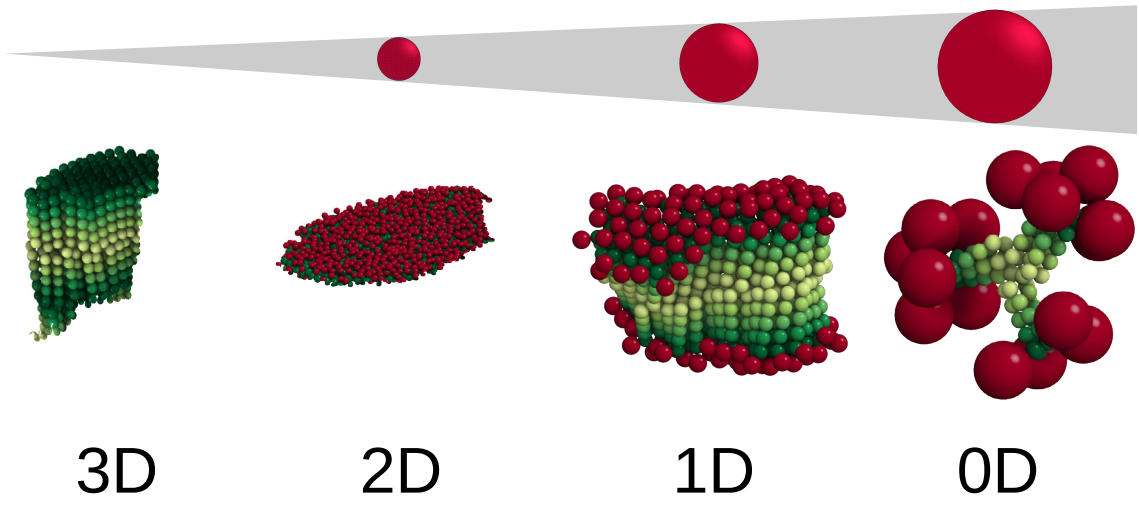
Sarthak Jadhaf, "Simulation of Selective Laser Melting (SLM) process for additive manufacturing"

The PhD project aims to develop computational simulation methods for elemtary processes in Selective Laser Melting (SLM) techniques. This includes DEM simulations in order to derive optimal strategies for the raking process of the powder bed using realistic material parameters, particle shapes, system geometries, and temperature depencence of the material parameters. It includes further the simulation of LASER melting processes using methods of particle-based fluid dynamics and ray-tracing techniques.
As an introducing mini-project to become familiar with the simulation techniques, we consider the formation of water drops in micro gravity. Aim of this mini-project is to develop a technique for producing spherical drops with minimal oscillations using the puddle jump effect, which is the ejection of drops from a mould with hydrophobic surface in the moment when gravity ceases. Oscillations can be reduced by chosing the geometric shape of the mold. Such a technique would help to perform experiments on imbibition of drops on porous surfaces in drop tower experiments.



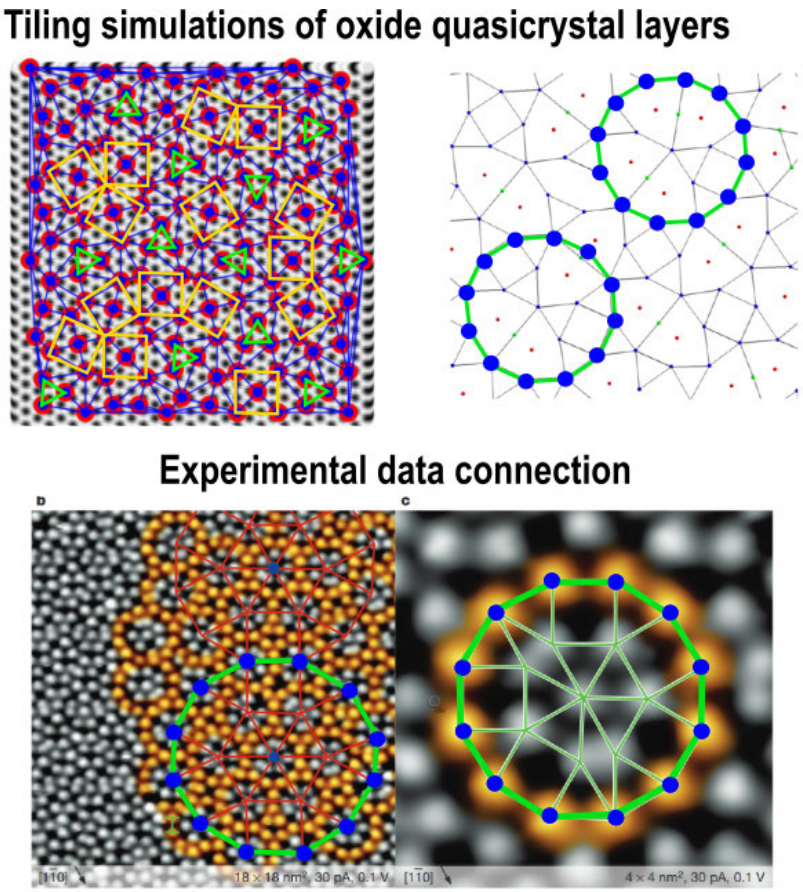
Federico Tomazic, “Modelling particle aggregation and assembly into optimal structures”

Nanoparticles and colloid building blocks are simulated via coarse-graining in order to predict and optimise the assembly of structural colour pigments and thin films and elucidate the aggregation processes which guide the synthesis of porous materials. In particular, new methods to model and simulate large numbers of complex, anisotropic particles are studied, in collaboration with the other groups part of the Collaborative Research Centre Design of Particulate Products. For example, the self-assembly of spherical nanoparticles grafted with polymers which exhibit directional crystallization are studied.



Nydia Roxana Varela-Rosales, "Simulations and thermodynamics of aperiodic crystals"

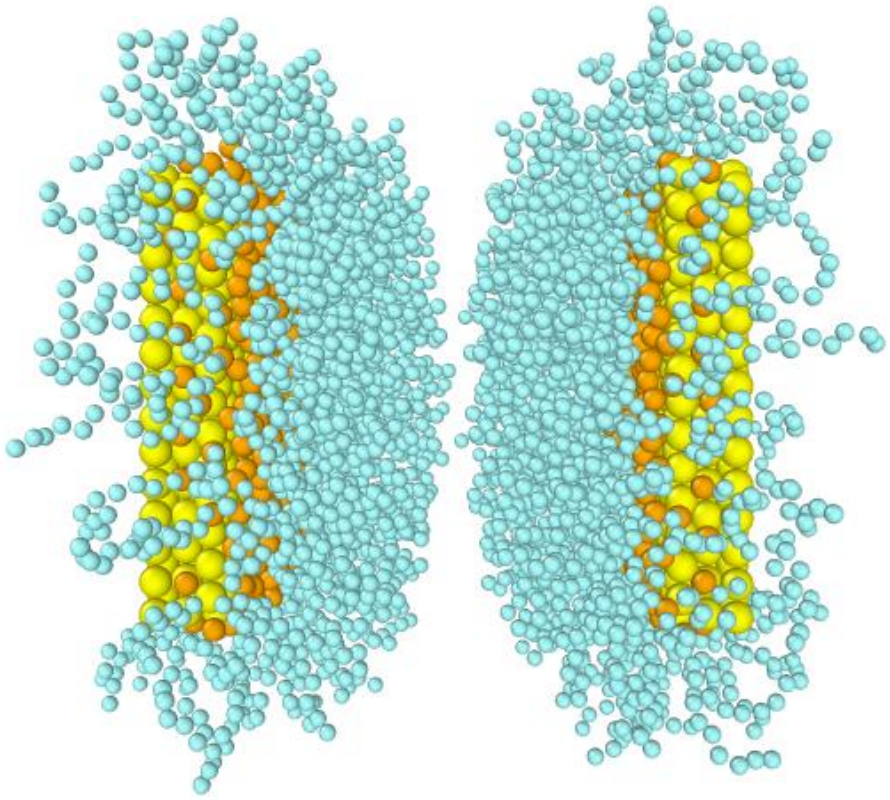
Quasicrystals are outstanding new materials that were recognized as stable phases a few years back. Because of their long-range order but lack of translational symmetry, these materials promise large technological applications in the fields of surface coatings, thermal insulators, photonic devices, etc. How can we simulate quasicrystals? This project consists of the study of the thermodynamics and simulations of these structures. In particular, we use free energy and point group analysis methods to characterize thermodynamic and symmetry properties of 2D and 3D quasicrystal structures. We have a close collaboration with experimentalists coming from an ANR-DFG French-German collaboration for joint projects in natural, life, and engineering sciences.



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

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

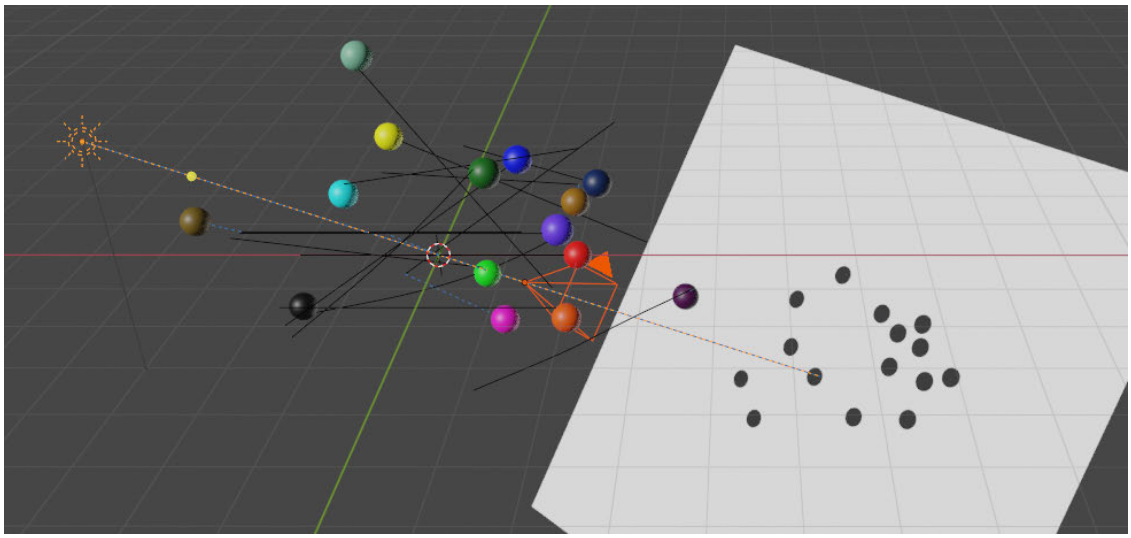
The purpose of this PhD research is to investigate the key factors that control the interaction between self-assembled monolayers, including temperature, pressure, ligand coverage, solvent effects, and the geometry of the surface. All research work is performed via molecular dynamics simulations in the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



Atharva Pandit, "Particle tracking and image reconstruction in multi-beam X-ray tomography"

The idea is to construct a device for full time-resoved (4D) Tomography. Instead of producing hundreds of images with one pair of x-ray source and detector and rotating the object to generate a 3d representation via Radon transformations or similar techniques, we use several pairs of X-ray sources and detectors. From these images, all made at the same time, we can locate the positions of many tracers and obtain 3D information with a time resolution of 100 fps or more.

The figure shows a simulation of dynamic tracer particles. Projections are cast on the detector due to the light emanating from the X-ray source



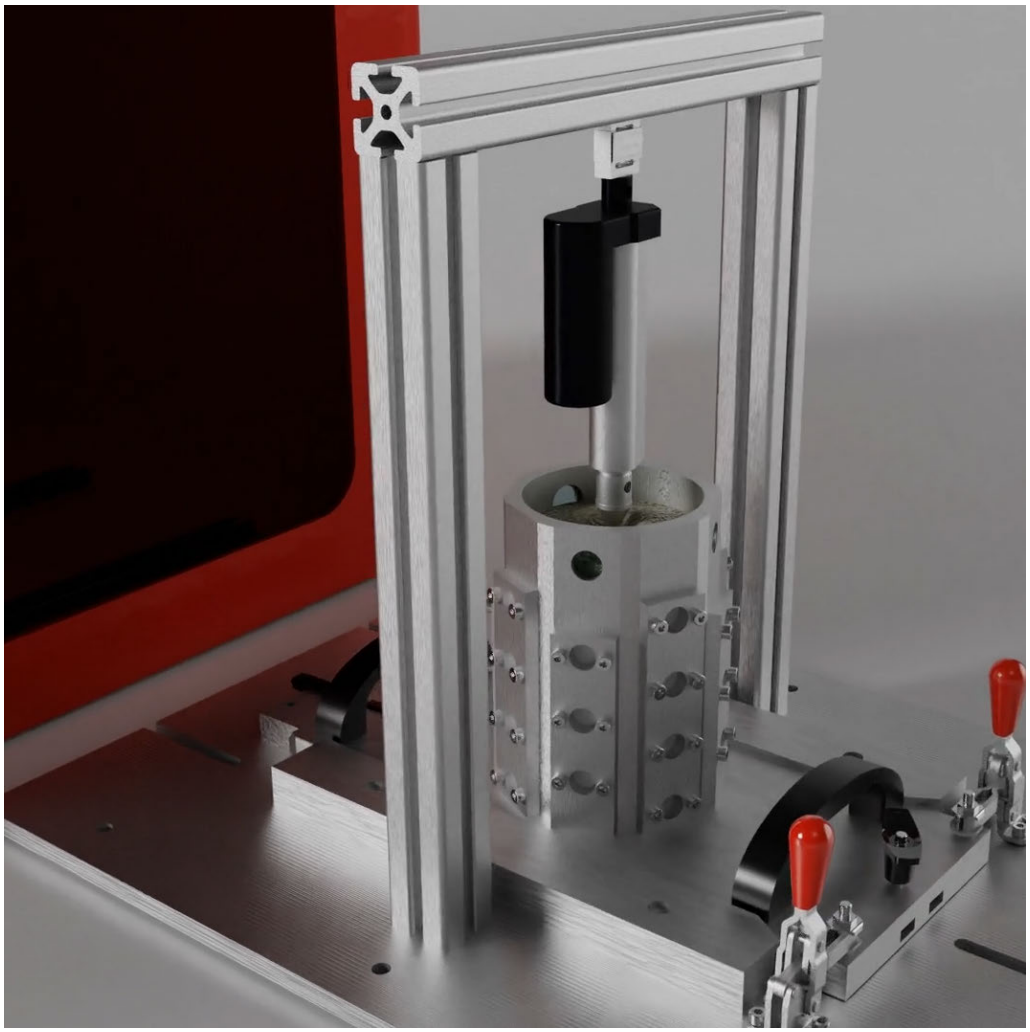
Valentina Marzulli, "Stress regimes within a layer of granular material during quasi-static penetration at different levels of gravity"

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

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

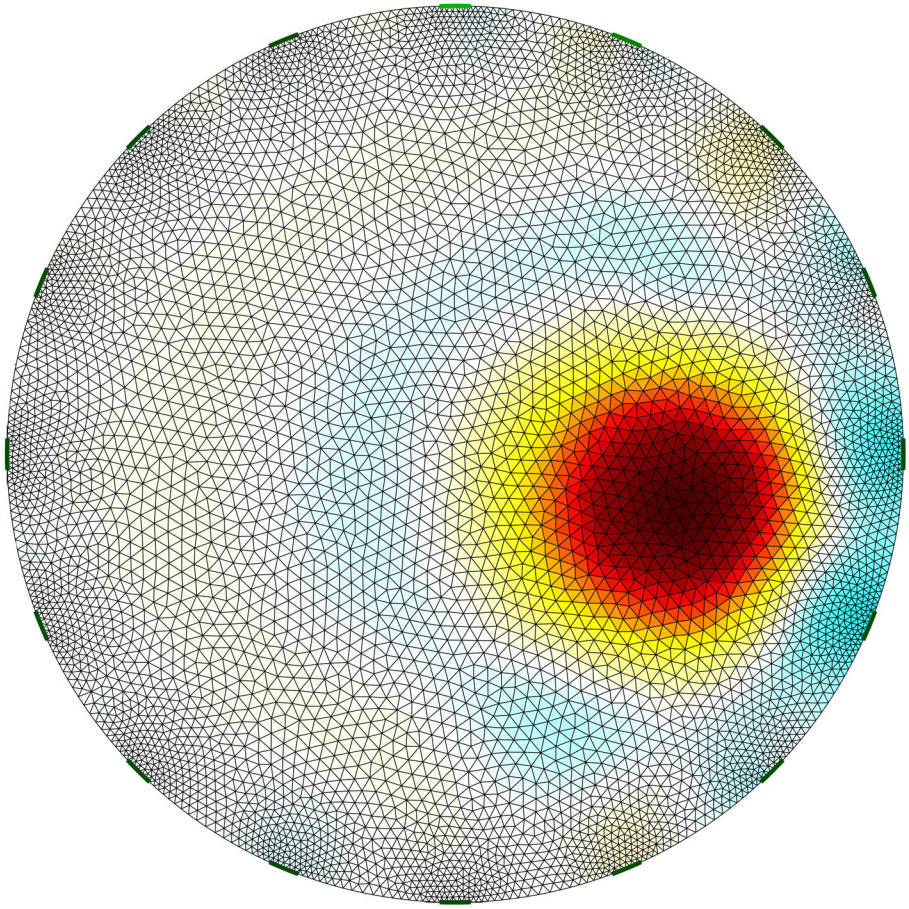
To gain further confidence to these results, complementary we will perform DEM simulations of the penetration process at $g < g_{\text{Earth}}$.

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



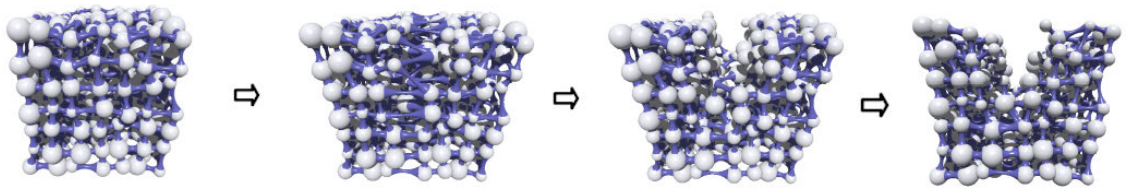
Ayman Ameen, "Image reconstruction for Electrical Impedance Tomography using AI approaches"

In this the thesis, we aim to explore and improve the state of the art techniques for image reconstruction of electrical impedance tomography (EIT). In the previous decades, EIT has gain a lot of interest due to its application in medicine and industrial applications. EIT has a lot of advantages compare to other visualization techniques such as non-invasiveness, and low cost.



