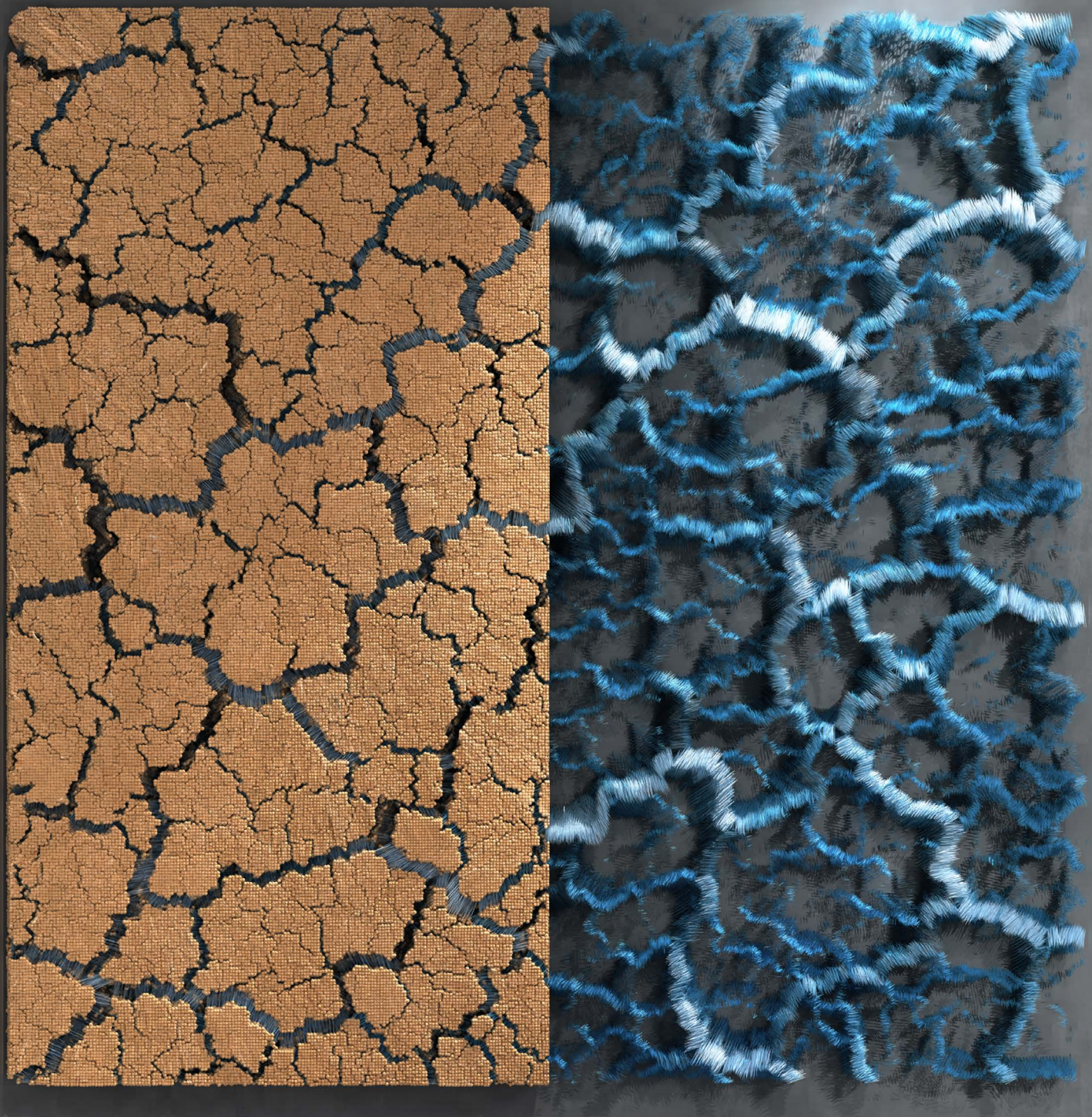
Institute for Multiscale Simulation

Prof. Thorsten Pöschel
Prof. Michael Engel

Friedrich-Alexander-Universität Erlangen-Nürnberg

2025
Annual Report



FAU Friedrich-Alexander-Universität Erlangen-Nürnberg

Institute for Multiscale Simulation
MSS

Institute for Multiscale Simulation

https://www.mss.tf.fau.de
Friedrich-Alexander-Universität Erlangen-Nürnberg
Cauerstraße 3, 91058 Erlangen

Editor: Geovane de Jesus Rodrigues

Front cover: Formation of cracks in drying suspension
Image by Meysam Bagheri

Back cover: Particle based simulation of reactive flows in micro-porous systems
Image by Felix Buchele

Institute for Multiscale Simulation

Annual Report 2025

Preface

The Institute for Multiscale Simulation of Particulate Systems at Friedrich-Alexander-Universität Erlangen-Nürnberg is dedicated to advancing the fundamental understanding of complex particulate and granular matter across scales. Our research combines rigorous multiscale simulations with carefully designed experiments to validate and refine theoretical models, connecting microscopic interactions to macroscopic behavior. By integrating computational physics, theory, and experimental insight, we aim to uncover the principles governing structure formation, dynamics, and functionality in complex matter.

Our activities span nanoscale, atomic, soft-matter, and granular systems and address chemical and physical processes in which collective behavior emerges from interactions among many components. A particular focus lies on self-assembly and self-organization—bottom-up processes through which simple building blocks spontaneously form complex, often highly functional structures. By investigating these mechanisms across length and time scales, we seek to deepen the understanding of emergent phenomena and contribute to the rational design of advanced materials and engineered systems.

In 2025, the Institute continued to expand its research portfolio, strengthen interdisciplinary collaborations, and foster an environment in which creativity, scientific rigor, and intellectual curiosity thrive. Alongside our scientific achievements, we remain committed to excellence in teaching, mentoring, and outreach. In this annual report, we present research highlights from the past year, summarize educational activities, and document our engagement within the scientific community and beyond.

Erlangen, December 2025

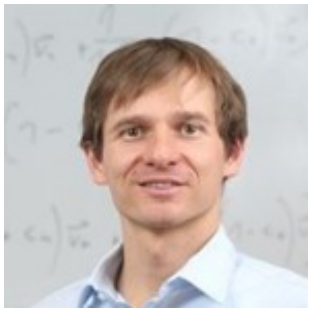
Thorsten Pöschel, Michael Engel

1. Staff Members

Professors

Prof. Dr.
Thorsten Pöschel

Prof. Dr.
Michael Engel



Priv.-Doz. Dr.
Patric Müller

Priv.-Doz. Dr.
Alberto Leonardi

Priv.-Doz. Dr.
Sudeshna Roy

Visiting Researchers

Prof. Dr.
Praveen Kumar Bommineni

Prof. Dr.
Tomoko Mizuguchi

Prof. Dr.
Sakurako Tanida

Habilitation Candidate

Dr.
Carlos L. Bassani

Postdoctoral Researchers

Dr.
Holger Götz

Dr.
Achim Sack

Dr.
Nydia Varela Rosales

PhD Students

Franziska Anderl
M. Sc.

Meysam Bagheri
M. Sc.

Felix Buchele
M. Eng.

Utku Canbolat
M. Sc.

Geovane de Jesus Rodrigues
M. Sc.

Mark Emmert
M. Sc.

Kai Ihrig
M. Sc.

Jyoti Pannu
M. Sc.

Wing To Ku
M. Sc.

Valentina Marzulli
M. Sc.

Arash Moradian
M. Sc.

Harsha Namdeo
M. Sc.

Luisa Nickl
M. Sc.

Navid Panchi
M. Sc.

Nicolas Pechler
M. Sc.

Huzaif Rahim
M. Sc.

Hakan Şanal
M. Sc.

Angel Santarossa
Lic. (M.Sc.)

Paul Scheuerlein
M. Sc.

Zhiyu Song
M. Sc.

Federico Tomazic
M. Sc.

Kaijie Zhao
M. Sc.