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 is going to be 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 shall be parallelized.



5. PhD Graduations

Marco Klement, "Computational Studies of Anisotropic Particles"

Faculty: Physics / Dr. rer. nat.
Date: 01.06.2021
Chairman of the examination committee: Prof. Dr. Wolfgang Achtziger
Members of the examination committee: Prof. Dr. Michael Schmiedeberg, Prof. Dr. Tobias Unruh, Prof. Dr. Jan Kierfeld

After PhD defense.

Marco's PhD hut.

Fru Mbah Chrameh: "Numerical simulation of colloidal self–assembly in spherical confinement: From kinetics and thermodynamics to photonic colour"

Faculty: Chemical Engineering / Dr.-Ing.
Date: 11.11.2021
Chairman of the examination committee: Prof. Dr. Harting
Members of the examination committee: Prof. Dr. Engel, Prof. Dr. Vogel , Prof. Dr. Rüde.

After PhD defense

Chrameh's PhD Committee

6. Teaching Activities

image: fau.de

Main Courses

- **Computeranwendungen in der Verfahrenstechnik 1 (CIV1)**
  Lecture (Prof. Thorsten Pöschel)
  Exercise (Holger Götz, Felix Buchele)
  Tutorial (Sarthak Jadhav)
  Lab Course – Praktikum (Holger Götz)
- **Simulation granularer und molekularer Systeme (SIMSYS)**
  Lecture (Prof. Michael Engel, Prof. Thorsten Pöschel)
  Exercise (Prof. Michael Engel, Prof. Thorsten Pöschel)
  Lab Course (Dr. Alberto Leonardi, Holger Götz)
- **Basics in Computational Materials Science and Process Simulation (B_Compu_1)**
  Lecture (Prof. Michael Engel, Prof. Andreas Bück, Dr. Manuel Münsch, Dr. Frank Wendler)
- **Selbstorganisationsprozesse (SOP)**
  Lecture (Prof. Michael Engel, Prof. Nicolas Vogel, Prof. Robin N. Klupp Taylor)
  Exercise (Prof. Michael Engel, Prof. Nicolas Vogel, Prof. Robin N. Klupp Taylor)
- **Partikelbasierte Strömungsmechanik (PSTM)**
  Lecture (Prof. Thorsten Pöschel)
  Exercise (Michael Blank)
- **Scannen und Drucken in 3D (SD3D)**
  Lecture (Dr. Patric Müller)
  Exercise (M. Sc. Felix Buchele, Dr. Patric Müller)
  Practicum (M. Sc. Felix Buchele, Dr. Patric Müller, M. Sc. Michael Blank, Dr. Achim Sack, Dr. Michael Heckel, Walther Pucheanu)
- **Maschinelles Lernen und Künstliche Intelligenz im Ingenieurwesen (KI-ING)**
  Lecture (Dr. Patric Müller)
  Exercise (M. Sc. Holger Götz, Dr. Patric Müller)
  Practicum (Dr. Patric Müller)

- **Digitale Bildverarbeitung (DBV)**
  Lecture (Dr. Achim Sack)
  Lab Course (Dr. Achim Sack)
- **Messtechnik 2 - Messmethoden und Analytik (MT2)**
  Lecture (Dr. Achim Sack)
  Lab Course (Dr. Achim Sack)

Smaller Courses

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

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

14.01.2021	Nydia Roxana Varela-Rosales	*Tiling simulations of oxide quasicrystal layers under external potential*
22.01.2021	Dr. Muttathukattil Narayanan Aswathy	*Grafted Polymers to Program Self assembly of Colloidal Nanoparticles*
29.01.2021	Nydia Roxana Varela-Rosales	*Solid-Angle Nearest Neighbors for Size-disperse Systems of Spheres*
05.02.2021	Luis Torres	*X-ray multiaxes reconstruction of granular flows: Calibration*
12.02.2021	Ali Mauricio Velasco Sabogal	*Multiscale Fractures in Granular Materials*
19.02.2021	Fru Mbah Chrameh	*Numerical simulation of colloidal self-assembly in spherical confinement*
26.02.2021	Prof. Leopoldo Gómez	*Structure of Entangled Filamentous Matter: Linear vs Rings*
12.03.2021	Federico Tomazic	*Numerical Methods for structural Colour Representation*
19.03.2021	Dr. Achim Sack	*In-Situ tracer generation in Eu:SrAl2O4*
26.03.2021	Michael Blank	*Simulation of the selective LASER melting process of titanium powder*
09.04.2021	Kamilia Gabaidullina	*Molecular simulation of the spray-drying process for the fabrication of magnetic supraparticles*
16.04.2021	Felix Buchele	*Optimizing Rover Wheel Geometries by Means of DEM Simulations*
23.04.2021	Dr. Igor Goychuk	*Nonequilibrium phase transition to superdiffusion in a basic model of nonlinear Brownian motion*
03.05.2021	Nydia Roxana Varela-Rosales	*Tiling simulations of oxide quasicrystal layers under external potential*
07.05.2021	Holger Götz	*Towards a granular neural network solver*
14.05.2021	Nydia Roxana Varela-Rosales	*Free energy calculations of quasicrystals*
04.06.2021	Prof. Leopoldo R. Gómez Dr. Nicolas García Prof. Thorsten Pöschel	*Ring-Linear Mixtures of Rubber Bands*

11.06.2021	Dr. Patric Müller	*Rarefied reactive gas flow in T-shape microreactors*
18.06.2021	Federico Tomazic	*Monte Carlo Ray Tracing for Structural Colour Representation*
25.06.2021	Dr. Achim Sack	*Granular flow in a rotating drum*
02.07.2021	Angel Santarossa	*3D Imaging of Hydraulic Fractures in gels by means of X-ray tomography*
16.07.2021	Dr. Muttathukattil Narayanan Aswathy	*Geometrically Frustrated Assembly*
16.07.2021	Michael Blank	*Contact angle, wetting and temperature gradient driven flow in free surface ISPH*
23.07.2021	Michael Blank	*Contact angle, wetting and temperature gradient driven flow in free surface ISPH*
06.08.2021	Felix Buchele	*Modelling of ceramic foams for SPH simulations*
13.08.2021	Sarthak Jadhav	*Size effect on surface segregation in bimetallic nanoparticles*
20.08.2021	Nydia Roxana Varela-Rosales	*Effect of external potential on 2d dodecagonal quasicrystal*
27.08.2021	Dr. Igor Goychuk	*Origin of nonequilibrium oscillations of overdamped Brownian particles in nonlinear viscoelastic media*
10.09.2021	Prof. Leopoldo Gómez	*Understanding Hydraulic Fracture through X-Ray Tomography*
17.09.2021	Dr. Patric Müller	*Soft particles reinforce robotic grippers: robotic grippers based on granular jamming of soft particles*
17.09.2021	Theresa Rogge	*Simulation des Ablagerungsprozesses von Metallpulvern fürSLM Prozesse*
24.09.2021	Federico Tomazic	*Coarse-Grained Simulation of Tripod Nanocrystal Assembly*
04.10.2021	Nydia Roxana Varela-Rosales	*Free energy calculations of 2D and 3D model quasicrystals*
08.10.2021	Michael Blank	*Simulation of wire-based LASER metal deposition of titanium using SPH*
15.10.2021	Meysam Bagheri	*Numerical Study of Solid Particle Transport in an Obstructed Channel Flow*

22.10.2021	Atharva Pandit	*Slow dynamics of dense colloidal suspensions in two and three dimensions*
29.10.2021	Holger Götz	*Simulating the Granular Gripper*
12.11.2021	Federico Tomazic	*Coarse-Grained Simulation of Tripod Nanocrystal Assembly*
19.11.2021	Dr. Patric Müller	*Soft particles reinforce robotic grippers: robotic grippers based on granular jamming of soft particles*
26.11.2021	Angel Santarossa	*Enhancing granular grippers´ performance through soft particles: Experimental part*
03.12.2021	Ali Mauricio Velasco Sabogal	*Fractures on brittle materials with Multi-sphere DEM grains linked by elastic beams*
10.12.2021	Felix Buchele	*SPH simulations in porous geometries*

Special course: Advanced Lattice Boltzmann Simulations

This course was done by Prof. José-Daniel Muñoz from the Simulation of Physical Systems Group, Department of Physics, Universidad Nacional de Colombia, Bogotá. It was a four-session crash course that introduced LBM and showed applications on waves, fluids and electromagnetic fields.

MSS-Seminar
CIP-Pool, Konrad-Zuse-Str. 3-5
16.11.21, 14:15-15:45 18.11.21, 14:15-15:45
23.11.21, 14:15-15:45 25.11.21, 14:15-15:45

MSS

Crash Course: Advanced Lattice Boltzmann Simulations

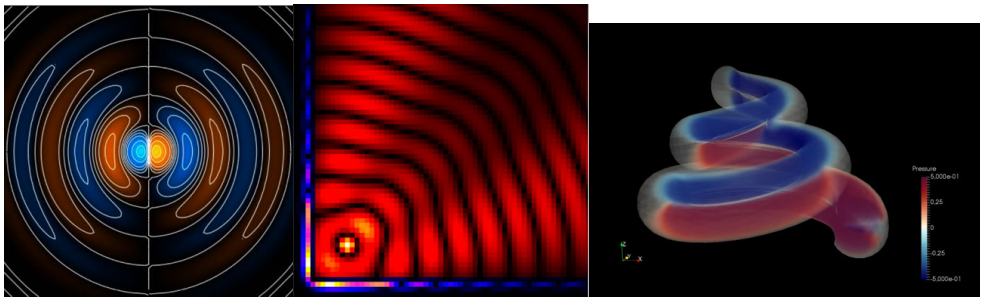
Prof. José-Daniel Muñoz

Simulation of Physical Systems Group, Department of Physics, Universidad Nacional de Colombia, Bogotá

In this seminar I will introduce a simple and scalable method developed in my group to produce a new class of complex functional nanomaterial. The approach is based around the heterogeneous nucleation and growth of thin noble metal coatings on spherical core particles. Depending on the conditions used, these coatings can be dense or fractal in nature. The system presents both opportunities and challenges. I will give details of our attempts to understand the formation mechanism of the coatings and also show how the optical properties strongly depend on the morphology. The latter support the in situ analysis of the coating formation and, in future could enable autonomous production of particles with targeted function.

Lattice-Boltzmann methods (LBM) are powerful schemes to reproduce the time evolution of many systems, including fluids, acoustics, electrodynamics, and even general relativity. In contrast with other methods that also divides the space into cells (like FEM or CFD), information flows from cell to cell transported by hypothetical particles that collide each other reproducing in the macroscopic limit the desired partial differential equations. So, each cell can evolve without asking the neighboring cells for information, making LBM full-parallelizable schemes. They are also very easy to implement, and results can be obtained from scratch in just a single session.

This four-session crash course introduces LBM and shows applications on waves, fluids and electromagnetic fields. It starts from scratch, intended for anyone programming on C++ or Python that has never tried a LBM before, but it also illustrates on further possibilities and introduces some advanced applications, like waves on curvilinear coordinates or electrodynamics. The course is planned as a hands-on workshop, where each one works on his/her laptop computer with a plain text editor (like Emacs), a plotter (like Gnuplot) and a C++ compiler (like g++). If you don't have those programs installed on your computer, a virtual machine will be also at disposal to download on a USB, that you can reboot and work from there.



7. Graduations

Master theses

- **Kamilia Gabaidullina, "Molecular simulation of the spray-drying process for the fabrication of magnetic supraparticles"**

  We simulate a supraparticle formation reproducing the spray drying process with the coarse-grained molecular dynamics using HOOMD-blue package. This project is in collaboration with The Supraparticle Group from the inorganic chemistry department. The aim of this work is to develop a new single droplet model that will help to predict the morphology of a supraparticle at various simulation parameters. The model consists of the mass-spring spherical confinement and colloidal particles generated inside it. We investigate the properties of the shell to ensure its stability and robustness. Different morphologies of supraparticles are observed and characterized in terms of segregation. Moreover, the pore-size distribution of porous supraparticles is calculated.

- **Theresa Rogge, "Simulation of the Recoating process of metal powder in SLM processes"**

  Additive manufacturing (AM) has already been on the rise for several years and offers many advantages, such as great freedom in geometry and material savings. However, the product quality is not yet high enough to become widely accepted in manufacturing. In laser-based processes such as selective laser melting (SLM), the formation of spatters can occur. These can lead to deterioration of the recoating and thus the powder layer, which can result in defect formation. Therefore, in this work, simulations of powder spreading in SLM are carried out using the discrete element method (DEM). In these simulations, a multi-sized, spherical titanium powder is simulated, taking into account cohesive forces, Van der Waals interactions and frictional forces. In order to simulate the powder as realistically as possible, the titanium powder from *APandC* with a size range of $15\mu m - 45\mu m$ is investigated and the results are taken into account in the simulations. Since the influence of spatters on the coating is to be investigated, a printed layer with an attached spatter is inserted into the simulation domain and its influence on the packing density, surface roughness and filling height of a recoated

powder layer is investigated. A blade is used for the recoating and the speed is varied between 140 mm/s and 60 mm/s. It was found that at a velocity of 60 mm/s the lowest roughness values and the highest packing densities as well as filling heights are obtained. Furthermore, it was found that the packing density and the filling height decrease with blade velocity, while the surface roughness increases. It was observed that, contrary to expectation, the presence of an obstacle such as a spatter has a positive influence on the packing density and the filling height. This leads to a lower sensitivity of the mentioned criteria to a fast velocity of the recoating device and is related to the build-up of powder in front of the obstacle.

- **Abeer Al-Ani, "Homogenization of fluid driven granular pipe flow"**

  The clogging of a dense stream of particles occurs vastly in both natural and industrial fields. Since most of jamming phenomena lead to negative effects on the flow stream, studying and preventing jamming is of critical importance. Following a previous work of [2], which investigated the clogging of particle gravity-driven flows in vacuum and affirmed the possibility of attaining steady material transport by adding a helical structure to the inner wall of the pipe without the need for energy input from any external source. In the current study, we reproduced and extended this method by using ANSYS Fluent and investigating the effect of air presence on the gravitationally driven pipe flow. We employed the Macroscopic Particle Model (MPM) for particles modelling and Computational Fluid Dynamics (CFD) for the two-way coupling of air-particle interaction. Results showed that flow in both vacuum and air is inhomogeneous and characterized by intermittent flow and density waves. We investigated the effect of the helical texture on particle flow by comparing gravity-driven flow with and without helix structure. We found that the helix texture promotes more homogenous particle flow along the pipe in vacuum, whereas the helix in the presence of air could not completely collapse the clusters, as there are still small groups of colloidal particles in some regions. Furthermore, we examined fluid-driven jamming and found that the complex effects of initial solid concentration and fluid velocity have a direct impact on the occurrence of jamming.

- **Alice Bellettini,"Free energy calculation in many-body particle systems with coupled molecular simulations"**

  Free energy calculations play a role in a broad field of applications, which involve the tailoring of particles self-assembly. In this work, some algorithms for free energy calculation, applied to (finite) hard-spheres systems are studied; the system evolution is here simulated via Monte Carlo sampling. The introduction is followed by an overview of the basics of classical statistical mechanics, limited to the concepts of use in this thesis. The starting point of the study is then a thermodynamic integration algorithm proposed by Frenkel and Ladd for crystalline phases. Following on from a previous work, this method is modied for applications to other phases and its performance is tested. High accuracies are achieved for fluid and crystalline systems outside the phase transition density range. Conversely, in such range, the systematic errors do not completely vanish, within a reasonable runtime. Further on, a new route for thermodynamic integration is introduced and tested ("coupling"). Here, the aim is to minimize the thermodynamic integration path in order to overcome the systematic errors still present via the first route. This method results to bring improved results only in very specific cases. Finally, a different approach for free energy calculations, based on sampling the system's trajectory in the phase space, is tested and its insights on the thermodynamics of hard-spheres discussed.

Miniprojects

- **Jonathan Martín González, "Monte Carlo Ray-Tracing Algorithm for Color Prediction of Photonic Crystals"**

  Photonic crystal are promising materials for their unique properties to control the light, prospected applications go from filters, to waveguiders or even optical transistors have been suggested. However, their properties are defined by their nanostructure, so being able to determine the given properties for a defined nanostructure, monitor their structure during the synthesis or the one of the final product is crucial for the further development of this type of materials. One way to learn about the nanostructure of these crystals is through their structural color. The approach of this project is the prediction of the structural color using a Monte Carlo ray-tracing algorithm, which will be studied and optimized for its application in 3D crystals.

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

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

- **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.