Master and Bachelor Students

Quirin Beckh
Bachelor student

Felix Böhmer
Bachelor student

Arne Bringewatt
Master student

Yi-Ting Chiang
Master student

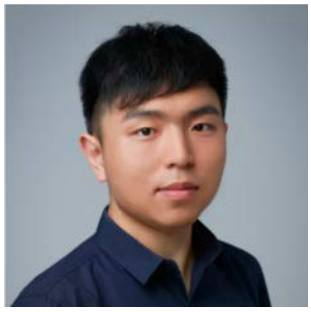
Suleyman Gafarli
Master student

Laura Steub
Master student

Technical and Administrative Staff

Stefanie Suttner
Team assistant

Walter Pucheanu
Master technician, head of the mechanics workshop



Hao Sheng
M.Sc.
System administrator,
X-ray tomography technician

Student Assistants

Mohammad Aminazadeh

Yaopeng Liu

Isabella Schneider

Sanjukta Chowdhury

2. Teaching Activities

image: fau.de

Simulation Granularer und Molekularer Systeme (SimSys)
Lecture Prof. Thorsten Pöschel
Prof. Dr. Michael Engel
Lab session Wing To Ku

Wissenschaftliches Rechnen für Ingenieure
Lecture Prof. Thorsten Pöschel
Exercise Felix Buchele

Scientific Computing in Engineering
Lecture Prof. Thorsten Pöschel
Exercise Felix Buchele

Photon and Neutron Scattering for Structure Determination
Lecture Priv.-Doz. Dr. Alberto Leonardi
Exercise Priv.-Doz. Dr. Alberto Leonardi

Messtechnik 2 - Messmethoden und Analytik (MT2)
Lecture Dr. Achim Sack
Exercise Nicolas Pechler

Digitale Bildverarbeitung (DBV)
Lecture Dr. Achim Sack
Exercise Dr. Achim Sack

Scanning and Printing in 3D (SD3D)
Lecture Priv.-Doz. Dr. Patric Müller
Exercise Priv.-Doz. Dr. Patric Müller
Lab session Priv.-Doz. Dr. Patric Müller
Walter Pucheanu
Felix Buchele
Nicolas Pechler

Maschinelles Lernen und Künstliche Intelligenz im Ingenieurwesen (KI-ING)
Lecture Priv.-Doz. Patric Müller
Exercise Priv.-Doz. Patric Müller
Utku Canbolat
Lab session Priv.-Doz. Patric Müller

Partikelbasierte Strömungsmechanik (PSTM)
Lecture Priv.-Doz. Dr. Patric Müller
Exercise Priv.-Doz. Dr. Patric Müller

Discrete Element Simulations
Lecture Dr. Holger Götz
Exercise Dr. Holger Götz
Lab Session Dr. Holger Götz

Granular Matter and Applications
Lecture Priv.-Doz. Dr. Sudeshna Roy

Selbstorganisationsprozesse (SOP)
Lecture Prof. Dr. Michael Engel
Dr. Giulia Magnabosco
Prof. Robin Klupp Taylor

Data Science for Engineers (DSE)
Lecture Prof. Dr. Michael Engel
Exercise Navid Panchi

Soft Matter Journal Club (SoftMat)
Lecture Prof. Dr. Michael Schmiedeberg
Prof. Dr. Michael Engel
Prof. Dr. Vasily Zaburdaev

Basics in Computational Materials Science and Process Simulation 1 (B_Compu_1)
Lecture Dr. Carlos L. Bassani

Projektkurs Chemische und Biologische Prozeßtechnik (CBPT)
Supervisor Geovane de Jesus Rodrigues
Nicolas Pechler

CEP Advanced Seminar
Lecture Prof. Robin Klupp Taylor
Supervisor Meysam Bagheri
Carlos L. Bassani
Nicolas Pechler
Huzaif Rahim

Multiphase Flows (MSS-MF)
Organizer Prof. Thorsten Pöschel

Multiscale Simulation Techniques (MSS-MS)
Organizer Prof. Thorsten Pöschel

Granular Matter - MSS Seminar (MSS-GM)
Organizer Prof. Thorsten Pöschel

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

17.01.2025	Huzaif Rahim	*Shear-induced pressure anisotropy in non-spherical particles*
24.01.2025	Angel Santarossa	*Granular jamming gripper with integrated suction*
31.01.2025	Jyoti	*Symmetry breaking and growth mechanism of multiply twinned nanoparticles*
07.02.2025	Kaijie Zhao	*Strain distribution and relaxation in pentatwinned nanocatalysts*
14.02.2025	Carlos L. Bassani	*Mesomorphology of clathrate hydrates from molecular ordering: I. Particle-based and continuum models of molecular attachment*
21.02.2025	Carlos L. Bassani	*Mesomorphology of clathrate hydrates from molecular ordering: II. Phase field models for the emergence and evolution of porous patterns*
07.03.2025	Wing To Ku	*Homogenization of granular pipe flow*
28.03.2025	Nicolas Pechler	*Generation of neural network training data to reconstruct two-phase flows in EIT*
11.04.2025	Felix Buchele	*The advent calendar problem*
18.04.2025	Suleyman Gafarli	*Development of a kinetic model for the methanol-to-olefins synthesis over an industrial catalyst*
25.04.2025	Marek Mihalkovic	*Composite alloys inspired by hard sphere mixtures and pair potentials*
02.05.2025	Navid Panchi	*Accurate, efficient and scalable implementation of Debye scattering equation solution*
09.05.2025	Felix Buchele	*Stochastic diffusion model for heterogeneous catalysis*
16.05.2025	Wing To Ku	*Mid-fidelity fluid structural simulation in rotorcraft aerodynamics*
23.05.2025	Harsha Namdeo	*Reconstruction of pair potential using nanoparticle configurational data*
05.06.2025	Felix Buchele	*A first principles based chemistry model*
13.06.2025	Hakan Şanal	*Finiteness Conditions in rings and modules with respect to isomorphism classes*
20.06.2025	Carlos L. Bassani	*Macromorphology evolution of gas hydrates under multiphase flow*
25.07.2025	Sakurako Tanida	*Elevator traffic jam: Why do they arrive together?*
01.07.2025	Zhiyu Song	*Effective interaction between ligand-coated nanoparticles*
22.08.2025	Geovane de Jesus Rodrigues	*Performing experiments under low/hypergravity*
29.08.2025	Meysam Bagheri	*Emergence of crack patterns in drying suspensions*

12.09.2025	Kamilla Zaripova	*Symmetry breaking of nanocrystal shapes via formation of surface defects with kinetic Monte Carlo*
03.10.2025	Felix Buchele	*An image-based approach to characterize porous media*
21.11.2025	Felix Buchele	*Bridging microkinetics and microstructure*

3. Granular Matter - MSS Seminar

190. **Prof. Hartmut Löwen**
Heinrich-Heine-Universität Düsseldorf, Germany
Odd and twisted: Dynamics of chiral active particles
February 5, 2025

191. **Prof. Daniel Bonn**
University of Amsterdam, Netherlands
Friction and contact mechanics visualized using fluorescent environmentally sensitive probes
February 12, 2025

192. **Prof. Scott Waitukaitis**
Institute of Science and Technology Austria, Klosterneuburg, Austria
Granular Goes Electric: Nabbing the Symmetry Breaker in Oxide Contact Electrification
February 19, 2025

193. **Prof. Frank Opferkuch**
Technische Hochschule Nürnberg Georg Simon Ohm, Germany
Challenges in the vaporization of working fluids and refrigerants in thermodynamic cycles.
March 19, 2025

194. **Dr. Holger Götz**
Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Jamming and convection in granulates
May 22, 2025

195. **Prof. Igor Ostanin**
University of Twente, Netherlands
DEM modeling framework enriched with the kernel-independent fast multipole method
April 2, 2025

196. **Prof. Nicolas Vogel**
Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Elliptical particles at liquid interfaces: from self-assembly to drying processes
April 23, 2025

197. **Dr. Jonathan Barés**
Université de Montpellier, France
Squishy granular matter: A story far beyond jamming
Mai 21, 2025

198. **Prof. Silvia Budday**
Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Exploring human brain mechanics
May 28, 2025

199. **Federico Tomazic**
Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Particle Self-Assembly into Complex Suprastructures: The Role of Shape and Interaction
June 3, 2025

200. **Prof. Hans Herrmann**
PMMH, ESPCI, Paris, France
Frustrated bearings
June 18, 2025

201. **Prof. Detlef Lohse**
University of Twente, Netherlands
The role of bubbles in electrolysis
June 25, 2025

202. **Dr. Reinhard Richter**
Universität Bayreuth, Germany
What you always wanted to know about intimate relationships but were afraid to ask
July 23, 2025

203. **Prof. Sakurako Tanida**
University of Tokyo, Japan
Dynamics, interactions, and frequency dependence of elevator traffic
September 17, 2025

204. **Prof. Mikio Sakai**
University of Tokyo, Japan
Advanced DEM modeling and its applications in data science
September 25, 2025

205. **Prof. Sergio Galindo Torres**
Westlake University, Hangzhou, China
Rheology of suspensions. Discrete Element - Lattice Boltzmann simulations
October 8, 2025

206. **Dr. Frank Smallenburg**
CNRS, Laboratoire de Physique des Solides, Orsay, France
Hard-sphere quasicrystals: A playground for entropy
October 15, 2025

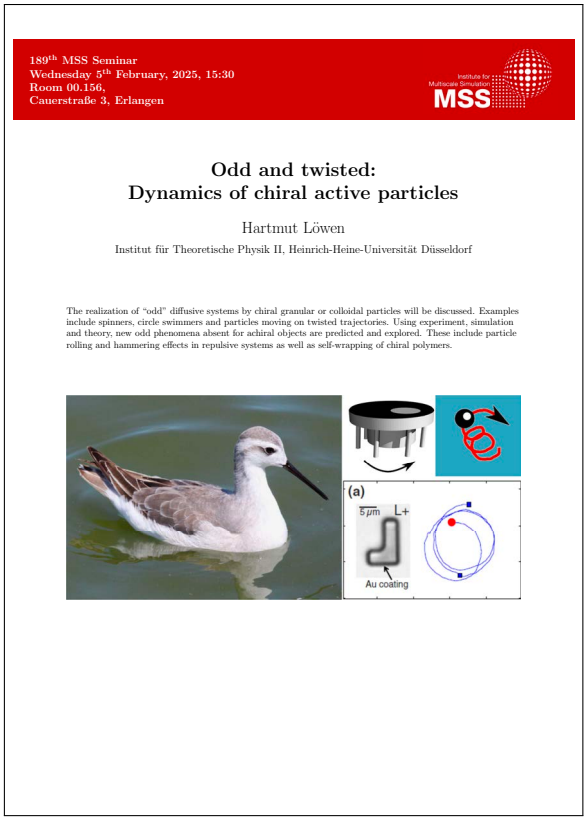
207. **Prof. Sergio Galindo Torres**
Westlake University, Hangzhou, China
Invariant forms of transport phenomena infracture networks
October 22, 2025

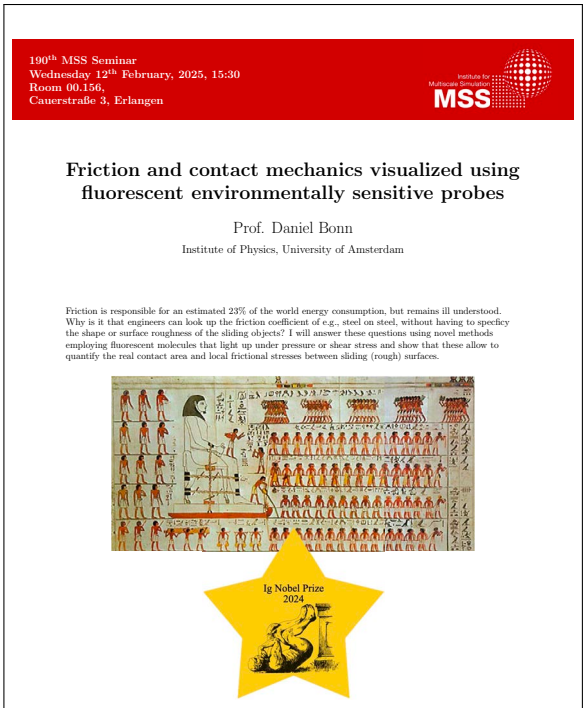
208. **Dr. Vinicius G. Poletto**
Federal University of Technology - Paraná, Curitiba, Brazil
Simulation of crystal deposition under flow
November 19, 2025

209. **Prof. Eric Opsomer**
GRASP, University of Liege, Belgium
When Grains Charge and Bend: Micro-Mechanisms Behind Granular
December 3, 2025

210. **Prof. Philipp Pelz**
Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Sub-Ångström 3D Resolution, Volume Imaging Beyond the Depth of Focus Limit, and Automated Tomography From Electron Scattering Experiments
December 10, 2025

211. **Dr. Giuseppe Soligno**
Utrecht University, Netherlands
Molecular dynamics (MD) models for the formation of low-dimensional nanomaterials
December 17, 2025





191st MSS Seminar
Wednesday 19th February, 2025, 15:30
Room Kurssaal 1 (KS1),
Cauerstraße 4, Erlangen

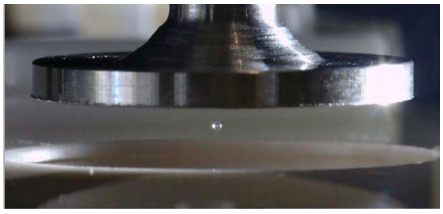
Granular Goes Electric:

Nabbing the Symmetry Breaker in Oxide Contact Electrification

Prof. Scott Waitukaitis

Institute of Science and Technology Austria, Klosterneuburg

Granular materials are constantly rubbing and rolling, sliding and colliding, grinding and crashing—and, as a consequence, they often become really (really) electrostatically charged. Why? In this talk, I will discuss our experiments using levitation to try and understand why grains made of identical oxide materials (*e.g.* SiO_2, Al_2O_3, ...) exchange electrical charge during contact. Although this topic is devilishly complicated, we're figuring big things out. Come to the seminar to find out more.



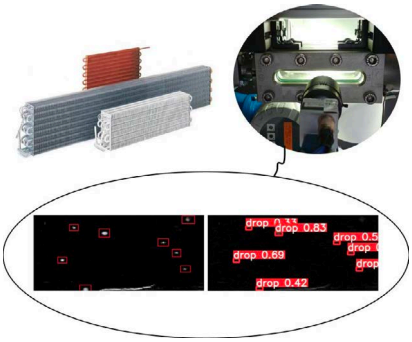
192nd MSS Seminar
Wednesday 19th March, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

Challenges in the vaporization of working fluids and refrigerants in thermodynamic cycles

Prof. Frank Opferkuch

Technische Hochschule Nürnberg Georg Simon Ohm

In Germany alone, 85 TWh of energy are used per year to generate cooling, and demand continues to rise steadily. To generate low temperatures, a gaseous refrigerant is compressed, condensed, expanded and finally evaporated again at low temperatures with the addition of heat. However, the design of evaporators is still only possible with a great deal of uncertainty. Optical methods for the investigation of thermohydraulic effects as well as the modeling and simulation of flow boiling can help to support the development of new evaporators and the use of new refrigerants. This talk will provide an insight into the technologies used and the challenges involved.



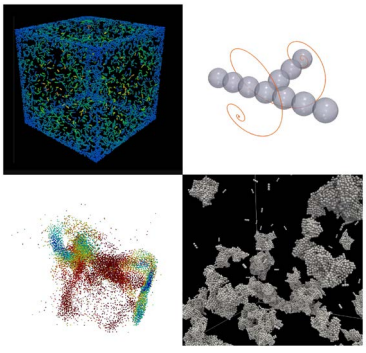
193rd MSS Seminar
Wednesday 2nd April, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

DEM modeling framework enriched with the kernel-independent fast multipole method

Prof. Igor Ostanin

University of Twente, Netherlands

In this talk, we discuss the coupling of the MercuryDPM particle dynamics code with the kernel-independent fast multipole method to capture long-range pair interactions between particles. The talk covers key implementation details, including coupling with rigid clumps, periodic boundary conditions, and OMP/MPI parallelization. Several examples from various application fields are presented to illustrate the method's capabilities.



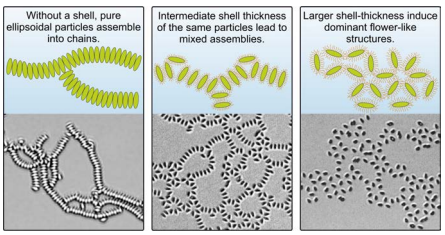
194th MSS Seminar
Wednesday 23rd April, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

Elliptical particles at liquid interfaces: from self-assembly to drying processes

Nicolas Vogel

Friedrich-Alexander-Universität Erlangen-Nürnberg

Colloidal particles adsorb to liquid interfaces. I will outline how this adsorption can be enhanced by adding polymer chains to particle surfaces and how this effect alters the drying behavior. Interestingly, the stretching of polymer particles into ellipsoids introduces such chains. This unintentional surface modification provides an alternative explanation for the famous shape-dependent drying behavior reported over a decade ago. Even though the shape anisotropy may not govern the drying behavior, it certainly affects the self-assembly at the air/water interface and provides a tool to control the preferred configuration at a liquid interface.



195th MSS Seminar
Wednesday 21st May, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

Institute for Multiscale Simulation
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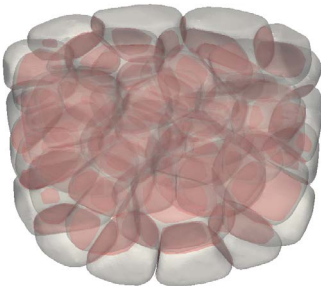
Squishy granular matter: A story far beyond jamming

Jonathan Barés
LMGC, Université de Montpellier, CNRS, Montpellier, France

Granular materials are ubiquitous in nature and industry, encompassing grains of diverse shapes, sizes, and, crucially, mechanical properties – even within the same packing. Among them, granular systems composed of highly deformable (*squishy*) particles exhibit particularly distinctive behaviors. These systems serve as fundamental models for biological tissues, soft cellular aggregates, liquid foams, emulsions, and sintered materials.
In this presentation, I will introduce an analytical model describing the deep jammed-state compaction of soft granular systems. This model will be validated through both 2D and 3D numerical simulations. Additionally, I will present novel experimental techniques designed to probe these systems at the sub-granular scale, providing crucial insights that definitively validate the model.



196th MSS Seminar
Wednesday 28th May, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

Institute for Multiscale Simulation
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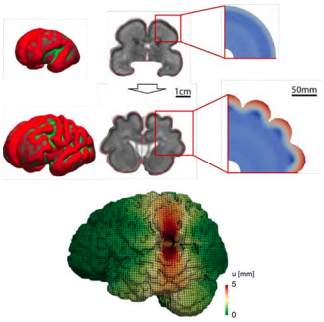
Exploring human brain mechanics

Prof. Silvia Budday
Institute of Continuum Mechanics and Biomechanics,
Friedrich-Alexander-Universität Erlangen-Nürnberg

The brain is arguably our most important and complex, but also least understood organ. Increasing evidence confirms that mechanics plays a critical role for brain function and dysfunction. Computational models can help understand basic processes in the brain, e.g., during development, injury, and disease, and facilitate early diagnosis and treatment of neurological disorders. By closely integrating biomechanical experiments on human brain tissue, microstructural analyses, continuum mechanics modeling, and finite element simulations, we develop computational tools that capture both biological processes at the cellular scale as well as macroscopic loading and pathologies at the tissue and organ scales.