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

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

- **Omar Zeair,, "Simulating Disorder Order Transformation in Cu Pd Alloy Nanoparticles"**

  We investigate disorder to order transformations of copper palladium alloy nanoparticles using a hybrid molecular dynamics Monte Carlo scheme. The scheme involves blocks of

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

8. Service for the Scientific Community

Editorial Boards

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physchem

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

Dr. Igor Goychuk
Editorial Board Member since 2021

Fluctuation and Noise Letters -
World Scientific

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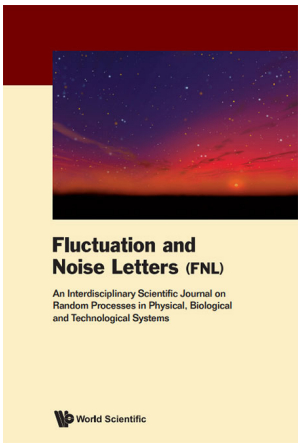

Dr. Igor Goychuk
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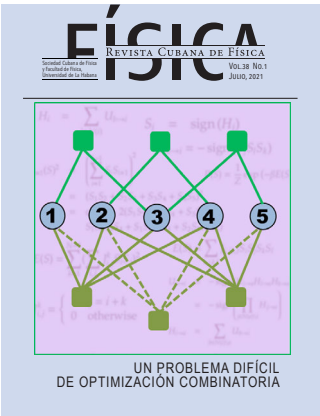

Prof. Thorsten Pöschel
Senior Editor since 2014

Computational Particle Mechanics
Springer/Nature

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

Prof. Thorsten Pöschel
Editorial Board Member since 2014
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Granular Matter
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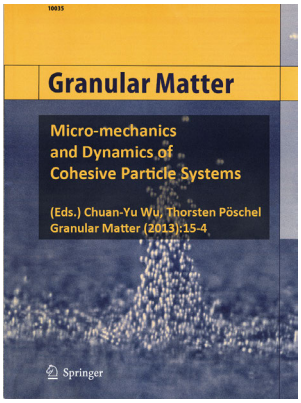

Prof. Thorsten Pöschel
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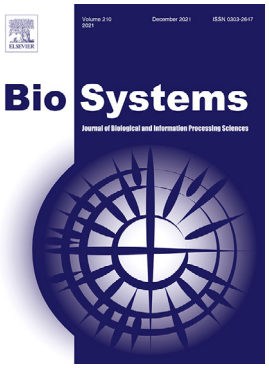

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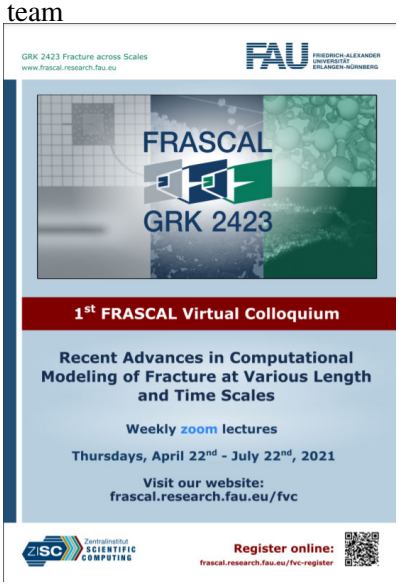
Associate Editor since 2003

Conference Organization

1st FRASCAL Virtual Colloquium
22 July, 2021, Erlangen, online

Ali Mauricio Velasco Sabogal – Organization team



Structure, modeling and properties of quasicrystals – Minisymposium
25th Congress of the International Union of Crystallography
22 July, 2021, Prague, online

Prof. Michael Engel – organizer

Artificial Intelligence & Optimisation
Virtual room at the 13th European Congress of Chemical Engineering
23 September, 2021, online

Prof. Michael Engel – organizer

Particles'2021

4.-6. October 2021, Hamburg, online

Prof. Thorsten Pöschel – Scientific Committee

Powders & Grains 2021

5. July - 6. August, 2021, Buenos Aires, online

Prof. Thorsten Pöschel – Scientific Committee

Online-Seminar: Geometry and Packing in Materials Science & Biology

`https://geompack.com`

Geometry and Packing in Materials Science and Biology is a series of webinars to share new insights into the application of geometry and packing problems to topics in materials science and biology. All researchers broadly interested in these topics are welcome to attend. The goal of these virtual meetings is to promote the exchange of ideas and foster collaboration.
Presentations are forty minutes long followed by another twenty minute period for questions and discussions.
The webinars will be via zoom and (depending on the discretion of the speaker) recordings of previous webinars will be available as YouTube videos.

Organizers: Adil Mughal, Greg Grason, Miranda Holmes-Cerfon, **Michael Engel**, Reidun Twarock, Stephane Douady, Joseph D. Paulsen

March 24, 2021	Elisabetta Matsumoto
	Twisted topological tangles or: the knot theory of knitting
April 7, 2021	Marjolein Dijkstra
	Packing, geometry & entropy: Crystallization of spheres in a sphere
April 21, 2021	Sascha Hilgenfeldt
	Placement and Symmetry of Singularities on Curved Surfaces
May 5, 2021	M. Lisa Manning
	Biological tissues as mechanical metamaterials
May 19, 2021	Vinothan N. Manoharan
	Braiding wires using capillary forces
June 2, 2021	Giuliana Indelicato
	From viral capsids to self-assembling nanoparticles
September 29, 2021	Joey Paulson
	The Wrinkle-to-Crumple Transition in Thin Elastic Solids
October 13, 2021	Sara Skrabalak
	Symmetry Making and Breaking in Seeded Syntheses of Metal Nanocrystals

October 27, 2021	Myfanwy Evans *From cylinder packings to auxetic periodic tensegrity structures*
November 10, 2021	Nicolas Vogel *Colloidal clusters from confined self-assembly: Structure – Thermodynamics – Formation kinetics*
November 24, 2021	Martin Lenz *Slimming down through frustration*
December 8, 2021	David Nelson *Fractional defect charges for liquid crystals on cones*

Activities within the University Self-Administration

Library Commission of the University, Representative of the Faculty of Engineering	Prof. Thorsten Pöschel
Central Institute for Scientific Computing of the Friedrich-Alexander University Erlangen-Nuremberg, executive board	Prof. Thorsten Pöschel
Competence Unit for Scientific Computing (CSC), founding member, head of “Application Lab Particles”	Prof. Thorsten Pöschel
[redacted]	
[redacted]	
Council of the Faculty of of Engineering	Prof. Michael Engel
Habilitation Committee of the Faculty of Engineering	Prof. Thorsten Pöschel
Council of the Department for Chemical and Biological Engineering	Prof. Thorsten Pöschel Dr. Patric Müller
Study Grants Committee	Prof. Michael Engel
Study Commission, Study program manager CEN	Prof. Michael Engel
Spokesman of the early-stage researchers (habilitands) of the Department for Chemical and Biological Engineering	Dr. Patric Müller
PR-Team of the Department for Chemical and Biological Engineering	Ulrike Hansl
Interdisciplinary Center for Nanostructured Films, cooperative head	Prof. Thorsten Pöschel
Executive Board Member and Focal Subject Head for Computational Materials Science and Process Simulation, Advanced Materials and Processes (MAP)	Prof. Michael Engel

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.

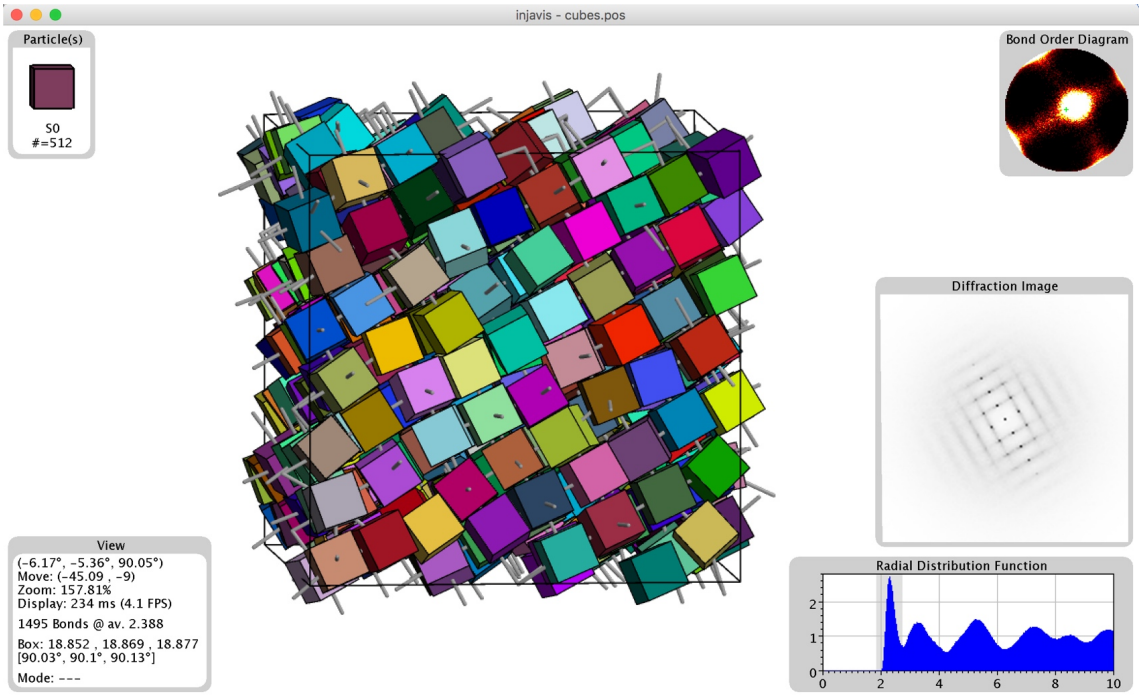


Figure: Screenshot of injavis showing a snapshot of a simulation of hard cubes. (top left) particle module; (top right) bonds module; (middle right) diffraction module; (bottom left) view module; (bottom right) RDF module

9. Awards

Humboldt fellow of MSS is awarded honoris causa doctorate

By the decision of the Academic Council of the ICMP of the National Academy of Sciences of Ukraine, the title of Doctor honoris causa was conferred on Stefan Sokołowski (Marie Curie-Skłodowska University, Lublin, Poland) for the development of the density functional theory for spatially restricted systems, pioneering studies on granular materials, adsorption, phase transitions, various mixing/demixing phenomena in fluids, simulations of polymers and hairy particles in bulk and in pores, as well as for your strong involvement in various forms of scientific collaboration with our Institute and your prolific contribution as an author and an active member of the Editorial board of the Condensed Matter Physics journal. `icmp.lviv.ua/en/content/stefan-sokolowski`
In 2012, Prof. Stefan Sokołowski was Humboldt fellow at our institute MSS. Currently, he works at the Department for Theoretical Chemistry of the Maria Curie-Skłodowska University in Lublin, Poland.

Prof. Stefan Sokołowski. Credits: https://icmp.lviv.ua/en/content/stefan-sokolowski
`lublin.gosc.pl/doc/6729146.Prof-Stefan-Sokolowski-doktorem-honoris-causa-Narodowej`

For more information on Stefan, see: M. Borówko, J. Ilnytskyi, O. Pizio: “Exploring fluid-solid interfaces with Stefan Sokołowski. Condensed Matter Physics **19**, 10101 (2016)

10. 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**

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

- “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. Dr. Ralf Stannarius (Otto-von-Guericke-Universität Magdeburg)

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

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

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

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

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

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

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

Germany), M. Sperl (Cologne, Germany), N. Vandewalle (Liège, Belgium)

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

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

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

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

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

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

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

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

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

Cooperations with Industry (Funding)

- "Tomographic Investigation of Failure in Ceramic Feedthroughs"
  Fa. BIOTRONIK SE & Co. KG, Berlin
  Entwicklungsservice CRM Komponenten, Nürnberg
  project lead **Dr. Achim Sack**
- "Simulationen der Warmeleitfähigkeit von Keramikschäumen und weiteren Dämmstoffen"
  ("Simulations of the thermal conductivity of ceramic foams and other insulating materials")

Fa. Schlagmann Poroton GmbH & Co. KG, Zeilarn
project lead **Dr. Patric Müller**

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

11. Publications

Scientific papers published by MSS in 2021 in reviewed journals

[1] Igor Goychuk and Thorsten Pöschel, "Nonequilibrium phase transition to anomalous diffusion and transport in a basic model of nonlinear Brownian motion", *Physical Review Letters*. 127, 110601. (2021).

[2] Igor Goychuk and Thorsten Pöschel, "Fingerprints of viscoelastic subdiffusion in random environments: revisiting some experimental data and their interpretations", *Physical Review E*. 104, 034125. (2021).

[3] Valentina Marzulli, Chitta Sai Sandeep, Kostas Senetakis, Francesco Cafaro, and Thorsten Pöschel, "Scale and water effects on the friction angles of two granular soils with different roughness", *Powder Technology*. 377, 813–826. (2021).

[4] Daniel S. Nasato, Heiko Briesen, and Thorsten Pöschel, "Influence of vibrating recoating mechanism for the deposition of powders in additive manufacturing: discrete element simulations of polyamide 12", *Additive Manufacturing*. 48, 102248. (2021).

[5] Christian Scholz, Anton Ldov, Thorsten Pöschel, Michael Engel, and Hartmut Löwen, "Surfactants and Rotelles in Active Chiral Fluids", *Science Advances*. 7, eabf8998. (2021).

[6] Tim Wenzel, Achim Sack, Patric Müller, Thorsten Pöschel, Sonja Schuldt-Lieb, and Henning Gieseler, "Stability of freeze-dried products subjected to microcomputed tomography radiation doses", *Journal of Pharmacy and Pharmacology*. 73, 212–220. (2021).

[7] Song-Chuan Zhao and Thorsten Pöschel, "Spontaneous formation of density waves in granular matter under swirling excitation", *Physics of Fluids*. 33, 081701. (2021).

[8] Holger Götz, Angel A. Santarossa, Achim Sack, Thorsten Pöschel, and Patric Müller, "Soft particles reinforce robotic grippers, Robotic grippers based on granular jamming of soft particles", *Granular Matter*. 24, 31. (2021).

[9] Ali Shakeri, Daniel Schiochet Nasato, Patric Müller, Harol Torres Menéndez, and Thorsten Pöschel, "A robust numerical method for granular Hydrodynamics in Three Dimensions", *Journal of Fluid Mechanics*. 917, A33. (2020).

[10] Mubashir Hussain and Patric Müller, "Rarefied reactive gas flow in T-shape microreactors", *Applied Thermal Engineering (submitted)*. 185, 116308. (2021).

[11] Thomas Weinhardt, Jeremy Lechman, and Thorsten Pöschel, "Fragmentation and Abrasion in Granular Matter Systems", *Computational Particle Mechanics*. 8, 1003–1004. (2021).

[12] Seyed Habibollah Ebrahimnazhad Rahbari, Michio Otsuki, and Thorsten Pöschel, "Fluctuations and like-torque clusters at the onset of the discontinuous shear thickening transition ingranular materials", *Nature-Communications Physics*. 4, 71. (2021).

[13] Prapanch Nair, Sebastian Mühlbauer, Shantanu Roy, and Thorsten Pöschel, "Can Minkowski tensors of a simply-connected porous microstructure characterize its permeability?", *Physics of Fluids*. 33, 042010. (2021).

[14] Igor Goychuk and Thorsten Pöschel, "Insufficient evidence for ageing in protein dynamics", *Nature*. 17, 773–774. (2021).

[15] Julián M. Gómez-Paccapelo, Angel A. Santarossa, H. Daniel Bustos, and Luis A. Pugnaloni, "Effect of the granular material on the maximum holding force of a granular gripper", *Granular Matter*. 23, 4. (2021).

[16] Alberto Leonardi, "Whole pair distribution function modeling: the bridging of Bragg and Debye scattering theories", *IUCrJ (International Union of Crystallography Journal)*. 8, 257–269. (2021).

[17] Yang Liu, Marco Klement, Yi Wang, Yaxu Zhong, Baixu Zhu, Jun Chen, Michael Engel, and Xingchen Ye, "Macromolecular Ligand Engineering for Programmable Nanoprism Assembly", *Journal of the American Chemical Society*. 143, 16163–16172. (2021).

[18] Marco Klement, Sangmin Lee, Joshua A. Anderson, and Michael Engel, "Newtonian Event-Chain Monte Carlo and Collision Prediction with Polyhedral Particles", *Journal of Chemical Theory and Computation*. 17, 4686–4696. (2021).

[19] Julia Dshemuchadse, Pablo F. Damasceno, Carolyn L. Phillips, Michael Engel, and Sharon C. Glotzer, "Moving Beyond the Constraints of Chemistry via Crystal Structure Discovery with Isotropic Multiwell Pair Potentials", *Proceedings of the National Academy of Sciences*. 118, e2024034118. (2021).

[20] Kwanghwi Je, Sangmin Lee, Erin G. Teich, Michael Engel, and Sharon C. Glotzer, "Entropic Formation of a Thermodynamically Stable Colloidal Quasicrystal with Negligible Phason Strain", *Proceedings of the National Academy of Sciences*. 118, e2011799118. (2021).

[21] Satoshi Takada, Dan Serero, and Thorsten Pöschel, "Transport coefficients of homogeneous dilute charged granular gases", *Journal of Fluid Mechanics (in press)*. (2021).

Book and book chapters published by MSS in 2021

[22] Вернер Эбелинг и Торстен Пёшель. *Лекции по квантовои статистике с приложениями к разресженным газам и плазме*. Москва, Ижевск: Институт компьютерных усследовауу, (2021).

[23] Werner Ebeling and Thorsten Pöschel. *Lectures in Quantum Statistics with Applications to Charged Gases and Plasmas (in Russian)*. Moscow, Izhevsk: IKI publisher, 2021.

[24] Nikolai V. Brilliantov, Alexander I. Orsinsky, and Thorsten Pöschel, "Boltzmann equation in aggregation kinetics", *(preprint)*. (2021).

[25] Thomas Weinhardt, Jeremy Lechman, and Thorsten Pöschel, editors. *Fragmentation and Wear in DEM Simulations*. Volume 8. Special Issue of Computational Particle Mechanics. Berlin: Springer, 2021.

Other publications published by MSS in 2021 and submitted manuscripts

[26] Leopoldo R. Gómez, Nicolás A. García, and Thorsten Pöschel, "Structure of Entangled Filamentous Matter: Linear vs Rings", *(in review)*. (2021).

[27] Sebastian Mühlbauer, Severin Strobl, Matthew Coleman, and Thorsten Pöschel, “Simulation of Catalytic Reactions in Open-cell Foam Structures”, *AIChE (submitted, arXiv:2010.03904)*. (2021).

[28] Song-Chuan Zhao and Thorsten Pöschel, “Collective motion in two-dimensional swirling granular matter”, *(in review)*. (2021).

[29] Harol Torres Menéndez, Ernesto Altshuler, Nikolai V. Brilliantov, and Thorsten Pöschel, “Lack of collective motion in purely rotating granular gases”, *(in review)*. (2021).

[30] Sebastian Mühlbauer, Severin Strobl, and Thorsten Pöschel, “Simulation of Reactive Flows Using Particle Methods”, *AIChE J. (submitted, arXiv:2010.03874)*. (2021).

[31] Kuang-Wu Lee and Patric Müller, “Spontaneous Size Segregation in Textured Granular Pipe Flow”, *(in review)*. (2021).

[32] Seyed Habibollah Ebrahimnazhad Rahbari, Hor Dashti-Naserabadi, Abbas Ali Saberi, Jürgen Vollmer, Thorsten Pöschel, and Hyunggyu Park, “Stochastic thermodynamics of the rheology of granular media”, *(in review)*. (2021).

Patent Application

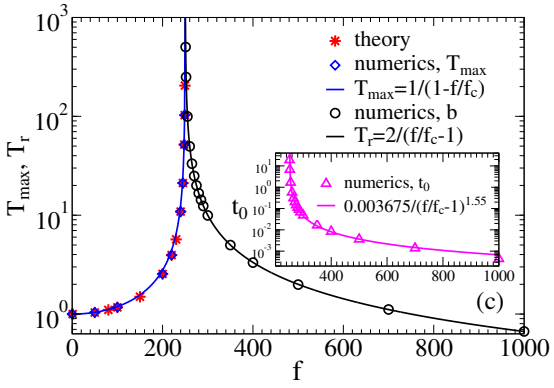
[33] Heiko Lehmann, Thorsten Pöschel, Michael Blank, Sebastian Mühlbauer, Patric Müller, and Michael Schmiedeberg. *Generator allgemeiner synthetischer Graphen mit vorgegebenen statistischen Eigenschaften*. Patentanmeldung 21167507.9 Europa. 2021.