197th MSS Seminar
Tuesday 3rd June, 2025, 16:15
Room 00.156,
Cauerstraße 3, Erlangen

Institute for Multiscale Simulation
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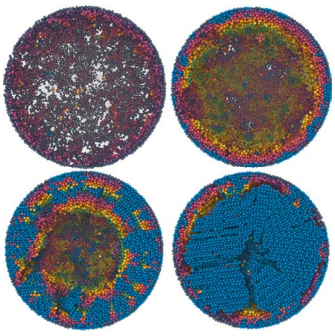
Particle Self-Assembly into Complex Suprastructures: The Role of Shape and Interaction

Federico Tomazic
Friedrich-Alexander-Universität Erlangen-Nürnberg

The relation betwen nanoparticle interaction and the formation of a desired self-assembled suprastructure can be understood by using computational techniques. We use coarse-grained models to represent nanoparticles and predict self-assembly outcomes, including the ordering of colloidal particles inside drying droplets, the formation of monolayers due to steric frustration and the self-assembly of regular porous structures caused by nanoparticle anisotropy.



198th MSS Seminar
Wednesday 18th June, 2025, 13:30
Room 00.156,
Cauerstraße 3, Erlangen

Institute for Multiscale Simulation
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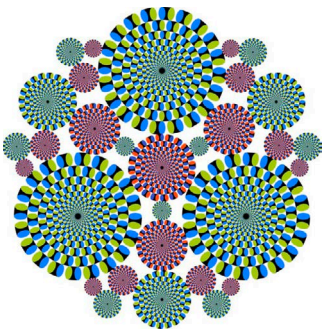
Frustrated Bearings

Prof. Hans Herrmann
PMMH, ESPCI, Paris, France

We will consider bearings, which are systems of touching spheres or disks that roll on each other without slip and will classify all the possible rotation modes. They can also be space-filling, resulting in "solid turbulence". We frustrate a system of touching spheres by imposing two different bearing states on opposite sides and search for the configurations of lowest energy dissipation. For Coulomb friction in two dimensions, the minimum cut separates he bearing states, while in three dimensions, intermediate bearing domains are energetically more favourable.

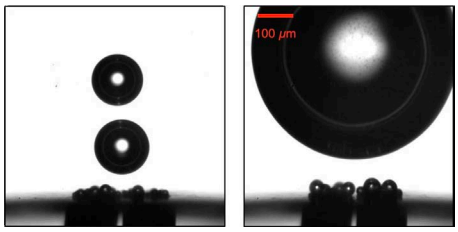


199th MSS Seminar
Wednesday 25th June, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

The role of bubbles in electrolysis

Detlef Lohse
University of Twente, Netherlands

Electrolysis is the key technology for the energy transition, converting renewable energy into hydrogen. However, a big stumbling block in achieving higher efficiency of this process are the bubbles created on the electrodes as they block them and enhance the resistance. In this talk I will report our latest experimental, theoretical, and numerical results on the role of bubbles in electrolysis and how to mitigate their harmful effect. In particular, I will address (i) the threshold current density for detachment of single electrolytic nanobubbles, (ii) the role of the electrolyte and of Marangoni convection on electrolytic bubbles, (iii) coalesence-driven electrolyte spraying: Why & when does it rain in electrolytic bubbles? (iv) To jump or not to jump: Coalescence driven departure of wall-attached electrolytic bubbles, and (v) Coalescence-driven departure of electrolytic bubbles.

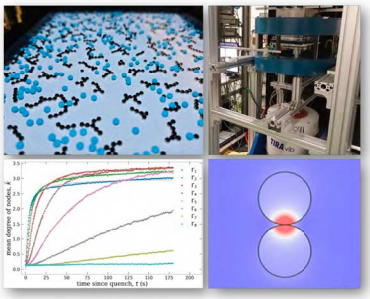


200th MSS Seminar
Wednesday 23rd July, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

What you always wanted to know about intimate relationships[1] but were afraid to ask

Reinhard Richter
Experimentalphysik V, Universität Bayreuth

We are reporting experiments on the aggregation process in a mixture of glass and magnetized steel spheres. Aggregation sets in after the amplitude of the vertical shaking is suddenly reduced. For a deep quench of the amplitude the magnetized beads quickly form a transient network that gradually develops into dense clusters. Conversely, with a smaller amplitude reduction the spheres directly aggregate into compact clusters. Utilizing network metrics we uncover two fundamental time scales, indicating that *viscoelastic phase separation* takes place.



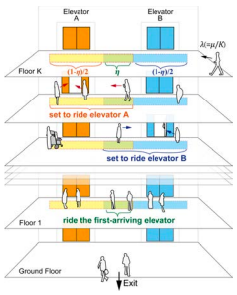
[1] of magnetized steel spheres

201st MSS Seminar
Wednesday 17th September, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

Dynamics, interactions, and frequency dependence of elevator traffic

Prof. Sakurako Tanida
Department of Aeronautics and Astronautics, Graduate School of Engineering, The University of Tokyo

Transportation systems are designed to move resources and people efficiently, yet they often exhibit unintended patterns of order. In this seminar, we focus on elevator traffic in crowded buildings, where multiple cars may respond to the same hall call almost simultaneously. We frame this as a synchronization problem and explore the underlying dynamics. The talk is organized into three themes: (1) single-car dynamics, (2) two-car interactions and synchronization, and (3) the role of periodicity and natural frequency.

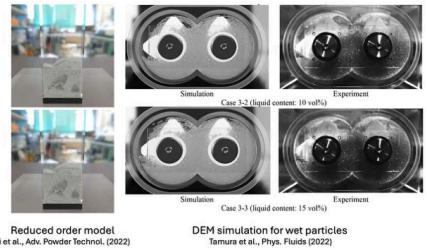


202nd MSS Seminar
Thursday 25th September, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

Advanced DEM modeling and its applications in data science

Prof. Mikio Sakai
University of Tokyo

The Discrete Element Method (DEM) is the standard tool for simulating granular dynamics and powder processing. Recent advances extend its capability to industrial-scale multiphase phenomena. My group has contributed by developing coarse-grained DEM for large systems, a DEM–VOF framework for gas–solid–liquid flows, and flexible boundary treatments via signed distance functions. These innovations expand DEM's scope but also generate vast data, creating challenges in extracting insights. To address this, we built a data-science framework: Proper Orthogonal Decomposition reveals dominant mixing and segregation, and neural-network integration yields reduced-order models that predict granular flows efficiently.



Reduced order model
Li et al., Adv. Powder Technol. (2022)

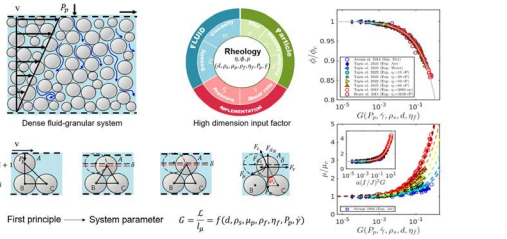
DEM simulation for wet particles
Tamura et al., Phys. Fluids (2022)

203rd MSS Seminar
Wednesday 8th October, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

Rheology of suspensions. Discrete Element – Lattice Boltzmann simulations

Prof. Sergio Galindo Torres
Westlake University, Hangzhou, China

This presentation shares recent findings on the rheology of suspensions and granular materials. Submarine landslides, for example, undergo continuous cycles of stagnation-creeping and fast flow stages. Through high-resolution simulations, we explored this mechanism and derived dimensionless numbers to quantify it. We further studied the contrasting rheological responses of suspensions under isochoric versus isobaric conditions. Despite their differences, both systems exhibit rheological transitions connected to granular cluster formation. Our latest work resolves a key aspect of this puzzle by linking cluster dynamics to these transitions through percolation theory. This approach yields scale-invariant universal relations that fully describe the observed behavior. These theoretical advances are expected to improve large-scale rheological models and ultimately enhance mitigation strategies for hazardous geophysical events.

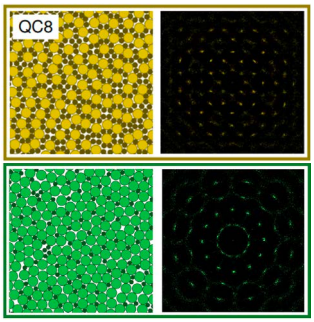


204th MSS Seminar
Wednesday 15th October, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

Hard-sphere quasicrystals: A playground for entropy

Frank Smallenburg
CNRS, Laboratoire de Physique des Solides, Orsay, France

Quasicrystals are exotic materials that break traditional rules of crystallography in metal alloys and soft-matter systems. This talk explores how a phase as complex as a quasicrystal can be stabilized by entropy alone, starting from simple hard spheres. We examine their self-assembly in simulations, determine the origin of their stability using free-energy calculations, and explore the emergence of point defects. Finally, I briefly highlight experiments that demonstrate a granular quasicrystal of millimeter-sized steel spheres.