Nonequilibrium phase transition to anomalous diffusion and transport in a basic model of nonlinear Brownian motion

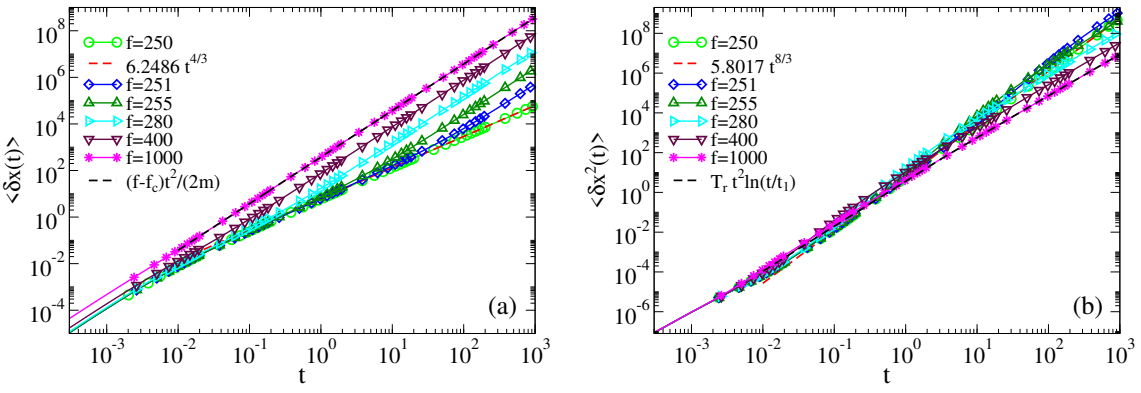
Igor Goychuk *and* ***Thorsten Pöschel***

Abstract:

We investigate a basic model of nonlinear Brownian motion in a thermal environment, where nonlinear friction interpolates between viscous Stokes and dry Coulomb friction. We show that superdiffusion and supertransport emerge as a nonequilibrium critical phenomenon when such a Brownian motion is driven out of thermal equilibrium by a constant force. Precisely at the edge of phase transition, diffusional fluctuations are maximized asymptotically, becoming strongly superballistic. The autocorrelation function of velocity fluctuations in this nonergodic regime exhibits a striking aging behavior.



Divergence of stationary kinetic temperature $T_{\max} = \langle \delta v^2 \rangle_{\rm st}$ characterizing the width of the velocity distribution at a critical value f_c of the driving force f. For $f > f_c$, the kinetic temperature $T_k(t) \sim T_r \ln(t/t_0)$ asymptotically diverges in time. The characteristic temperature T_r and time t_0 (see inset) are also diverging at the critical point. The numerical and theoretical results are depicted with various symbols. Full lines present their fits.



(a) Mean distance and (b) variance of the particle positions as functions of time for critical and supercritical transport and diffusion, respectively, at several values of force f shown in the plots (full lines with symbols). Dashed lines present various fits discussed in the paper.

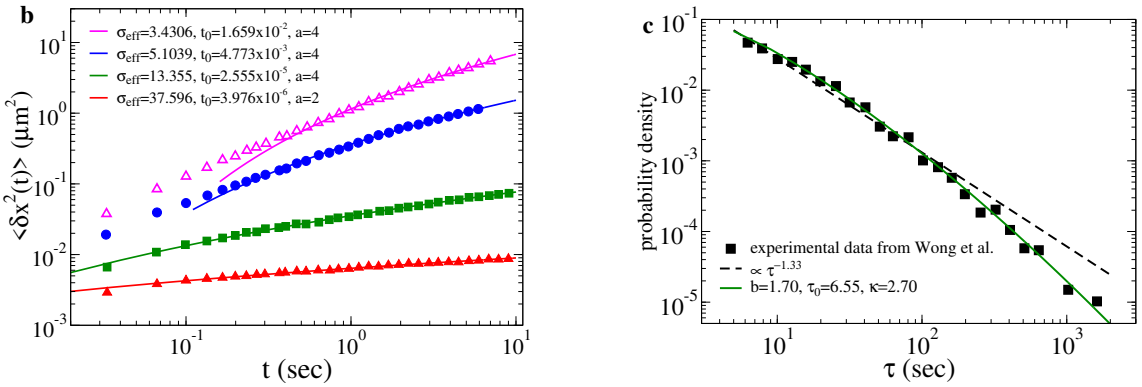
[1] Igor Goychuk and Thorsten Pöschel, "Nonequilibrium phase transition to anomalous diffusion and transport in a basic model of nonlinear Brownian motion", *Physical Review Letters*. 127, 110601. (2021).

Fingerprints of viscoelastic subdiffusion in random environments: revisiting some experimental data and their interpretations

Igor Goychuk and *Thorsten Pöschel*

Abstract:

Many experimental studies revealed subdiffusion of various nanoparticles in diverse polymer and colloidal solutions, cytosol and plasma membrane of biological cells, which are viscoelastic and, at the same time, highly inhomogeneous randomly fluctuating environments. The observed subdiffusion often combines features of ergodic fractional Brownian motion (reflecting viscoelasticity) and nonergodic jump-like non-Markovian diffusional processes (reflecting disorder). Accordingly, several theories were proposed to explain puzzling experimental findings. Below we show that some of the significant and profound published experimental results are better rationalized within the viscoelastic subdiffusion approach in random environments, which is based on generalized Langevin dynamics in random potentials, than some earlier proposed theories.



Experimental data extracted using Engauge Digitizer from Wong, *et al.*, Phys. Rev. Lett. **92**, 178101 (2004) and their fits. In (b), the ensemble-averaged mean-square displacement (MSD) *vs.* time is taken from Fig. 1 in Wong, *et al.* (symbols). In all cases, the radius of diffusing particle is the same, $R = 0.25\ \mu$m, however, the mean mesh size of an entangled actin filament network varies from $\xi = 0.75\ \mu$m (empty magenta triangles), through $\xi = 0.55\ \mu$m (filled blue circles) and $\xi = 0.30\ \mu$m (filled green squares) to $\xi = 0.25\ \mu$m (filled red triangles). The original data are alternatively fitted with the Sinai-like dependence $\langle \delta x^2(t)\rangle = \xi^2 |\ln(t/t_0)/\sigma_{\rm eff}|^a$ and the parameters shown in the plot. It fits the data better than the original power law fits (not shown). In (c), the data on the residence time distribution from Fig. 3(b) of Wong, *et al.* for $\xi = 0.31\ \mu$m and the same R are fitted by (i) power-law dependence $\psi(\tau) \propto \tau^{-1-\alpha}$ with $\alpha = 0.33$, which was used in this paper (black dashed line), and (ii) a generalized log-normal distribution $\psi(\tau) \propto e^{-|\ln(\tau/\tau_0)/\kappa|^b}/\tau$ (green full line), with the parameters given in plot. The latter fit is evidently better.

[2] Igor Goychuk and Thorsten Pöschel, "Fingerprints of viscoelastic subdiffusion in random environments: revisiting some experimental data and their interpretations", *Physical Review E*. 104, 034125. (2021).

Scale and water effects on the friction angles of two granular soils with different roughness

Valentina Marzulli**, Chitta Sai Sandeep, Kostas Senetakis, and Francesco Cafaro, and **Thorsten Pöschel

Abstract:

An integrated experimental study is presented which aims at relating the frictional properties at the particle scale to the bulk mechanical behavior for two different types of sands. We performed direct shear tests and inter-particle tests on lunar regolith simulant DNA-1A and Ottawa sand (benchmark material) under both dry and wet conditions. We found higher macroscopic friction angles for the lunar simulant in both dry and wet conditions, a smaller strength decay for Ottawa sand during reversal direct shear tests and similar strength envelopes of both materials under wet and dry conditions. Particle-scale tests evidenced higher inter-particle friction for DNA-1A in wet conditions with respect to the dry case for normal force lower than 2–3 N. For the lunar simulant, the differences between bulk and inter-particle friction appeared to be emphasized in dry condition and an evident effect of water on the friction coefficient was found only at the micro-scale.

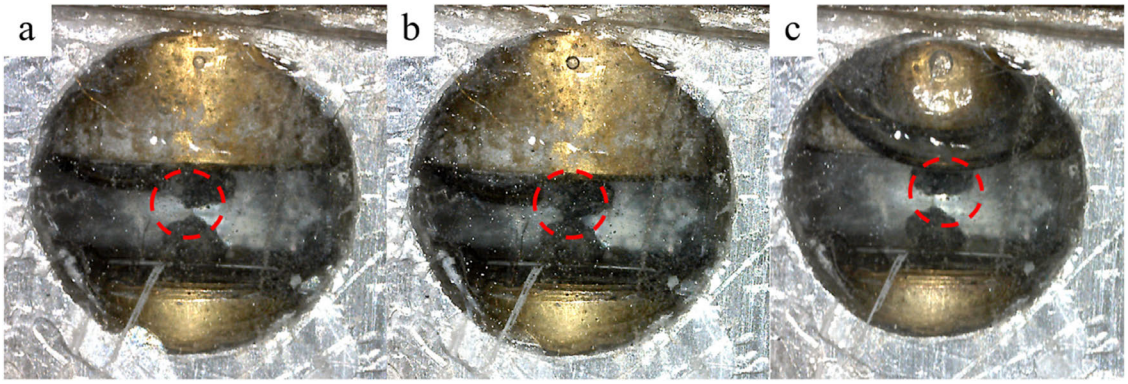


Figure: DNA-1A grain pair tested in submerged condition (a) before the micromechanical tests (b) during loading (c) after the loading. The dashed red circle shows the damage of asperities on the top grain after the micromechanical test.

[3] Valentina Marzulli, Chitta Sai Sandeep, Kostas Senetakis, Francesco Cafaro, and Thorsten Pöschel, “Scale and water effects on the friction angles of two granular soils with different roughness”, *Powder Technology*. 377, 813–826. (2021).

Influence of vibrating recoating mechanism for the deposition of powders in additive manufacturing: Discrete element simulations of polyamide 12

Daniel S. Nasato, Heiko Briesen, and ***Thorsten Pöschel***

Abstract:

Improving the quality of the powder layers used in selective laser melting is a crucial step in bringing additive manufacturing to an industrial standard process. In this work, the effect of vibrations applied to the recoating mechanism (standard blade and roller) on the quality of the powder bed is evaluated. A numerical study using a realistic particle model of polyamide 12 is performed to evaluate the influence of frequency and amplitude in the porosity of the powder layer. Small frequency and amplitude, combined with small recoating velocity, lead to a reduction in the porosity of the granular bed. Large frequency and amplitude, however, lead to a vibro-fluidized state of the particles, loosening the granular bed and increasing the porosity. For practical applications, the choice of frequency and amplitude must be considered in combination with a specific translational velocity of the recoating mechanism.

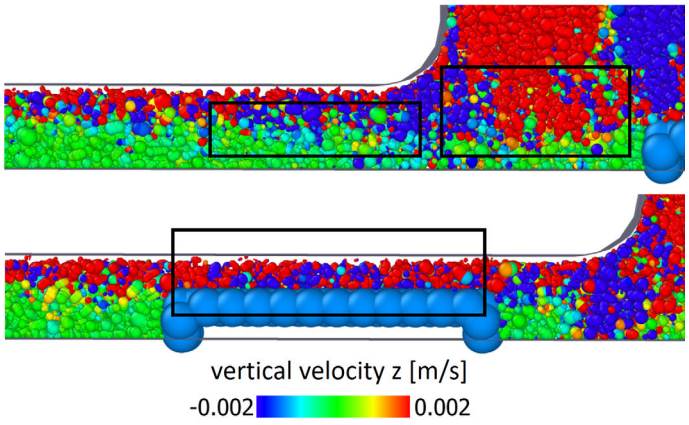


Figure: Compression of the granular bed due to the blade vibration. Top: vertical motion of the particles can be seen in the deep layers of the granular bed (see black boxes). Bottom: this compaction is limited to the recoated layer above the rigid part.

[4] Daniel S. Nasato, Heiko Briesen, and Thorsten Pöschel, "Influence of vibrating recoating mechanism for the deposition of powders in additive manufacturing: discrete element simulations of polyamide 12", *Additive Manufacturing*. 48, 102248. (2021).

Surfactants and rotelles in active chiral fluids

Christian Scholz, Anton Ldov, ***Thorsten Pöschel****,* ***Michael Engel****, and Hartmut Löwen*

Abstract:
Surfactant molecules migrate to interfaces, reduce interfacial tension, and form micelles. All of these behaviors occur at or near equilibrium. Here, we describe active analogs of surfactants that operate far from equilibrium in active chiral fluids. Unlike molecular surfactants, the amphiphilic character of surfactants in active chiral fluids is a consequence of their activity. Our fluid of choice is a mixture of spinners that demixes into left-handed and right-handed chiral fluid domains. We realize spinners in experiment with three-dimensionally printed vibrots. Vibrot surfactants are chains of vibrots containing both types of handedness. Experiments demonstrate the affinity of double-stranded chains to interfaces, where they glide along and act as mixing agents. Simulations access larger systems in which single-stranded chains form spinning vesicles, termed rotelles. Rotelles are the chiral ana- logs of micelles. Rotelle formation is a ratchet mechanism catalyzed by the vorticity of the chiral fluid and only exist far from equilibrium.

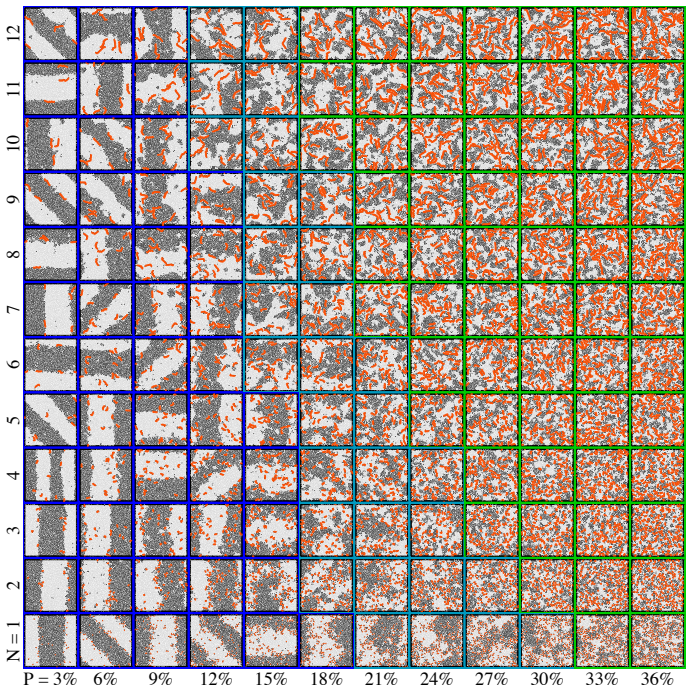


Figure: Parameter space map of double-stranded vibrot chains in a mixed vibrot fluid. Snapshots show steady states as a function of the parameters chain length N and chain concentration P from simulations with periodic boundary conditions. The density 50%, which corresponds to 2348 vibrots. For low concentration of chains, full demixing is observed (dark blue frames). With increasing chain fraction, demixing is suppressed, which first leads to partial demixing (light blue frames) and eventually to complete mixing (green frames). The onset of demixing increases with chain length.

[5] Christian Scholz, Anton Ldov, Thorsten Pöschel, Michael Engel, and Hartmut Löwen, “Surfactants and Rotelles in Active Chiral Fluids”, *Science Advances*. 7, eabf8998. (2021).

Stability of freeze-dried products subjected to microcomputed tomography radiation doses

Tim Wenzel, ***Achim Sack, Patrick Müller, Thorsten Pöschel****, Sonja Schuldt-Lieb, and Henning Gieseler*

Abstract:

Objectives: Microcomputed tomography (μCT) is a powerful analytical tool for non-invasive structural analysis.The stability of drug substances and formulations subjected to X-ray radiation may be a concern in the industry. This study examines the effect of X-ray radiation on the stability of freeze-dried pharmaceuticals. The investigation is a proof of concept study for the safety of μCT X-ray radiation doses during the non-destructive investigation of freeze-dried products.

Methods: Different formulations of clotrimazole, insulin and l-lactate dehydrogenase were freeze-dried and the products exposed to a defined dose of radiation by μCT. Conservative freeze-drying conditions were used. Irradiated and normal samples were analysed for their stability directly after freeze-drying and after stability testing.

Key findings: The stability of model compounds was well maintained during freeze-drying. Some degradation of all compounds occurred during accelerated stability testing.The results showed no differences between the irradiated and normal state directly after freeze-drying and accelerated stability testing.

Conclusions: No evidence of a detrimental effect of 100 Gy X-ray exposure on a model small molecule, peptide and protein compound was found while useful structural information could be obtained. Consequently, the technology may be useful as a non-destructive tool for product inspections if the formulation proves stable.

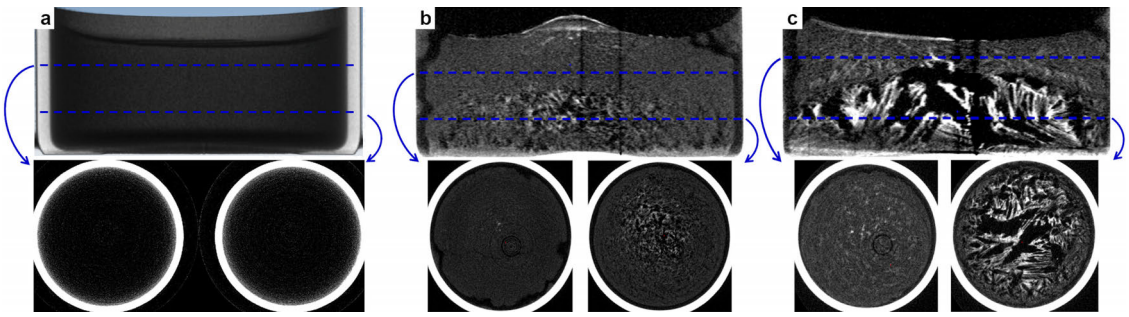


Figure: Example vertical section of the middle of the products and horizontal sections at two different heights by *mu*CT scans. Comparative images of a homoge- neous 70 mg/ml mannitol and 30 mg/ml SAM product (a), a 100 mg/ml SAM product with minor collapse confined to the centre of the product (b).

[6] Tim Wenzel, Achim Sack, Patric Müller, Thorsten Pöschel, Sonja Schuldt-Lieb, and Henning Gieseler, “Stability of freeze-dried products subjected to microcomputed tomography radiation doses”, *Journal of Pharmacy and Pharmacology*. 73, 212–220. (2021).

Spontaneous formation of density waves in granular matter under swirling excitation

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

Abstract:

We study here the spontaneous clustering of a submonolayer of grains under horizontal circular shaking. The clustering of grains occurs when increasing the oscillation amplitude beyond a threshold. The dense area travels in a circular fashion at the driving frequency, which even exceeds the speed of driving. It turns out that the observed clustering is due to the formation of density waves. The analysis of a phenomenological model shows that the instability of the uniform density profile arises by increasing the oscillation amplitude and captures the non-monotonic dependence of the transition amplitude of the clustering on the global density of the system. Here, the key ingredient is that the velocity of individual grains increases with the local density. The interplay of the dissipative particle–particle interaction and frictional driving of the substrate results in this dependence, which is tested with discrete element method simulations.

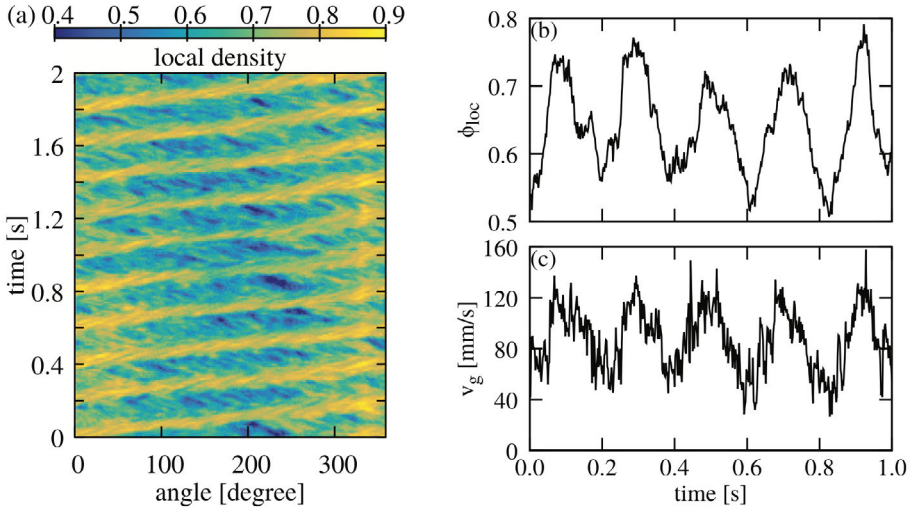


Figure: (a) Local density profile along a circular path vs time for $A = 11\,\text{mm}$ and $\phi_{\text{tot}} = 0,505$, where clustering close to the center is observed. The exact position of the path is given in the main text. For the same experiment, the local density ϕ_{loc} and the velocity of a grain v_g on the circular path are plotted vs time in (b) and (c), respectively. See the main text for the definition of ϕ_{loc}.

[7] Song-Chuan Zhao and Thorsten Pöschel, “Spontaneous formation of density waves in granular matter under swirling excitation”, *Physics of Fluids*. 33, 081701. (2021).

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

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

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

Figure: Experimental setup for automatic holding force measurements.

[8] Holger Götz, Angel A. Santarossa, Achim Sack, Thorsten Pöschel, and Patric Müller, “Soft particles reinforce robotic grippers, Robotic grippers based on granular jamming of soft particles”, *Granular Matter*. 24, 31. (2021).

A robust numerical method for granular hydrodynamics in three dimensions

Ali Shakeri**, Daniel Schiochet Nasato, **Patric Müller**, **Harol Torres Menéndez**, and **Thorsten Pöschel

Abstract:

Granular systems are of a discrete nature. Nevertheless, it can be advantageous to describe their dynamics by means of continuum mechanical methods. The numerical solution of the corresponding hydrodynamic equations is, however, difficult. Therefore, previous numerical simulations are typically geared towards highly specific systems and frequently restricted to two dimensions or mild driving conditions. Here, we present the first robust general simulation scheme for granular hydrodynamics in three dimensions which is not bound to the above limitations. The performance of the simulation scheme is demonstrated by means of three applications which have been proven as notoriously difficult for numerical hydrodynamic description. Although, by construction, our numerical method covers grain-inertia flows, the presented examples demonstrate that it produces reliable results even in the jammed or high density limit.

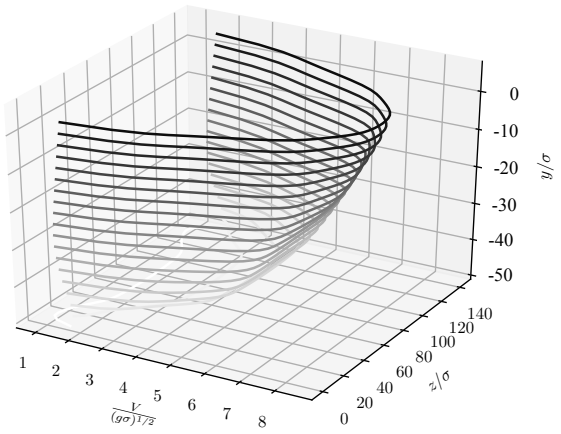


Figure: The three-dimensional velocity profile for a granulate flowing down an inclined pile between two rough sidewalls shows that the maximum velocity is attained on the top surface of the granulate and on the centreline between the two sidewalls. The vertical axis is chosen such that $y/\sigma = 0$ is the height of a fixed plane near the surface of fluctuating height. Thus, at $y\sigma \approx -50$, the flow velocity almost ceases. The coefficient of restitution was $\varepsilon = 0.9$.

[9] Ali Shakeri, Daniel Schiochet Nasato, Patric Müller, Harol Torres Menéndez, and Thorsten Pöschel, "A robust numerical method for granular Hydrodynamics in Three Dimensions", *Journal of Fluid Mechanics*. 917, A33. (2020).

Rarefied reactive gas flow in T-shape microreactors

Mubashir Hussain *and* ***Patric Müller***

Abstract:

The present study investigates the reactive gas flows in T-shape microreactors by means of a 3D direct simulation Monte-Carlo method (DSMC). The reactive process is modeled by incorporating a single step irreversible exothermic reaction of gas species A and B. The energy released in each reaction is added to the system by increasing the kinetic energy of the product gas specie C. The reactive collisions are modeled by means of a momentum preserving hard sphere collision model in 3D DSMC. We analyzed several process and gas parameters to observe their extent of influence on the characteristics of the reactive flow. The T-microreactor with thermal walls showed much higher mass carrying capacity as compared to the specular walls. The reaction front, which initially for maximum reaction rate was close to the inlet of gas specie of higher mass density, moved towards the center of the inlet part of the T-channel and eventually dissolved with decreasing reaction rates. This transition was smooth in the T-channel with thermal walls, whereas, quite abrupt in case of specular walls. Moreover, in T-microreactors with thermal walls, the amount of A and B converted to C follows an exponential decrease especially in moderate to low reaction rates. Further, with a clear separation between high and low reactive regimes, a piece-wise exponential decay in concentration of C with respect to decreasing reaction rates was also observed in the T-channel with specular walls.

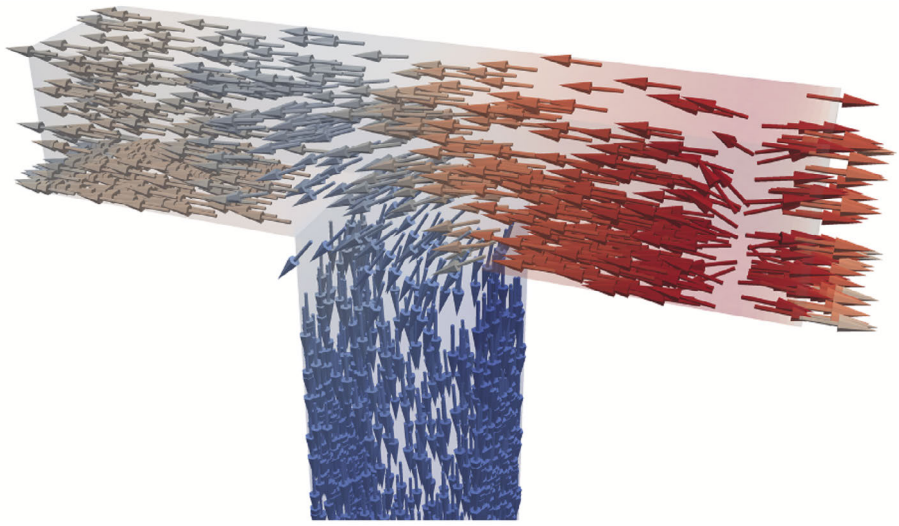


Figure: Mass density and flow field of the gas species *C* for specular walls.

[10] Mubashir Hussain and Patric Müller, “Rarefied reactive gas flow in T-shape microreactors”, *Applied Thermal Engineering (submitted)*. 185, 116308. (2021).

Fragmentation and abrasion in granular matter systems

Thomas Weinhart, Jeremy Lechman, and ***Thorsten Pöschel***

Abstract:
Fragmentation and abrasion are fundamental particle-level processes that affect many macroscopic properties of granular media, from the particle size distribution to the stress–strain relationship to the wear of process equipment. Studying those processes is essential in many fields, including the geotechnical engineering, mining, pharmaceutical, and chemical industries.
Fragmentation and abrasion in granular systems can be described on at least two complementary scales. On the intra-particle scale, one needs to understand the fracture behavior of a single particle. Such fractures are affected by the material properties and the internal structure of the particle. Pore structure, pre-cracks, material plasticity, and the particles' geometric shape affect the particles' fracture behavior. Modeling the intra-particle scale allows characterizing the fragmentation behavior of granules, resulting in fracture models for multi-particle simulations. As particle properties vary within a granular bulk, usually those fracture models rely on a statistical approach; thus, they describe the average fracture behavior of a particle. Fracture models derived in this way can then be used to understand the macroscopic behavior of the bulk material.

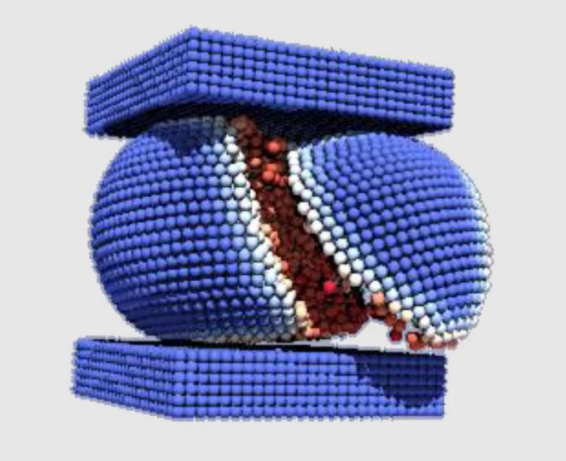


Figure: S. Silling, C. Barr, M. Cooper, J. Lechman, D. Bufford, Comp. Part. Mech. **8**, 1005 (2021), Fig. 7

[11] Thomas Weinhardt, Jeremy Lechman, and Thorsten Pöschel, "Fragmentation and Abrasion in Granular Matter Systems", *Computational Particle Mechanics*. 8, 1003–1004. (2021).

Fluctuations and like-torque clusters at the onset of the discontinuous shear thickening transition in granular materials

Seyed Habibollah Ebrahimnazhad Rahbari, Michio Otsuki, and ***Thorsten Pöschel***

Abstract:

The main mechanism driving rheological transitions is usually mechanical perturbation by shear unjamming mechanism. Investigating discontinuous shear thickening is challenging because the shear counterintuitively acts as a jamming mechanism. Moreover, at the brink of this transition, a thickening material exhibits fluctuations that extend both spatially and temporally. Despite recent extensive research, the origins of such spatiotemporal fluctuations remain unidentified. Here, we numerically investigate the fluctuations in injected power in discontinuous shear thickening in granular materials. We show that a simple fluctuation relation governs the statistics of power fluctuations. Furthermore, we reveal the formation of like-torque clusters near thickening and identify an unexpected relation between the spatiotemporal fluctuations and the collective behavior due to the formation of like-torque clusters. We expect that our general approach should pave the way to unmasking the origin of spatiotemporal fluctuations in discontinuous shear thickening.

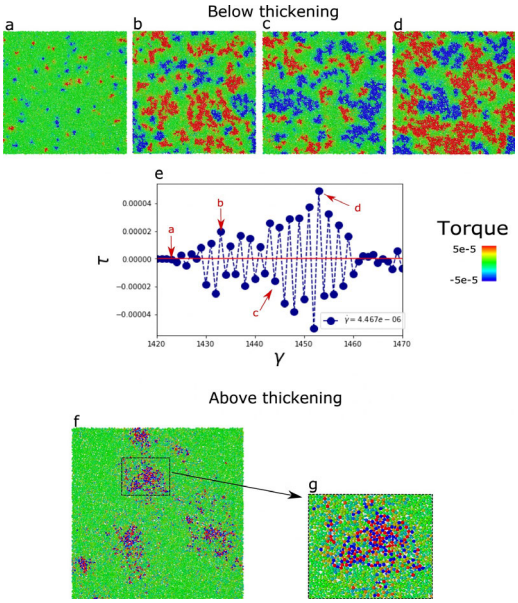


Figure: Torque across discontinuous shear thickening transition. Panels (a–d) show subsequent snapshots of the system as it undergoes instability. The color-coding corresponds to the total torque of each particle; the green particles have nearly 0 torque. As the system is sheared, domains of like-torque particles nucleate and grow, thus resulting in an enhancement in the rotational degrees of freedom, which underlies the well-known instability near the thickening transition. The mean torque as a function of strain is shown in panel (e), where the position of each snapshot as a function of strain is marked.

[12] Seyed Habibollah Ebrahimnazhad Rahbari, Michio Otsuki, and Thorsten Pöschel, “Fluctuations and like-torque clusters at the onset of the discontinuous shear thickening transition ingranular materials”, *Nature-Communications Physics*. 4, 71. (2021).

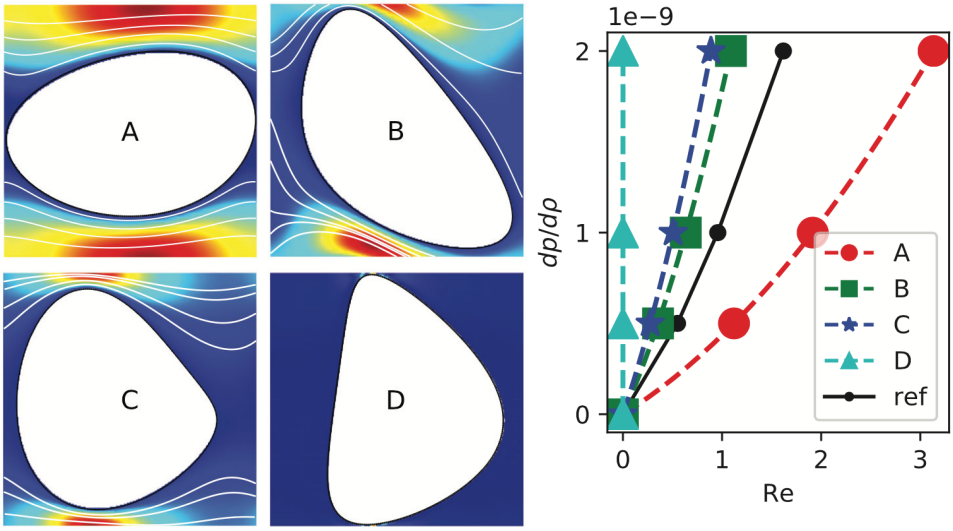
Can Minkowski tensors of a simply connected porous microstructure characterize its permeability?

THIS PAPER WAS SELECTED AS AN EDITOR'S PICK

Prapanch Nair, ***Sebastian Mühlbauer***, *Shantanu Roy, and* ***Thorsten Pöschel***

Abstract:

We show that the permeability of periodic simply connected porous media can be reliably predicted from the Minkowski tensors (MTs) describing the pore microstructure geometry. To this end, we consider a large number of two-dimensional simulations of flow through periodic unit cells containing complex-shaped obstacles. The prediction is achieved by training a deep neural network using the simulation data with the MT elements as attributes. The obtained predictions allow for the conclusion that MTs of the pore microstructure contain sufficient information to characterize the permeability, although the functional relation between the MTs and the permeability could be complex to determine.



(a) (b)

Figure: Flow through four representative shapes for $m = 2$: A and D correspond to the shapes with maximum and minimum permeability in the dataset, respectively. (a) The contours correspond to the velocity component in the x-direction and the white lines represent the flow streamlines; (b) shows the fit of Eq. (5) for the velocity values (normalized as Re) for varying pressure gradient (in the x-direction). The solid line denotes the circular shape used as a reference shape.

[13] Prapanch Nair, Sebastian Mühlbauer, Shantanu Roy, and Thorsten Pöschel, "Can Minkowski tensors of a simply-connected porous microstructure characterize its permeability?", *Physics of Fluids*. 33, 042010. (2021).

Insufficient evidence for ageing in protein dynamics

Igor Goychuk *and* ***Thorsten Pöschel***

Abstract:

In a fascinating Letter, Nature Phys. **12**, 171 (2016), the authors claim that the non-equilibrium dynamics of single protein molecules exhibits ageing over thirteen (!) decades of time. This is a genuinely revolutionary claim that contradicts accepted knowledge in biophysics. If true, such ageing may cover a whole life span duration of many proteins. For this reason, the Letter was the subject of an enthusiastic comment "Forever ageing", Nature Phys. **12**, 113 (2016), and continues to attract the attention of many researchers. In our Matters Arising comment, we critically re-examine the claim's foundation and show that it is unfortunately based on a fallacy that neither the authors nor the readers of this remarkable work noticed earlier.