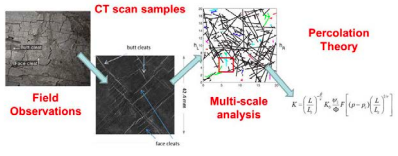


205th MSS Seminar
Wednesday 22nd October, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

Invariant forms of transport phenomena in fracture networks

Prof. Sergio Galindo Torres
Westlake University, Hangzhou, China

Transport phenomena in complex hydrological systems remain one of the most challenging modeling problems in environmental science, with no universally satisfactory solutions for general scenarios. In this talk, we present a novel approach addressing the flow and scalar transport in fracture networks. For fracture networks, a key obstacle is the scarcity of field data on fracture apertures, orientations, and sizes, necessitating reliance on statistical descriptors. By using percolation theory, we derive invariant formulations for hydraulic permeability and longitudinal dispersion coefficients. These models are rooted in first principles, require no parameter fitting, and explicitly incorporate statistical fracture properties, ensuring practical applicability in engineering contexts

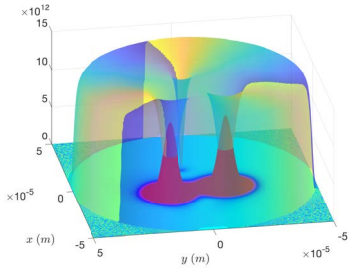


206th MSS Seminar
Wednesday 12th November, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

Massive quantum vortices in binary Bose-Einstein condensates

Alice Bellettini
Department of Applied Science and Technology, Politecnico di Torino, 10129 Torino, Italy

Quantum bosonic gases, due to their manipulability, provide the perfect platform for observing macroscopic quantum many-body phenomena. These can be for example quantum vortices ("topological defects"), being the hallmark of superfluidity, or Josephson supercurrents. Such collective effects have been recently employed in the context of quantum simulation and atomtronics. Here, I will introduce the basics of ultracold quantum gases and present my research on the properties of massive quantum vortices in different configurations, and on vortex-supported supercurrents.



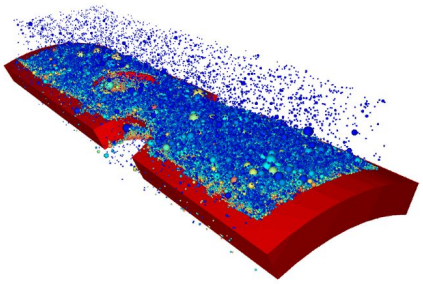
207th MSS Seminar
Wednesday 19th November, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

Simulation of Crystal Deposition under Flow

Vinicius G. Poletto

Research Center for Rheology and Non-Newtonian Fluids,
Federal University of Technology - Paraná, Curitiba, Brazil

This talk presents a multidisciplinary framework for modeling and simulating crystal deposition processes coupled with fluid dynamics, liquid–solid two-phase flow, and thermodynamics. The investigated phenomena include nucleation, agglomeration, crystal growth, adhesion, and particle–fluid interactions. The proposed model integrates population balance equations for crystal kinetics, CFD–DEM for multiphase flow, and DEM-based calibration of adhesion forces. Applications in downhole oil wells are discussed, emphasizing the spatiotemporal distribution of scaling mass at operationally critical components such as valves.



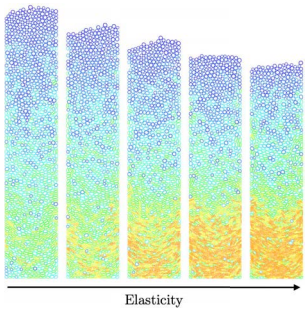
208th MSS Seminar
Wednesday 3rd December, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

When Grains Charge and Bend: Micro-Mechanisms Behind Granular Flow

Eric Opsomer

GRASP, University of Liege, Belgium

Granular materials display rich behaviors driven by particle-scale interactions. This seminar connects two mechanisms to show how microscopic physics shapes macroscopic flow and stress patterns. First, I will discuss triboelectric charging in flowing powders, modeled through DEM simulations of patchy particles. Then, we turn to simulations of deformable rings in a silo revealing that particles deep in the pile buckle. Together, these results illustrate how local charging or deformation can reorganize granular assemblies and govern their global mechanical response.



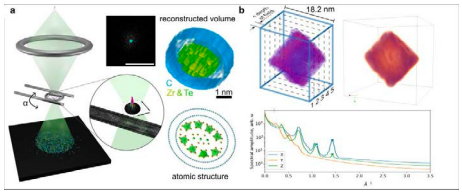
209th MSS Seminar
Wednesday 10th December, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

Sub-Ångstrom 3D Resolution, Volume Imaging Beyond the Depth of Focus Limit, and Automated Tomography From Electron Scattering Experiments

Prof. Philipp Pelz

Friedrich-Alexander-Universität Erlangen-Nürnberg

Electron ptychography is rapidly emerging as a way to turn scattered electron waves into precise three-dimensional atomic maps, effectively solving a challenging inverse problem that links measurement, modeling, and reconstruction. By combining multi-slice physics, joint optimization, and automated data collection, we can now recover sub-Ångström 3D structures even when the experiment violates classical limits such as depth of focus and tomographic completeness. These methods dramatically expand the range of materials and volumes that can be imaged at true atomic resolution, opening the door to data that is richer, more robust, and more compatible with theory and simulation. The result is a practical platform that bridges experiment and computational modeling through a unified, physics-based reconstruction framework.



210th MSS Seminar
Wednesday 17th December, 2025, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

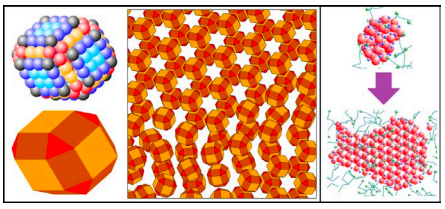
Molecular dynamics (MD) models for the formation of low-dimensional nanomaterials

Dr. Giuseppe Soligno

Debye Institute for Nanomaterials Science, Utrecht University (Utrecht, The Netherlands)
Soligno Technologies (Utrecht, The Netherlands)

In the first part, I will present a versatile coarse-grained MD model to investigate the dynamics of (anisotropic) nanoparticles, showing how this model was applied to simulate the self-assembly of 5-nm nanocrystals in 2D superlattices observed at fluid-fluid interfaces.

In the second part, I will show preliminary results from a fully atomistic MD model for the growth and morphological evolution of a nanocrystal (e.g., a 0D amorphous CdSe cluster evolving into a 2D crystalline nanoplatelet).



4. Conference Presentations

Talks

Thorsten Pöschel	*LASER-Wire deposition welding in zero gravity* DLR Symposium "Forschung und Exploration" Bonn | Germany, 12 - 14.3.2025
Thorsten Pöschel	*Charged granular gases* Charged Matter Klosterneuburg | Austria, 26 - 28.3.2025
Carlos L. Bassani	*Kinetic Monte Carlo Simulations for Nanocrystal Shape Control* Materials Research Society Spring Meeting Seattle | USA, 7 – 11.4.2025
Thorsten Pöschel	*Fractal Packing of Nanomaterials* Discrete Simulation and Continuum Modeling of Granular Matter Puglia | Italy, 3 – 9.5.2025
Michael Engel	*Shaping Nanocrystals Beyond Equilibrium* Crystallization and Self-Assembly: from Soft Matter to Pharmaceuticals to Biomineralisation Roscoff | France, 5 – 7.5.2025
Carlos L. Bassani	*Kinetic Monte Carlo Simulations for Nanocrystal Shape Control* Gold 2025 San Sebastian | Spain, 11 – 14.5.2025
Alberto Leonardi	*Operando study of the nucleation and co-growth dynamics of multiple intermetallic phases in solidification of Al-Mn alloys by simultaneous synchrotron X-ray diffraction and tomography* 7th International Conference on Advances in solidification Processes Madrid | Spain, 10 - 13.6.2025
Alberto Leonardi	*Unlocking Mechanical Secrets in Nano-architectured Materials* FAU Tag des CBI 2025 Erlangen | Germany, 18.6.2025
Alberto Leonardi	*Exploration of melt inclusion geometry, entrapment and post-entrapment processes in 3D using X-Ray and diffraction computed tomography* IAVCEI 2025 Scientific Assembly Erlangen | Germany, 29 - 4.7.2025
Thorsten Pöschel	*Discrete Elements Simulations including Fragmentation - Models and Challenges* DEM10 - 10th International Conference on Discrete Element Methods Himeji | Japan, 1 – 5.7.2025

Felix Buchele	*Image-based spherical decomposition of 3D geometries* DEM10 - 10th International Conference on Discrete Element Methods Himeji | Japan, 1 – 5.7.2025
Alberto Leonardi	*In situ study of strains in a 3D Printed Composite (basalt-polylactic acid) by Dual X-Ray Imaging and Diffraction* 19th International Conference on Advances in Experimental Mechanics London | UK, 2 - 4.9.2025
Alberto Leonardi	*Synchrotron Radiation Tomography Study on Degradation of Magnesium Chloride-containing Bioactive Glasses in Osteoporotic Rat Skull Defect Repair* ToScA UK & Europe 2025 Grenoble | France, 10 - 12.9.2025
Alberto Leonardi	*Synchrotron Radiation Tomography Study on Degradation of Magnesium Chloride-containing Bioactive Glasses in Osteoporotic Rat Skull Defect Repair* ToScA UK & Europe 2025 Grenoble | France, 10 - 12.9.2025
Alberto Leonardi	*Unravelling Cs and Sr Uptake Mechanisms in Natural Zeolites Using DIAD for Nuclear Waste remediation* ToScA UK & Europe 2025 Grenoble | France, 10 - 12.9.2025
Alberto Leonardi	*Using a digital twin of a synchrotron beamline to understand alignment of laminography experiments* ToScA UK & Europe 2025 Grenoble | France, 10 - 12.9.2025
Kaijie Zhao	*A Unified Framework for Strain Analysis in Pentatwinned Nanoparticles* ECCOMAS 8th Young Investigators Conference, organized by the University of Chieti-Pescara Pescara | Italy, 17 – 19.9.2025
Thorsten Pöschel	*Active granular gases - non-equilibrium steady states emerging from dissipative collective behavior* SOEAM25 - Self-Organizing and Evolving Active Matter Dresden | Germany, 22 – 26.9.2025
Carlos L. Bassani	*Kinetic Monte Carlo Simulations for Nanocrystal Shape Control* International Congress on Particle Technology Nürnberg | Germany, 23 – 25.9.2025
Carlos L. Bassani	*Kinetic Monte Carlo Simulations for Nanocrystal Shape Control* Particle-Based Materials Symposium 2025 Erlangen | Germany, 7 – 8.10.2025
Thorsten Pöschel	*Event-driven Dynamics of Soft-sphere Systems: Briding Newtonian Mechanics and Non-Smooth Dynamics* 12th Sysmposium of the European Network for Nonsmooth Dynamics (ENNSD) Erlangen | Germany, 30 – 2.10.2025
Carlos L. Bassani	*Kinetic Monte Carlo Simulations for Nanocrystal Shape Control* Materials for Sustainable Development Conference Fall Valencia | Spain, 20 – 24.10.2025
Sudeshna Roy	*Supression Mechanisms of Particle-Filled Flexible Shells for Small Body Landings* 9th International Conference on Vibration Engineering (ICVE 2025) Nanjing | China, 24 – 26.10.2025

Posters

Harsha Namdeo	*Reconstruction of pair potential using nano-configurational data* Particle-Based Materials Symposium 2025 Erlangen | Germany, 7 – 8.10.2025
Jyoti Pannu	*Off-Lattice Kinetic Monte Carlo Simulations of Multiply Twinned Nanoparticles* Particle-Based Materials Symposium 2025 Erlangen | Germany, 7 – 8.10.2025
Navid Panchi	*AES-Debye: Accurate and Efficient Implementation of Debye Scattering Equation* Particle-Based Materials Symposium 2025 Erlangen | Germany, 7 – 8.10.2025
Kaijie Zhano	*A Unified Framework for Strain Analysis in Pentatwinned Nanoparticles* Particle-Based Materials Symposium 2025 Erlangen | Germany, 7 – 8.10.2025
Kaijie Zhao	*Simulated formation of a primitive icosahedral quasicrystal across a wide density range* Particle-Based Materials Symposium 2025 Erlangen | Germany, 7 – 8.10.2025
Achim Sack	*Strömungslinien in Granularer Materie* Lange Nacht der Wissenschaften Erlangen | Germany, 23.10.2025
Harsha Namdeo, Jyoti Pannu	*Modeling of colloidal interactions and assemblies for optimal functional properties* Annual retreat of SFB1411 Design of particulate products Waischenfeld | Germany, 24 - 26.11.2025
Thorsten Pöschel, Sudeshna Roy	*Efficient numerical integration of rigid body dynamics* Powders & Grains 2025 Goa | India, 8 – 12.12.2025

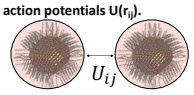
Reconstruction of Pair Potential using Nano-configurational Data

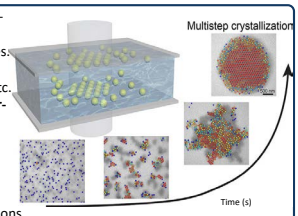
Harsha Namdeo[1,2], Navid Panchi[1], Michael Engel[1,2]

[1]Institute for Multiscale simulation (MSS), IZNF, Friedrich-Alexander-Universität Erlangen-Nürnberg (Germany)
[2]Collaborative Research Center 1411 – Design of Particulate Products (CRC1411), Friedrich-Alexander-Universität Erlangen-Nürnberg (Germany)

Motivation

- **Inverse design** – Determine interactions or structural parameters yielding target material properties.
- **Influencing factors**: solvent, electron dose rate, shape, size, etc.
- Captured **effectively** by **pair interaction potentials U(r$_{ij}$).**



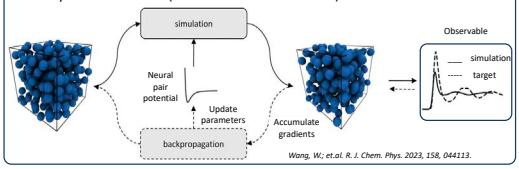


Goal: Link experiments and simulations to tune nanoparticle self-assembly

Zhong, Y.; et.al. Am. Chem. Soc. 2022, 144, 14915−14922.

Background and scope

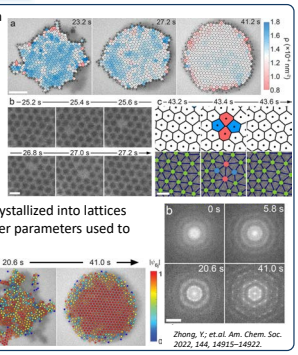
- Force/observable matching: extract interaction potentials.
- Needs accurate experimental particle configurational data.
- Limited tracking → ensemble observables linked to interaction energies.
- IBI key observable: RDF (Radial distribution function)



Wang, W.; et.al. R. J. Chem. Phys. 2023, 158, 044113.

Experimental details

- Gold nanospheres (68.1 nm) with thiol-terminated polystyrene ligands.
- Observed using LCTEM (Liquid Cell TEM).
- Maps constructed: Individual nanoparticles in solvent → superlattice formation
- Solvent dependence:
  - Octane – dispersed
  - Butanol – aggregated,
  - Octane: Butanol (1:1 v/v) – crystallized into lattices
- Analyzed using local & global order parameters used to describe long-range order

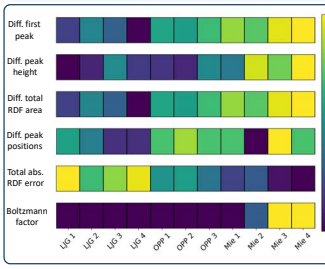


Zhong, Y.; et.al. Am. Chem. Soc. 2022, 144, 14915−14922.

Simulation details

- Modeling **2D isotropic** particles (no explicit solvent and ligands)
- **NVT ensemble** ~ liquid-cell conditions
- **Target RDF** from experimental data
- **Liquid** phase – ensure sufficient particle motion
- **Methods to reconstruct potentials:**
  - RDF matching for a class of potentials
  - Neural Network potentials
  - Iterative Boltzmann Inversion (IBI) scheme

RDF matching for a class of potentials



- Brute-force parameter matching.
- Potential Classes - LJG, OPP, and Mie potentials.
- Compare RDF features of simulations and experiments.
- Confusion Matrix to identify the optimal potential parameters (lowest error).
- Many candidate solutions.
- Inefficient optimization as limited class of potentials.

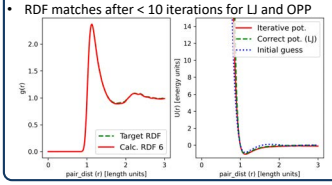
Iterative Boltzmann Inversion (IBI) scheme

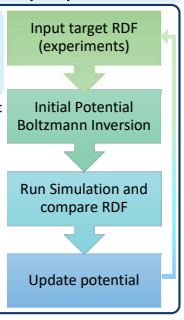
$$U_{i+1}(r_j) \leftarrow U_i(r_j) + k_B T \ln\left[\frac{g_{IBI}(r_j)}{g^{target}(r_j)}\right]$$

$$For\ i = 0,$$

$$U_0(r_j) = -k_B T \ln g^{target}(r_j) \quad \{also\ called\ PMF\}$$

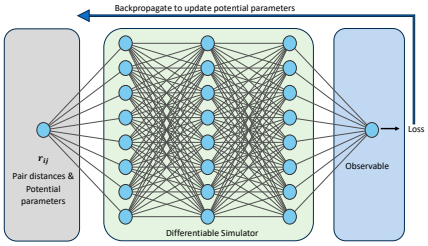
- Iterative method: match the simulation RDF to target
- 1st iteration use potential of mean force (PMF)
- RDF matches after < 10 iterations for LJ and OPP



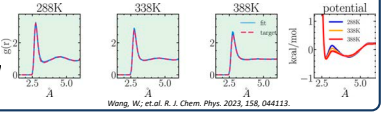


Neural Network potentials

- Goal match observable then optimize using neural networks
- Need a starting potential to constraint (Morse here)



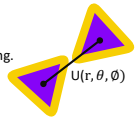
- Adjust **simulation temperature** for best match
- Possible to get **any functional form** for potential



Wang, W.; et.al. R. J. Chem. Phys. 2023, 158, 044113.