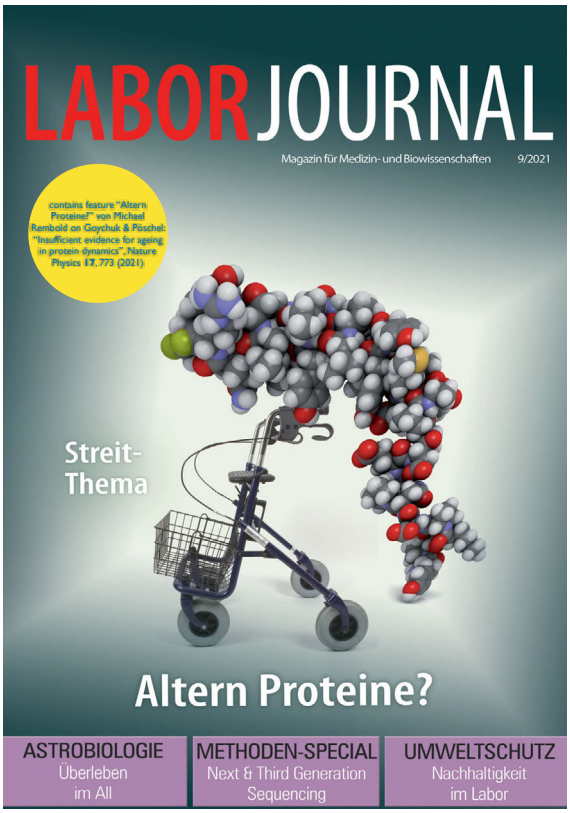


Figure: Title page of "Laborjournal". Our paper was featured by a 4-pages article in Laborjournal: Mario Rembold: "Kontrovers: Altern Proteine oder nicht?", LaborJournal **9**, 16-20 (2021)

[14] Igor Goychuk and Thorsten Pöschel, "Insufficient evidence for ageing in protein dynamics", *Nature*. 17, 773–774. (2021).

Effect of the granular material on the maximum holding force of a granular gripper

Julián M. Gómez–Paccapelo, ***Angel A. Santarossa****, H. Daniel Bustos, and Luis A. Pugnaloni*

Abstract:
A granular gripper is a device used to hold objects by taking advantage of the phenomenon of Reynold's dilatancy. A membrane containing a granular sample is allowed to deform around the object to be held and then vacuum is used to jam the granular material inside the membrane. This allows to hold the object against external forces since deformation of the granular material is prevented by not allowing the system to increase its volume. The maximum holding force supported by the gripper depends on a number of variables. In this work, we show that in the regime of frictional holding (where the gripper does not interlock with the object), the maximum holding force as a function of the penetration of the object in the gripper does not depend on the granular material used to fill the membrane. Results for a variety of granular materials can be collapsed into a single curve if maximum holding force is plotted against the penetration depth achieved. The results suggest that a robotic arm capable of sensing the penetration depth can use this master curve to estimate the maximum holding force at each gripping operation.

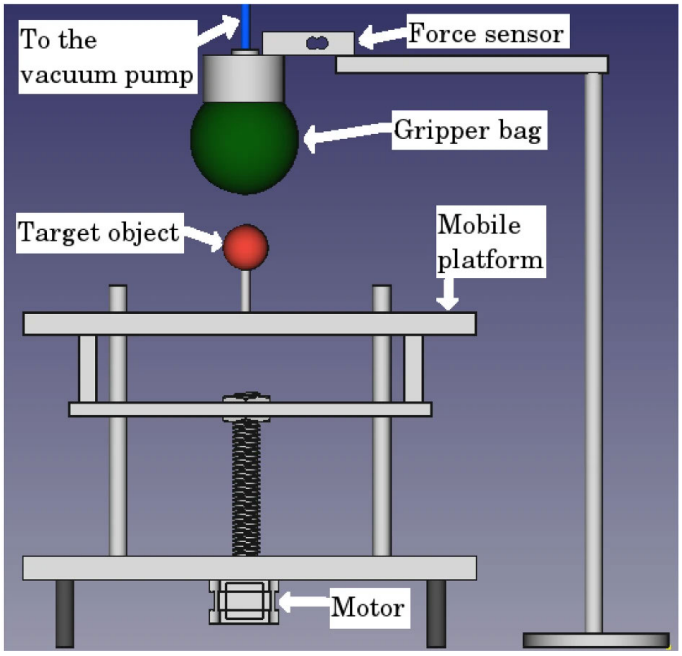


Figure: Sketch of the experimental apparatus

[15] Julián M. Gómez-Paccapelo, Angel A. Santarossa, H. Daniel Bustos, and Luis A. Pugnaloni, "Effect of the granular material on the maximum holding force of a granular gripper", *Granular Matter*. 23, 4. (2021).

Whole pair distribution function modeling: the bridging of Bragg and Debye scattering theories

Alberto Leonardi

Abstract:

Microstructure-based design of materials requires an atomic level understanding of the mechanisms underlying structure-dependent properties. Methods for analyzing either the traditional diffraction profile or the pair distribution function (PDF) differ in how the information is accessed and in the approximations usually applied. Any variation of structural and microstructural features over the whole sample affects the Bragg peaks as well as any diffuse scattering. Accuracy of characterization relies, therefore, on the reliability of the analysis methods. Methods based on Bragg's law investigate the diffraction peaks in the intensity plot as distinct pieces of information. This approach reaches a limitation when dealing with disorder scenarios that do not conform to such a peak-by-peak basis. Methods based on the Debye scattering equation (DSE) are, otherwise, well suited to evaluate the scattering from a disordered phase but the structure information is averaged over short-range distances usually accessed by experiments. Moreover, statistical reliability is usually sacrificed to recover some of the computing-efficiency loss compared with traditional line-profile-analysis methods. Here, models based on Bragg's law are used to facilitate the computation of a whole PDF and then model powder-scattering data via the DSE. Models based on Bragg's law allow the efficient solution of the dispersion of a crystal's properties in a powder sample with statistical reliability, and the PDF provides the flexibility of the DSE. The whole PDF is decomposed into the independent directional components, and the number of atom pairs separated by a given distance is statistically estimated using the common-volume functions. This approach overcomes the need for an atomistic model of the material sample and the computation of billions of pair distances. The results of this combined method are in agreement with the explicit solution of the DSE although the computing efficiency is comparable with that of methods based on Bragg's law. Most importantly, the method exploits the strengths and different sensitivities of the Bragg and Debye theories.

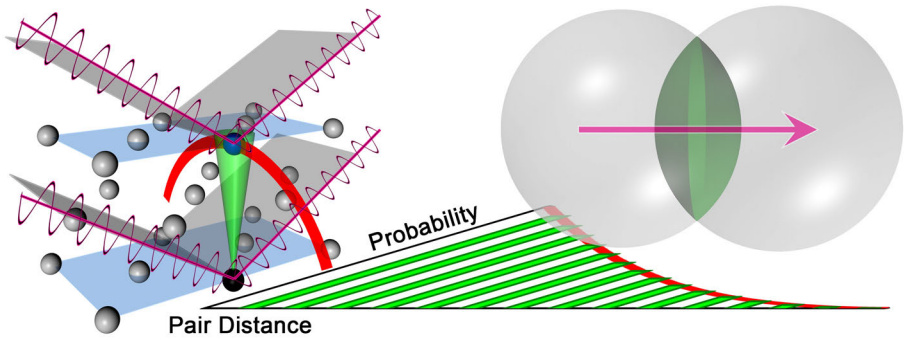


Figure: The whole pair distribution function modeling (WPDFM) method is introduced to overcome the separation between Bragg and Debye theories in analysis of powder scattering data. Bragg's models, such as the common volume function, are used to facilitate the computation of a whole pair distribution function and then solve the Debye scattering equation

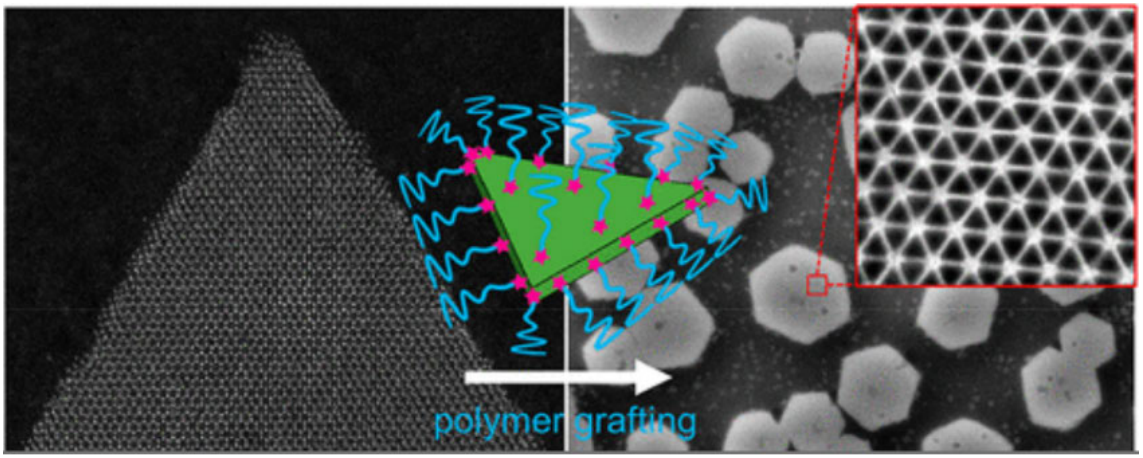
[16] Alberto Leonardi, "Whole pair distribution function modeling: the bridging of Bragg and Debye scattering theories", *IUCrJ (International Union of Crystallography Journal)*. 8, 257–269. (2021).

Macromolecular Ligand Engineering for Programmable Nanoprism Assembly

Yang Liu, ***Marco Klement****, Yi Wang, Yaxu Zhong, Baixu Zhu, Jun Chen,* ***Michael Engel****, and Xingchen Ye*

Abstract:

Ligands play a central role for the energetics and kinetics of nanocrystal assembly. Yet, the precise and simultaneous manipulation of ligands to dictate assembly outcome has proven difficult. Here, we present macromolecular ligand-engineering strategies to control, characterize, and model four molecular parameters of grafted polymer chains: chain length, chain dispersity, grafting density, and chain distribution. Direct ligand-exchange between nanoprisms and polymers functionalizes facets selectively and produces patchy nanocrystals. We develop a generalizable two-step ligand-exchange approach for the independent control of the two emergent brush parameters, brush thickness and brush softness. The resultant polymer-grafted prismatic nanocrystals with programmable ligand brushes self-assemble into thin-film superstructures of different wallpaper symmetries and faceted supracrystals. Our experiments are complemented by coarse-grained computer simulations of nanoprisms with directional, facet-specific interactions. This work paves the way for the precision synthesis of polymer–nanocrystal hybrid materials and enables the further refinement of theoretical models for particle brush materials.



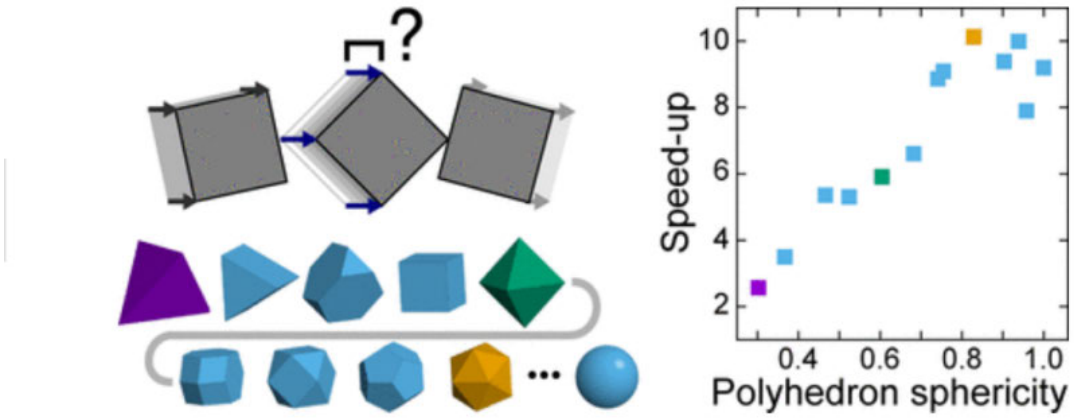
[17] Yang Liu, Marco Klement, Yi Wang, Yaxu Zhong, Baixu Zhu, Jun Chen, Michael Engel, and Xingchen Ye, “Macromolecular Ligand Engineering for Programmable Nanoprism Assembly”, *Journal of the American Chemical Society*. 143, 16163–16172. (2021).

Newtonian Event-Chain Monte Carlo and Collision Prediction with Polyhedral Particles

Marco Klement**, Sangmin Lee, Joshua A. Anderson, and **Michael Engel

Abstract:

Polyhedral nanocrystals are building blocks for nanostructured materials that find applications in catalysis and plasmonics. Synthesis efforts and self-assembly experiments have been assisted by computer simulations that predict phase equilibria. Most current simulations employ Monte Carlo methods, which generate stochastic dynamics. Collective and correlated configuration updates are alternatives that promise higher computational efficiency and generate trajectories with realistic dynamics. One such alternative involves event-chain updates and has recently been proposed for spherical particles. In this contribution, we develop and apply event-chain Monte Carlo for hard convex polyhedra. Our simulation makes use of an improved computational geometry algorithm XenoSweep, which predicts sweep collision in a particularly simple way. We implement Newtonian event chains in the open-source general-purpose particle simulation toolkit HOOMD-blue for serial and parallel simulation. The speedup over state-of-the-art Monte Carlo is between a factor of 10 for nearly spherical polyhedra and a factor of 2 for highly aspherical polyhedra. Finally, we validate the Newtonian event-chain algorithm by applying it to a current research problem, the multistep nucleation of two classes of hard polyhedra.



[18] Marco Klement, Sangmin Lee, Joshua A. Anderson, and Michael Engel, “Newtonian Event-Chain Monte Carlo and Collision Prediction with Polyhedral Particles”, *Journal of Chemical Theory and Computation*. 17, 4686–4696. (2021).

Moving Beyond the Constraints of Chemistry via Crystal Structure Discovery with Isotropic Multiwell Pair Potentials

Julia Dshemuchadse, Pablo F. Damasceno, Carolyn L. Phillips, ***Michael Engel****, Sharon C. Glotzer*

Abstract:

Which crystal structures are possible if the restrictions of the quantum realm are lifted? Our knowledge of ordered particle geometries was previously restricted to the kinds of structures observable in hard condensed matter—on the atomic scale. Here, we use freely tunable computational models to represent particles with variable properties, and we determine the crystal structures into which they self-assemble. The resulting arrangements often correspond to structures known from atomic-scale materials; however, we discover a comparable number of previously unknown crystal structures with different local coordination motifs, incompatible with the limitations of the chemical bond. Our results can be used to engineer soft condensed matter with unprecedented, ordered geometries, paving the way toward materials with potentially novel properties.

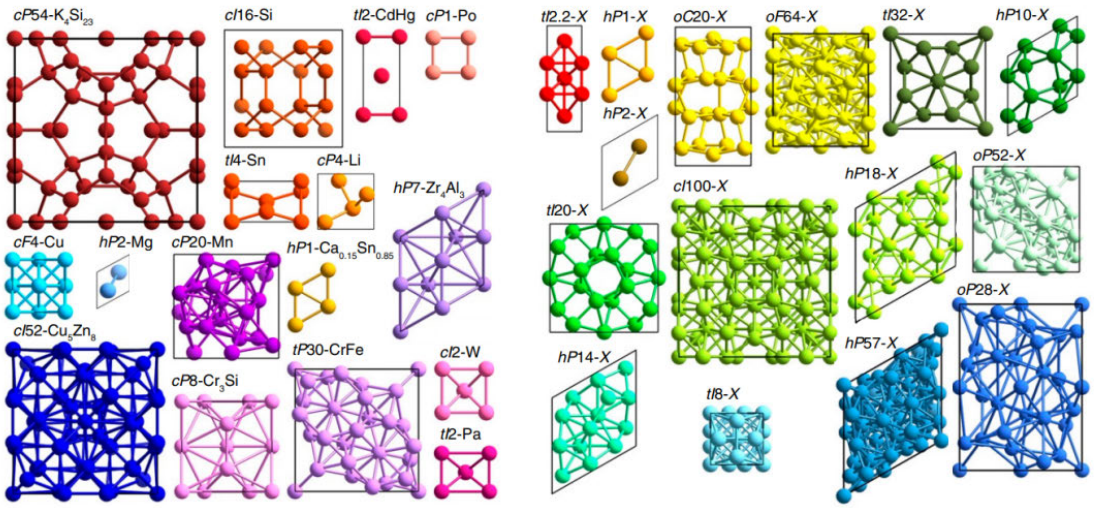


Figure: Unit cells of the crystal structures reported in this study. Unit cells of all 16 known crystal structures (left) and all 15 previously unknown crystal structures (right) are shown

[19] Julia Dshemuchadse, Pablo F. Damasceno, Carolyn L. Phillips, Michael Engel, and Sharon C. Glotzer, "Moving Beyond the Constraints of Chemistry via Crystal Structure Discovery with Isotropic Multiwell Pair Potentials", *Proceedings of the National Academy of Sciences*. 118, e2024034118. (2021).

Entropic formation of a thermodynamically stable colloidal quasicrystal with negligible phason strain

Kwanghwi Je, Sangmin Lee, Erin G. Teich, ***Michael Engel****, and Sharon C. Glotzer*

Abstract:

Quasicrystals have been discovered in a variety of materials ranging from metals to polymers. Yet, why and how they form is incompletely understood. In situ transmission electron microscopy of alloy quasicrystal formation in metals suggests an error-and-repair mechanism, whereby quasiperiodic crystals grow imperfectly with phason strain present, and only perfect themselves later into a high-quality quasicrystal with negligible phason strain. The growth mechanism has not been investigated for other types of quasicrystals, such as dendrimeric, polymeric, or colloidal quasicrystals. Soft-matter quasicrystals typically result from entropic, rather than energetic, interactions, and are not usually grown (either in laboratories or in silico) into large-volume quasicrystals. Consequently, it is unknown whether soft-matter quasicrystals form with the high degree of structural quality found in metal alloy quasicrystals. Here, we investigate the entropically driven growth of colloidal dodecagonal quasicrystals (DQCs) via computer simulation of systems of hard tetrahedra, which are simple models for anisotropic colloidal particles that form a quasicrystal. Using a pattern recognition algorithm applied to particle trajectories during DQC growth, we analyze phason strain to follow the evolution of quasiperiodic order. As in alloys, we observe high structural quality; DQCs with low phason strain crystallize directly from the melt and only require minimal further reduction of phason strain. We also observe transformation from a denser approximant to the DQC via continuous phason strain relaxation. Our results demonstrate that soft-matter quasicrystals dominated by entropy can be thermodynamically stable and grown with high structural quality—just like their alloy quasicrystal counterparts.

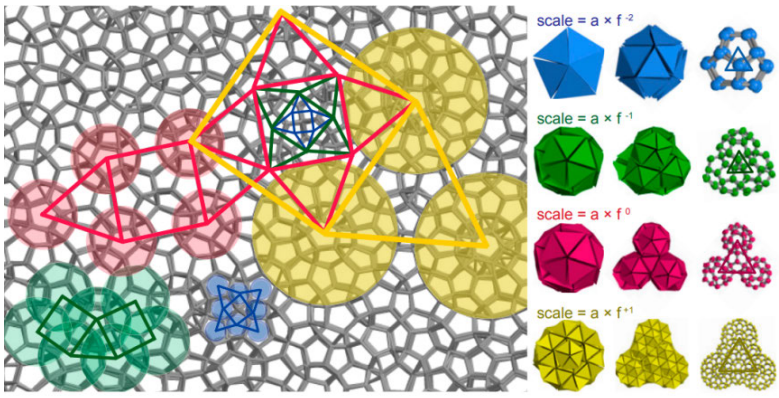


Figure: Tiling hierarchy in the DQC from hard regular tetrahedra. (A) Thick gray lines connect the centers of nearest-neighbor tetrahedra. The DQC can be described as a decorated tiling on different hierarchy levels as indicated by colors

[20] Kwanghwi Je, Sangmin Lee, Erin G. Teich, Michael Engel, and Sharon C. Glotzer, “Entropic Formation of a Thermodynamically Stable Colloidal Quasicrystal with Negligible Phason Strain”, *Proceedings of the National Academy of Sciences*. 118, e2011799118. (2021).

Transport coeffcients for granular gases of electrically charged particles

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

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

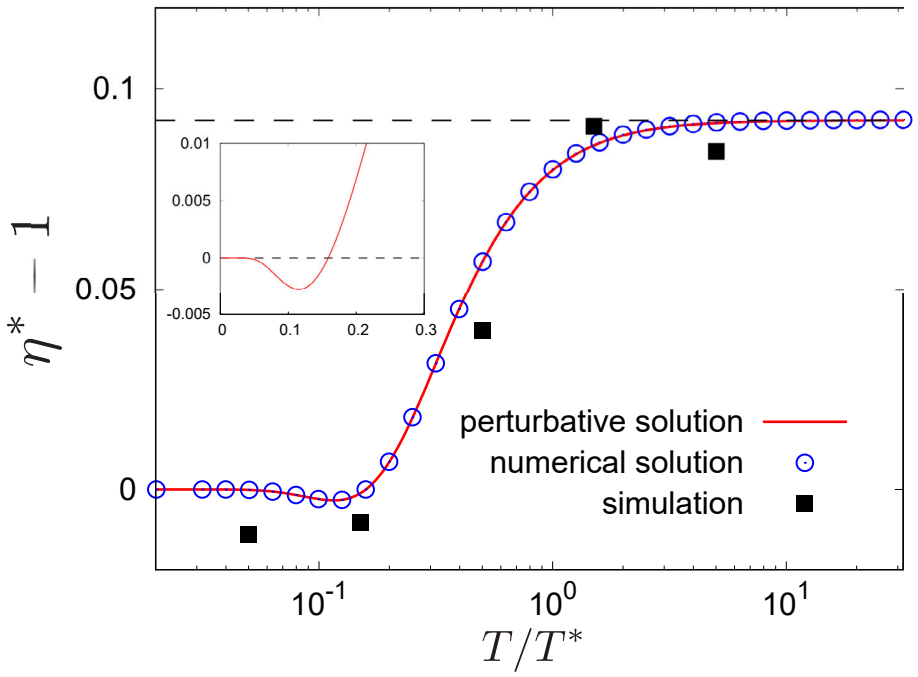


Figure: Shear viscosity as a function of granular temperature obtained from the kinetic theory perturbatively (solid line) and numerically (open circles) for $e^* = 0.8$. The filled squares show results obtained from an event-driven molecular dynamics simulation. The dashed line is the shear viscosity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

[21] Satoshi Takada, Dan Serero, and Thorsten Pöschel, "Transport coefficients of homogeneous dilute charged granular gases", *Journal of Fluid Mechanics (in press)*. (2021).

Лекции по квантовои статистике с приложениями к разресзенным газам и плазме

Lectures in Quantum Statistics with Applications to Charged Gases and Plasmas (in Russian)

Werner Ebeling and ***Thorsten Pöschel***

Abstract:

Most of the matter in our universe is in a gaseous or plasma state. Yet, most textbooks on quantum statistics focus on examples from and applications in condensed matter systems, due to the prevalence of solids and liquids in our day-to-day lives. In an attempt to remedy that oversight, this book consciously focuses on teaching the subject matter in the context of (dilute) gases and plasmas, while aiming primarily at graduate students and young researchers in the field of quantum gases and plasmas for some of the more advanced topics. The majority of the material is based on a two-semester course held jointly by the authors over many years, and has benefited from extensive feedback provided by countless students and co-workers. The book also includes many historical remarks on the roots of quantum statistics: firstly because students appreciate and are strongly motivated by looking back at the history of a given field of research, and secondly because the spirit permeating this book has been deeply influenced by meetings and discussions with several pioneers of quantum statistics over the past few decades.

[22] Вернер Эбелинг и Торстен Пёшель. *Лекции по квантовои статистике с приложениями к разресзенным газам и плазме*. Москва, Ижевск: Институт компьютерных усследовауу, (2021).

[23] Werner Ebeling and Thorsten Pöschel. *Lectures in Quantum Statistics with Applications to Charged Gases and Plasmas (in Russian)*. Moscow, Izhevsk: IKI publisher, 2021.

Boltzmann equation in aggregation kinetics

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

Abstract:

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

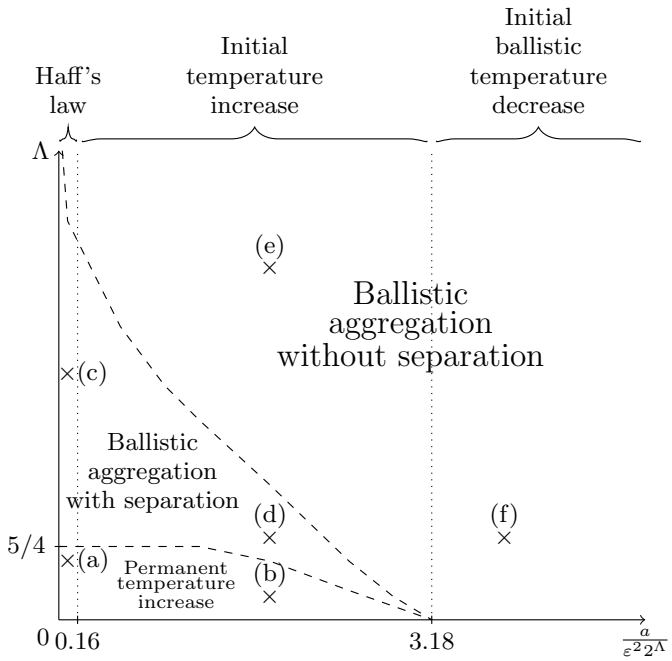


Figure: Phase diagram for the temperature-dependent Smoluchowski equations. Different kinetic regimes are separated by dashed lines. The simulations were performed for $\varepsilon = 0.99$, $m_1 = 1$ and $\sigma_1 = 1$, for mono-disperse initial conditions, initial dimensionless density $(\pi/6)n_1(0)\sigma_1^3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

[24] Nikolai V. Brilliantov, Alexander I. Orsinsky, and Thorsten Pöschel, "Boltzmann equation in aggregation kinetics", *(preprint)*. (2021).

Fragmentation and Wear in DEM Simulations

Special Issue of "Computational Particle Mechanics" (Springer, Berlin)
Edited by Thomas Weinhart, Jeremy Lechman, and ***Thorsten Pöschel***

[25] Thomas Weinhardt, Jeremy Lechman, and Thorsten Pöschel, editors. *Fragmentation and Wear in DEM Simulations*. Volume 8. Special Issue of Computational Particle Mechanics. Berlin: Springer, 2021.

Structure of Entangled Filamentous Matter: Linear vs Rings

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

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

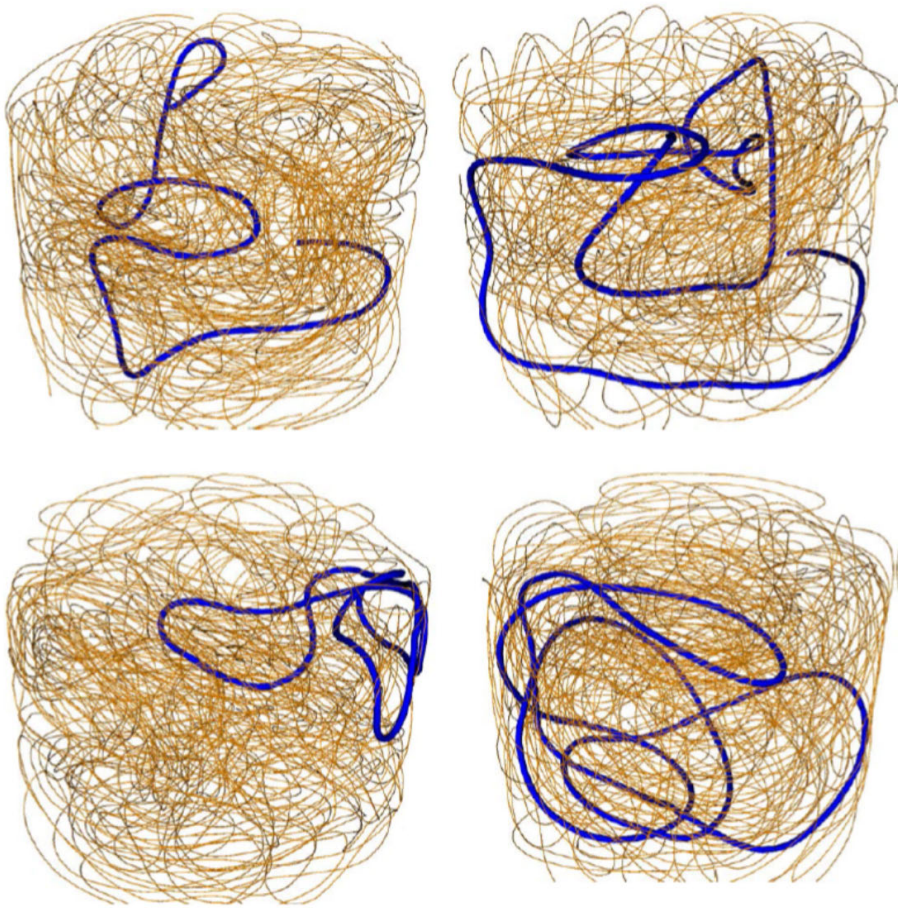


Figure: Packing structure of linear and rings rubber bands. In each assembly a single rubber band is highlighted to better appreciate the configurations.

[26] Leopoldo R. Gómez, Nicolás A. García, and Thorsten Pöschel, “Structure of Entangled Filamentous Matter: Linear vs Rings”, *(in review)*. (2021).

Simulation of catalytic reactions in open-cell foam structures

Sebastian Mühlbauer**, **Severin Strobl**, **Matthew Coleman**, and **Thorsten Pöschel

Abstract:

We describe a technique for particle-based simulations of heterogeneous catalysis in open-cell foam structures, which is based on isotropic Stochastic Rotation Dynamics (iSRD) together with Constructive Solid Geometry (CSG). The approach is validated by means of experimental results for the low temperature water-gas shift reaction in an open-cell foam structure modeled as inverse sphere packing. Considering the relation between Sherwood and Reynolds number, we find two distinct regimes meeting approximately at the strut size Reynolds number 10. For typical parameters from the literature, we find that the catalyst density in the washcoat can be reduced considerably without a notable loss of conversion efficiency. We vary the porosity to determine optimum open-cell foam structures, which combine low flow resistance with high conversion efficiency and find large porosity values to be favorable not only in the mass transfer limited regime but also in the intermediate regime.

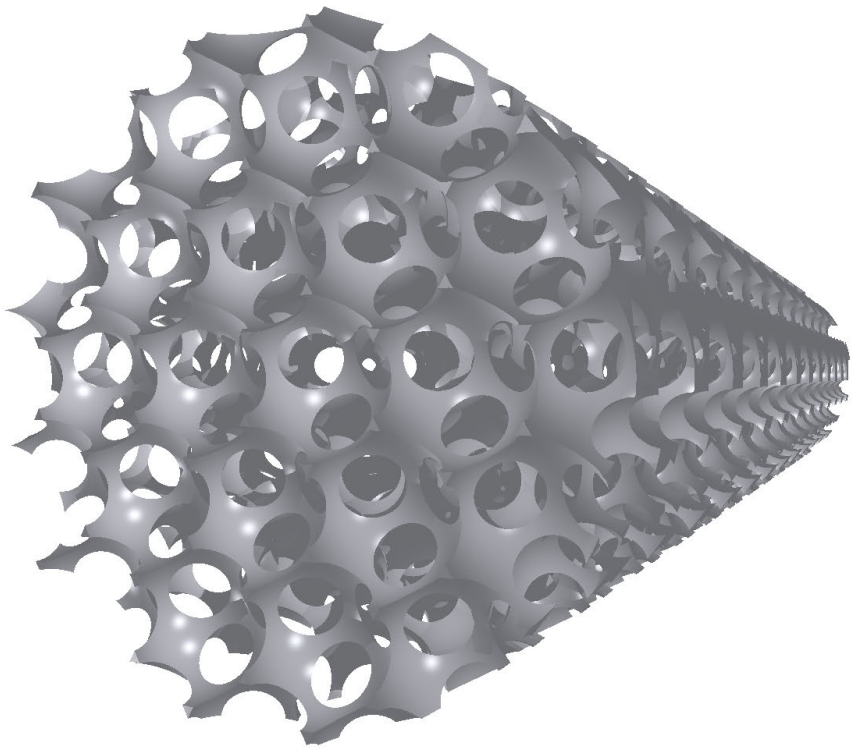


Figure: Cylindrical cutout of a foam structure modeled as an inverse sphere packing.

[27] Sebastian Mühlbauer, Severin Strobl, Matthew Coleman, and Thorsten Pöschel, "Simulation of Catalytic Reactions in Open-cell Foam Structures", *AIChE (submitted, arXiv:2010.03904)*. (2021).

Collective motion in two-dimensional swirling granular matter

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

Abstract:

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

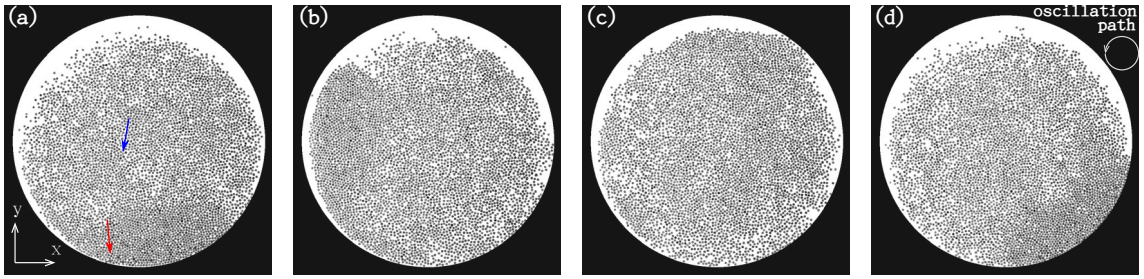


Figure: Snapshots of the packing of $\varphi = 0.57$ and $A = 7\,\mathrm{mm}$ at the middle of (a) cycle 1, (b) cycle 5, (c) cycle 9 and (d) cycle 13. In the inset of (d) the oscillation path of the amplitude $A = 10\,\mathrm{mm}$ is drawn up to scale.

[28] Song-Chuan Zhao and Thorsten Pöschel, "Collective motion in two-dimensional swirling granular matter", *(in review)*. (2021).

Lack of collective motion in purely rotating granular gases

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

Abstract:

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

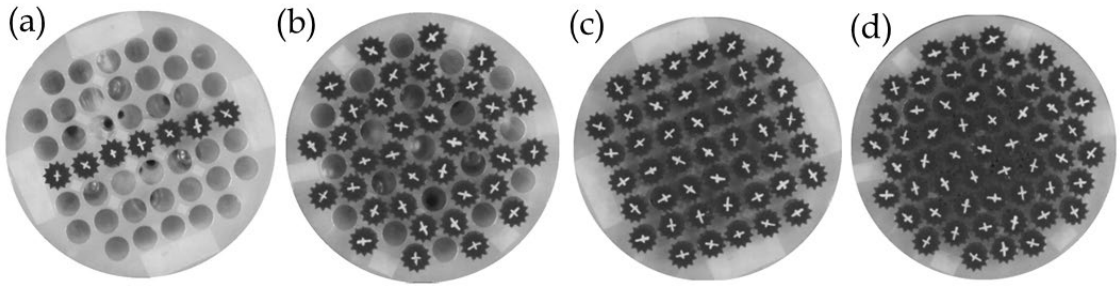


Figure: Rotational granular gas lattices. (a) two neighbors; (b) three neighbors; (c) four neighbors; (d) six neighbors. Also, the lattice constant, a, and the clearance, $R = r_h - r_l$, can be chosen

[29] Harol Torres Menéndez, Ernesto Altshuler, Nikolai V. Brilliantov, and Thorsten Pöschel, "Lack of collective motion in purely rotating granular gases", *(in review)*. (2021).

Simulation of reactive flows using particle methods

Sebastian Mühlbauer**, **Severin Strobl**, and **Thorsten Pöschel

Abstract:
We describe a new computational method for the numerically stable particle-based simulation of open-boundary flows, including volume conserving chemical reactions. The novel method is validated for the case of heterogeneous catalysis against a reliable reference simulation and is shown to deliver identical results while the computational efficiency is significantly increased.