Conclusion and Outlook

- **Explored three** approaches to recover pair potentials from experimental data.
- Without particle tracking, rely on ensemble **observables.**
- RDF matching: brute force → inconclusive.
- **Neural network potentials**: **generalizable** but require tuning.
- **IBI**: effective for **liquid-phase** systems.
- **Isotropic** case: **RDF sufficient** to recover potentials.
- **Anisotropic** case: RDF insufficient → need **orientational** observables.



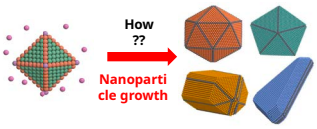
Acknowledgements:
This work was supported by the IRTG-ParSciTech (Project D04) and by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation (project No. 416229255). Computational resources and support provided by the Erlangen Regional Computing Center (RRZE) are gratefully acknowledged.

Off-Lattice Kinetic Monte Carlo Simulation of Multiply Twinned Nanoparticles

Friedrich-Alexander-Universität Erlangen-Nürnberg

Jyoti Pannu, Carlos L. Bassani and Michael Engel*
Institute of Multiscale Simulation (MSS),
Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Institute for Multiscale Simulation MSS

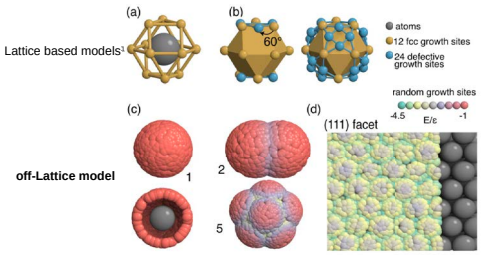


Motivation

- **What are the atomistic growth mechanisms of Multiply Twinned Nanoparticles?**
- **What kinetic processes drive the formation of symmetry broken nanoparticles shapes?**
- **What effect do crystallographic defects, such as stacking faults, have on the growth and shape of nanoparticles?**

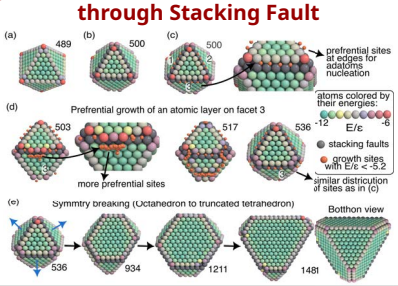
Off-lattice kinetic Monte Carlo simulations

- Growth of **noble metal** nanocrystals with **Lennard Jones** potentials using KMC simulations



- The probability of atom growing at certain growth site depends on the **Boltzmann factor**.
- The system **kinetically trapped** in local energy minima, resulting in the formation of twinned nanoparticles such as decahedra and icosahedra during growth

Symmetry Breaking into an Tetrahedron through Stacking Fault



Conclusions

- We reveal the atomistic growth mechanisms of twinned nanoparticles like decahedra, icosahedra, pentagonal rod.
- We found that the quantity and alignment of stacking faults directly relates to the final morphology of the nanoparticles.
- By controlling the nucleation of planar defects during the growth, we can synthesis the nanocrystals of desired shapes.

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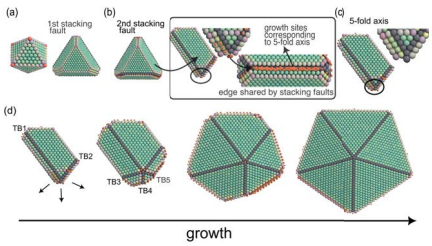
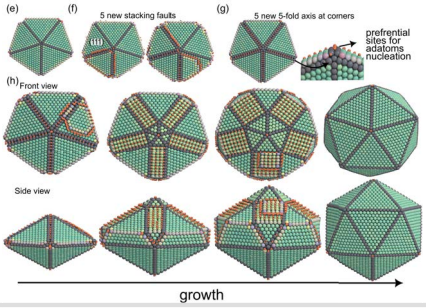
Growth Mechanism of Decahedral and Icosahedral Nanoparticles

- Formation of 5-fold axis by two stacking faults leads to the growth of Decahedral nanoparticles[3]

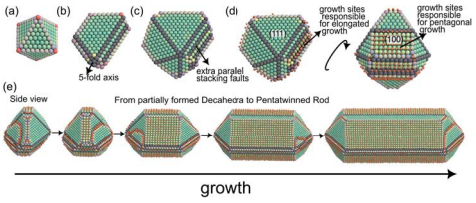


- Growth of new stacking faults on the (111) facets of Decahedra trigger the shape transformation to Icosahedron, through the Decmon structure[4]



Formation of Pentatwinned rods

- The preferential growth of atoms on (111) facets of Decahedra leads to the formation of Pentatwinned rods.



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[1] Bassani, C. L.; Engel, M. Kinetically Trapped Nanocrystals with Symmetry-Preserving Shapes. Journal of the American Chemical Society 2025, 147, 9487–9495.
[2] Du, J. S.; Zhou, W.; Rupich, S. M.; Mirkin, C. A. Twin pathways: discerning the origins of multiply twinned colloidal nanoparticles. Angewandte Chemie 2021, 133, 6934–6939.
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[4] alomares-Báez, J. P.; Montejano-Carrizales, J. M.; Guisbiers, G.; José-Yacamán, M.; Rodríguez-López, J. L. The Decmon: a new nanoparticle shape along the truncation path from the icosahedron to the decahedron. Nanotechnology 2019, 30, 425701

AES-Debye: Accurate, Efficient and Scalable Implementation of Debye Scattering Equation

Navid Panchi[1,2], Sebastian Kuckuk[2], Markus Whittmann[2], Michael Engel[1], Alberto Leonardi[1,3]

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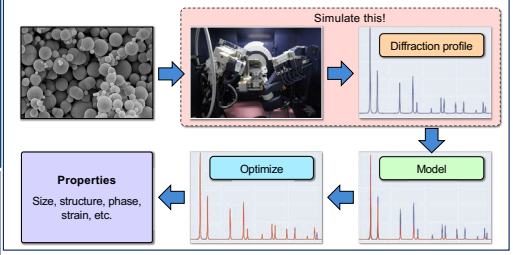
[2]Erlangen National High Performance Computing Center (NHR@FAU), Friedrich-Alexander-Universität Erlangen-Nürnberg (Germany)
[3]UKRI-STFC Rutherford Appleton Laboratory, Diamond Light Source (United Kingdom)

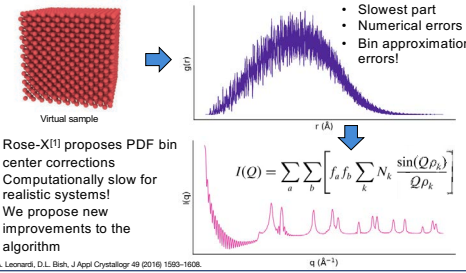
Motivation

- Debye scattering equation is crucial for total scattering analysis
- Enables calculation of powder diffraction patterns for virtual samples
- Requires extensive computational resources



Debye Scattering Equation (DSE)

Calculate pair distribution function (PDF)



- Slowest part
- Numerical errors
- Bin approximation errors!

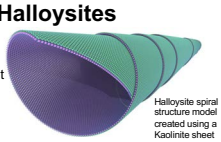
$$I(Q) = \sum_a \sum_b \left[f_a f_b \sum_k N_k \frac{\sin(Q\rho_k)}{Q\rho_k} \right]$$

- Rose-X[1] proposes PDF bin center corrections
- Computationally slow for realistic systems!
- We propose new improvements to the algorithm

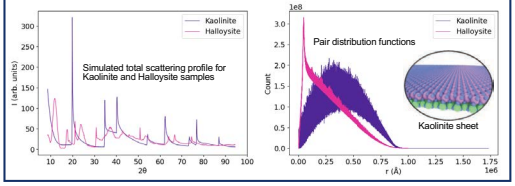
[1] A. Leonardi, D.L. Bish, J Appl Crystallogr 49 (2016) 1593–1608.

Application 1: Halloysites

- Kaolinite clay structures crystallized in spiral shapes[2]
- Challenging to model the pattern without using the atomic structures
- Each tube of up to 50 nm (100M atoms)
- Parallelized over 720 cores ~ 3 mins for 10M atoms (current sample)



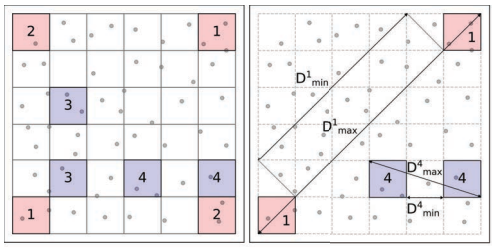
[2] J.M. Falcón, T. Sawczen, I.V. Aoki, Front. Mater. 2 (2015).