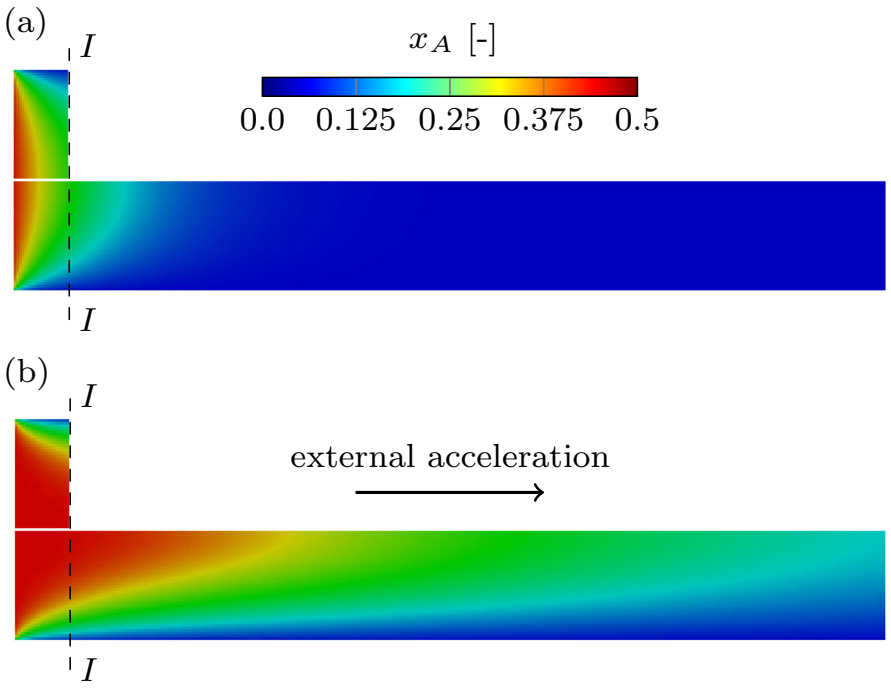


Figure: Profiles of reactant mole fraction, x_A, along the channels for the case of (a) pure diffusion and (b) a flow driven by an external acceleration. In both cases the upper part of the image shows the short channel using the novel boundary condition and the lower part shows the reference channel.

[30] Sebastian Mühlbauer, Severin Strobl, and Thorsten Pöschel, "Simulation of Reactive Flows Using Particle Methods", *AIChE J. (submitted, arXiv:2010.03874)*. (2021).

Spontaneous Size Segregation in Textured Granular Pipe Flow

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

Abstract:

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

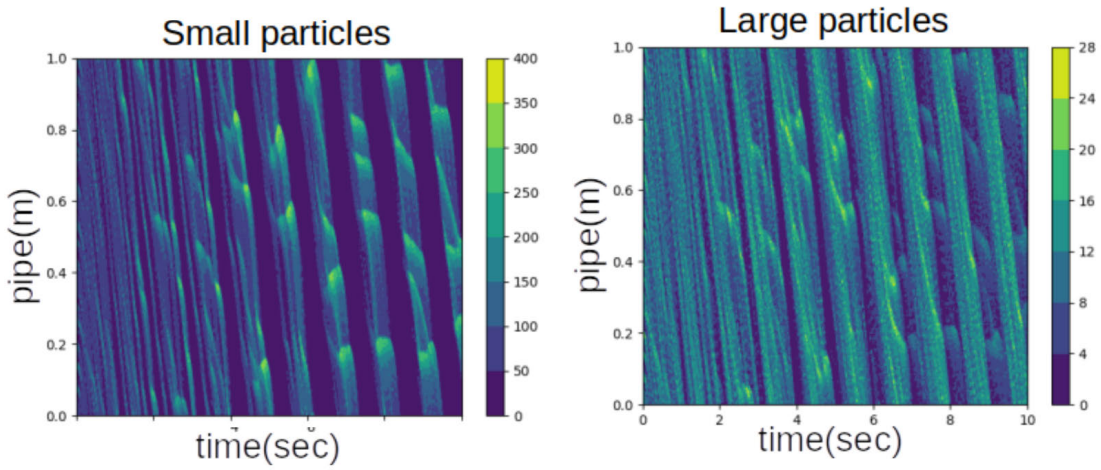


Figure: A typical size segregation of polydisperse granular particles in the pipe flow. The case shown here is for volume fraction $V_\varphi = 0.2$ and aspect ratio $D_\varphi = 5$. The upper panel is the time evolution of small particles, while the lower panel is for large particles. The colormap indicates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

[31] Kuang-Wu Lee and Patric Müller, "Spontaneous Size Segregation in Textured Granular Pipe Flow", *(in review)*. (2021).

Stochastic Thermodynamics of the Rheology of Granular Media

Seyed Habibollah Ebrahimnazhad Rahbari , Hor Dashti-Naserabadi, Abbas Ali Saberi, Jürgen Vollmer, ***Thorsten Pöschel****, and Hyunggyu Park*

Abstract:

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

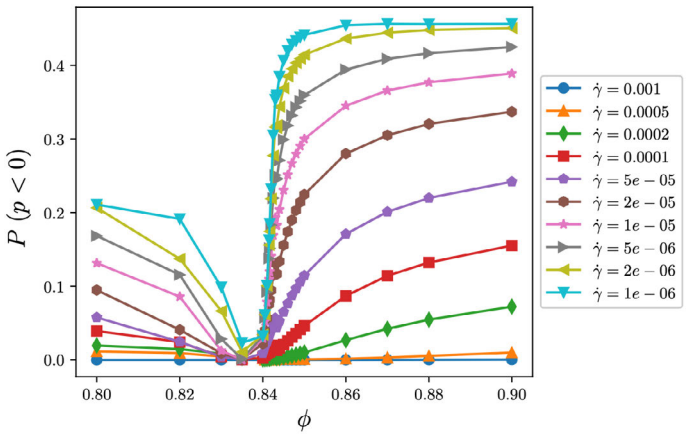


Figure: The probability for negative power $P(p<0)$ vs packing fraction ϕ. Each color corresponds to a shear rate that is given in the legend. The number of particles vary from $N = 61941$ to 69684 for $\phi = 0.8$ and 0.9, respectively, at a fixed system size $L = 300$. Each curve has a global minimum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

[32] Seyed Habibollah Ebrahimnazhad Rahbari, Hor Dashti-Naserabadi, Abbas Ali Saberi, Jürgen Vollmer, Thorsten Pöschel, and Hyunggyu Park, "Stochastic thermodynamics of the rheology of granular media", *(in review)*. (2021).

Patentanmeldung: Generator allgemeiner synthetischer Graphen mit vorgegebenen statistischen Eigenschaften

(Generator of general synthetic graphs with given statistical properties)

Heiko Lehmann, ***Thorsten Pöschel, Michael Blank, Sebastian Mühlbauer,*** ***Patric Müller****, and Michael Schmiedeberg*

Abstract:

Krankheitserreger, wie z.B. Viren, werden von Organismus zu Organismus übertragen. Entsprechend der Reisetätigkeit eines Wirts kann sich ein Virus so entlang von Flugknotenpunkten über weite Distanzen, aber auch entlang des Straßennetzes über kurze Distanzen ausbreiten. Die Personen, die dabei miteinander in Kontakt stehen, bilden ein Netzwerk.

Weitere Beispiele für Netzwerke sind die Freundschaftsbeziehung in einem sozialen Netzwerk, die Referenzen in wissenschaftlichen Arbeiten oder das Internet. Jedes Netzwerk weist dabei charakteristische statistische Eigenschaften auf, die sich aus der Verknüpfung der Knoten ergibt. Ein Beispiel für eine solche Eigenschaft ist die Freundschaftsverteilung auf Facebook.

Will man die Ausbreitung eines Virus oder Computervirus in einem solchen Netzwerk zurückverfolgen muss dieses zunächst anhand der zugrunde liegenden statistischen Eigenschaften erzeugt werden, sofern dieses nicht bereits vorhanden ist.

Das Patent beschreibt einen Algorithmus, der Netzwerke anhand vorgegebener statistischer Zielverteilungen erzeugt.

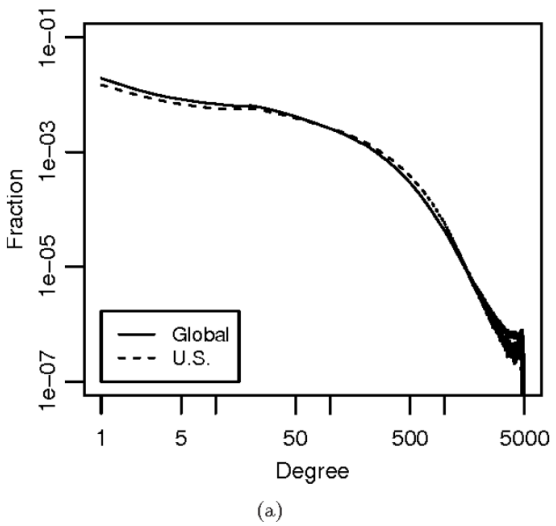


Figure: Anteil der Personen über Anzahl der Freundschaftsbeziehungen auf Facebook (J. Ugander et al. “The anatomy of the facebook social graph”. preprint arXiv:1111.4503 (2011))

[33] Heiko Lehmann, Thorsten Pöschel, Michael Blank, Sebastian Mühlbauer, Patric Müller, and Michael Schmiedeberg. *Generator allgemeiner synthetischer Graphen mit vorgegebenen statistischen Eigenschaften*. Patentanmeldung 21167507.9 Europa. 2021.

12. Public Attention and Public Outreach

MSS festured by a SINTERIT-User Case Study "Printing accurate and durable phantom to mimic human organs"

www.sinterit.com/printing-accurate-and-durable-phantom-to-mimic-human-organs/

MSS paper festured by BILD

MSS paper "Surfactants and rotelles in active chiral fluids" by C. Scholz, A. Ldov, **T. Pöschel**, **M. Engel**, and H. Löwen, *Science Advances* **7**, eabf8998, was featured by BILD on April 17, 2021.

Uni Erlangen forscht

MINI-ROBOTER AUS 3D-DRUCKER

Diese Vibrots sind einen Zentimeter groß. Die Neigung ihrer Füßchen bestimmt die Rotationsrichtung

Nürnberg/Erlangen – **Kleine Roboter, große Wirkung.**

Wissenschaftler der Friedrich-Alexander-Universität (FAU) forschen mit Mini-Robotern. Die Mikro-Roboter werden im 3D-Drucker hergestellt, sind ein Zentimeter groß und wiegen ein Gramm. Wenn man sie in Vibration versetzt, beginnen sie sich zu drehen, deshalb werden sie Vibrots genannt. Die Neigung ihrer sieben Beine bestimmt die Rotationsrichtung.

Der Clou: gleichdrehende Vibrots schließen sich zu Ketten zusammen.

Diese Wirkung der Mikro-Roboterketten könnte in Zukunft beispielsweise dabei helfen, ölverseuchte Gewässer zu reinigen, indem die Ketten Öl einschließen, das so leichter abgefischt werden kann.

Dazu ist ein nächster Schritt nötig: Die Vibrots müssen noch viel viel kleiner werden. *(lau)*

Foto: CHRISTIAN SCHOLZ/HHU

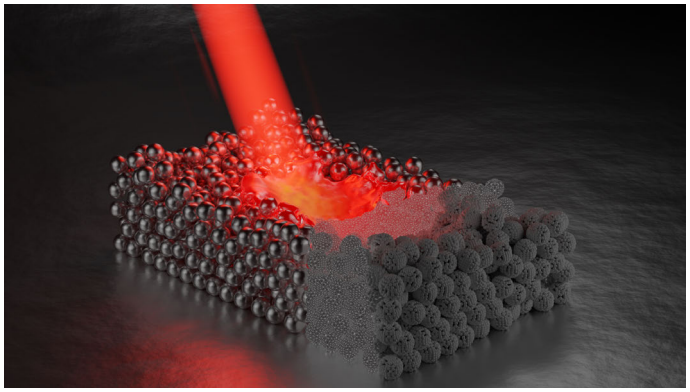
www.fau.eu/2021/04/15/news/research/quite-a-turnaround-what-microrobots-have-in-common-with-soap/

MSS paper featured by Laborjournal

Our Nature-Physics paper "Insufficient evidence for ageing in protein dynamics" by Igor Gochuk and Thorsten Pöschel was featured by a 4-pages article in Laborjournal: Mario Rembold: "Kontrovers: Altern Proteine oder nicht?", LaborJournal **9**, 16-20 (2021) www.laborjournal.de/rubric/hintergrund/hg/hg_21_09_01.php

MSS image by Michael Blank wins DFG photo competition and appears on the official DFG calendar 2022

German Science Foundation (DFG) issues a themed wall calendar every year, with twelve photo motifs from DFG-funded projects illustrating the project's research work. The image by Michael Blank will appear on the October page of the official DFG-Calendar 2022.



Simulation of selective laser melting of titanium powder. The titanium particles have a diameter of 45 μm and the size of the powder bed is $(0.2 \times 0.4 \times 1.0)\,\mathrm{mm}^3$. The simulation method is based on Smoothed Particle Hydrodynamics (SPH) in combination with ray tracing. The figure illustrates the simulation method at different scales of modeling.

MSS goes Girl's Day

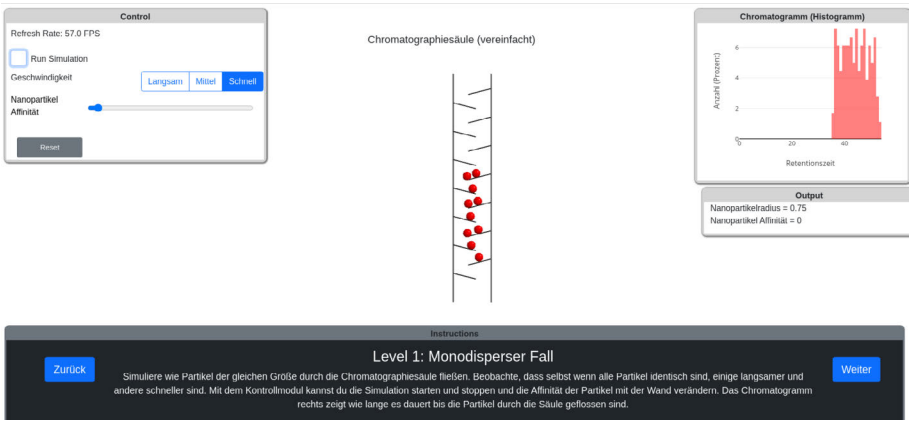
On 28.04.2021 the Girls' Day for schoolgirls of the 5th - 11th grade took place at the Faculty of Engineering. Girls can get an insight into technical courses of study at various experimental stations. This year, the event took place virtually.
From MSS, Dr. Achim Sack partcipated supported by Dr. Michael Heckel. Achim gave a 2 hour presentation "Light into the Dark" ("Licht ins Dunkel bringen"). He explained Computed Tomography starting from the properties of x-rays to a full scan of a Kinder-Surprise egg.
`www.maedchen-technik.de`

Mädchen und Technik

MSS participated in the “Mädchen und Technik” event September 6-10 with the experiment “Light into the Dark”. In 5 shows, around 40 girls of classes 6-11 had the opportunity to experience X-ray tomography in practice. A clear explanation introduced the subject of X-ray, radiographs and tomography. Afterwards, the participants were able to pursue their curiosity about science and technology and, under guidance, make radiographs and X-ray tomographies of objects of their own choice (e.g. Kinder surprise, headphones and RFID cards).

g’scheid schlau - das Lange Wochenende der Wissenschaften, 21. – 24. Oktober 2021

MSS members participated by an oral presentation on Sunday 24.10 at 15.00. For this opportunity, an online chromatography simulation tool had been developed. This tool was elaborated in the framework of the Collaborative Research Centre 1411 by Prof. Michael Engel, Navid Panchi, Nydia Varela Rosales and Federico Tomazic.
`www.mss.cbi.fau.de/personal/engellab/crc/front_page.html`



Screenshot of the Chromatography Simulation Tool

Lehromat 1000

lehromat.de

Governments' responses to the spreading Covid-19 pandemic have thrown the entire society into crisis. For the large group of students in elementary and secondary schools, this means cancelled classes for a long time, or at least irregular classes.

Remote teaching via the Internet offers a way out, but it cannot replace face-to-face contact and group dynamics among students. This concerns both the contact of the students in the classroom and the development and maintenance of social contacts and social behavior outside the classroom.

An alternative to distance learning is alternate teaching. Here, the classes are taught in half the class size at the school, while the other half of the students are taught remotely at home. The groups change every week. Alternating instruction is more appropriate for fostering the social development of the students, but is particularly challenging and time-consuming for the teachers, since both parts of the class must be approached in completely different ways in order to teach the subject matter equally.

The Lehromat 1000 is a device designed to assist the teacher in alternate teaching. With its help, the non-present students are fully involved in what is happening in the classroom.

Currently the Lehromat is used at several public schools in Nuremberg and Neumarkt.

A full description including all instructions for assembling your own Lehromat can be found at lehromat.de.

Lehromat was featured by several publications:

www.fau.de/2021/05/news/fau-entwickelt-lehrhilfe-zum-selbstbau-fuer-schulen
www.nordbayern.de/region/neumarkt/lehromat-sendet-live-aus-der-klasse-1.11017665
www.neumarkt-tv.de/neumarkt-tv/aktuell/der-lehromat-neues-projekt-am-ostendorfer-gymnasium/
wochenblatt-neumarkt.de/neumarkt-tv/aktuell/der-lehromat-neues-projekt-am-ostendorfer-gymnasium/
www.youtube.com/watch?v=kI7nbdVNni8
www.webundmobile.de/beyond-dev/editor/lehrhilfe-selbstbau-schulen-2667539.html

BILDUNG

Klassenzimmer für zu Hause

28. April 2021
17:14 Uhr

Dank „Lehromat“ sind Neumarkter Schüler auch im Distanzunterricht live dabei. Das erleichtert den Alltag in der Pandemie.

Von Josef Wittmann

Sara Hammesfahr unterrichtet in der Französischstunde mit dem „Lehromat“ ihre Präsenz- und Homeschüler der 11. Jahrgangsstufe in Neumarkt gleichzeitig. Foto: JOSEF WITTMANN

NEUMARKT. „Bon jour“, begrüßt Studienrätin Sara Hammerfahr ihre Q11 zur Französischstunde. „Bon jour Mademoiselle Hammerfahr“, antworten nicht nur die Anwesenden, sondern auch neun Stimmen aus dem Lautsprecher. Normal ist das in Corona-Zeiten nicht, denn wie alle bayerischen Abschlussklassen sind auch die Ostendorfer wegen der aktuellen Sieben-Tage-Inzidenz im Wechselunterricht. Da sehen sich Schüler und Lehrer in Coronazeiten nur jeden zweiten Tag. „Ich habe manche schon seit Weihnachten nicht mehr gesehen“, sagt die Schülerin Lea und freut sich wie alle anderen, dass das nun ein Ende hat.

www.mittelbayerische.de/region/neumarkt-nachrichten/klassenzimmer-fuer-zu-hause-21102-art1999547.html

13. Social Activities

Group Excursion July 2021

This year we finally had another group excursion. We went hiking and did Via Ferrata climbing near Hirschbach in the Hersbrucker Alb. Great fun!

In front of the Noristörl

Crossing the Noris-Brettl