Other features

- Open source
- Python interface for ease of use
- Minimal dependencies
- Supported on Windows, Linux and Mac OS
- Can also be used for high accuracy PDF calculations
- Supports Nvidia and AMD GPUs
- LAMMPS plugin in-coming!
- Easily extensible

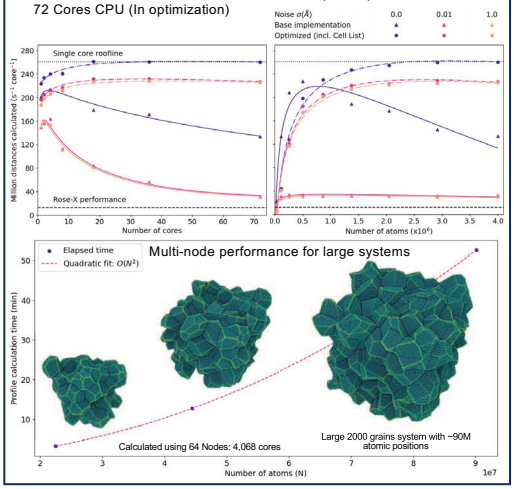
Domain Decomposition



- Divide the box into equal cells
- Distribute atoms into different cells
- Create pairs of equidistant cells
- Equidistant pairs access same part of the PDF data structure memory
- Efficient cache utilization on CPU

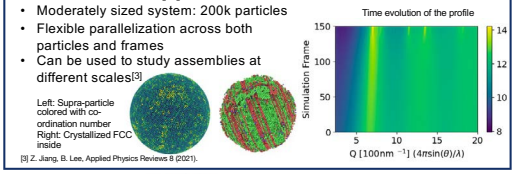
Performance

- Rose-X suffers from memory bandwidth limitation
- ~ 2x faster on Nvidia a100 GPU vs 72 Cores CPU (In optimization)
- Cells based approach helpful for realistic systems
- ~ 20x speed-up vs Rose-X



Application 2: Colloids

- Moderately sized system: 200k particles
- Flexible parallelization across both particles and frames
- Can be used to study assemblies at different scales[3]



[3] Z. Jiang, B. Lee, Applied Physics Reviews 8 (2021).

Acknowledgements:
This work was supported by Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) through grant No. LE4543/2-1 as well as through KONWIHR (STAR-MISI) grant. Computational resources and support provided by the Erlangen Regional Computing Center (RRZE) are gratefully acknowledged.

Simulated formation of a primitive icosahedral quasicrystal across a wide density range

Kaijie Zhao[1], Michael Engel[1]

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

Motivation

- Primitive icosahedral quasicrystal has never been assembled in simulation with simple isotropic pair potential in a single-component system
- Traditional tiling approach usually only allows for a slight local disorder and large-scale imperfections are not observed

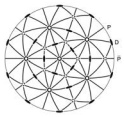
Method: Higher-dimensional analysis for Icosahedral Quasicrystal

- IQC can be generated via **the cut-project method**[1] from 6 dimension
- Three hypercubic lattice in 6D: **Primitive,** Body-centered[2] and Face-centered[3]
- Embedding matrices with respect to $\boldsymbol{V}^{\parallel}$ and $\boldsymbol{V}^{\perp}$:

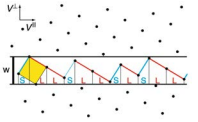
$$\boldsymbol{M}_{\parallel} = [\boldsymbol{a}_i^*]_{i=1}^6 = (2\tau^2+2)^{-\frac{1}{2}} \begin{bmatrix} 0 & \tau & 1 & 0 & -\tau & 1 \\ \tau & 1 & 0 & -\tau & 1 & 0 \\ 1 & 0 & \tau & 1 & 0 & -\tau \end{bmatrix}, \quad \boldsymbol{M}_{\perp} = (2\tau^2+2)^{-\frac{1}{2}} \begin{bmatrix} 0 & -1 & \tau & 0 & 1 & \tau \\ -1 & \tau & 0 & 1 & \tau & 0 \\ \tau & 0 & -1 & \tau & 0 & 1 \end{bmatrix},$$

where $\tau = \frac{1+\sqrt{5}}{2}$

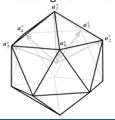
Icosahedral symmetry projection



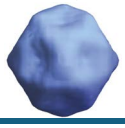
Cut-project method



Embedding matrix in $\boldsymbol{V}^{\parallel}$

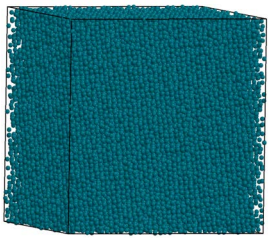


Atomic surface of body-centered IQC[2]

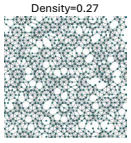


Structural information of the primitive IQC

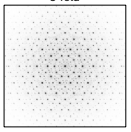
- Self-assembly via MD simulations in NPT ensemble
- FFT & BOD indicate the presence of primitive IQC
- Density flexible in a range from 0.27 to 0.42
- Smeared peaks already observed in liquid state



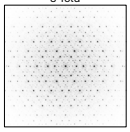
Density=0.27



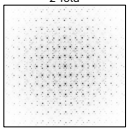
5-fold



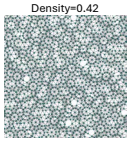
3-fold

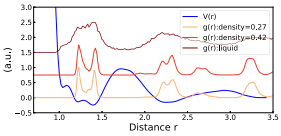


2-fold

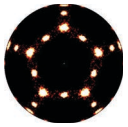


Density=0.42

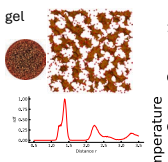


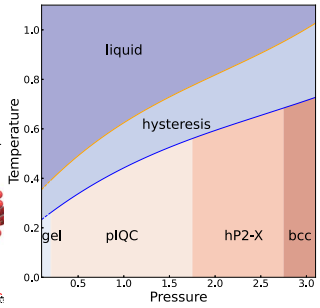


BOD



Phase Diagram





Conclusions

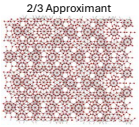
- A primitive IQC is self-assembled via a simple isotropic pair potential in a single-component system
- The primitive IQC qualitatively matches the structure generated by a triacontahedral atomic surface in **Density, Free energy and Atomic distribution in complementary space**
- The wide density range of its existence demonstrates an unexpectedly **high flexibility of the atomic surface**

References

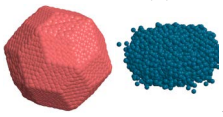
[1] Walter S, Deloudi S. Springer Science & Business Media, 2009.
[2] Engel M, Damasceno P F, Phillips C L, et al.. Nature materials, 2015, 14(1): 109-116.
[3] Yamada, T., Takakura, H. & Yamamoto, A. , Acta Cryst. 2024, A80, 422&438.

Comparison with model: Real space & Complementary space

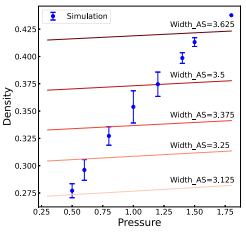
2/3 Approximant

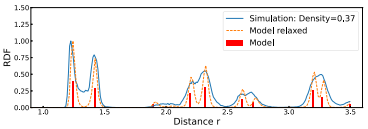


Atomic surfaces (AS)

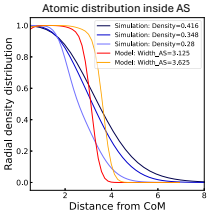


Density vs Pressure

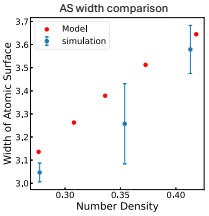




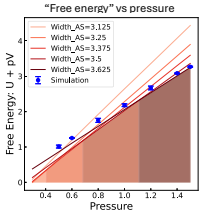
Atomic distribution inside AS



AS width comparison



"Free energy" vs pressure



- Existence of **single cluster** when hyperatoms are projected onto complementary space supports the hypothesis of a **primitive hypercubic lattice**
- Variation of radial distribution confirms the **increase of AS radius with density**
- Size of the simulated atomic surface qualitatively matches that of the model

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A Unified Framework for Strain Analysis in Pentatwinned Nanoparticles

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[2]*Department of Chemistry, Rice University, Houston, TX, United States*

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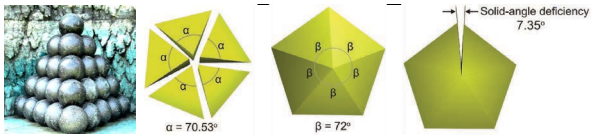
[4]*Smalley-Curl Institute & Rice Advanced Materials Institute, Rice University, Houston, Texas 77005, United States*

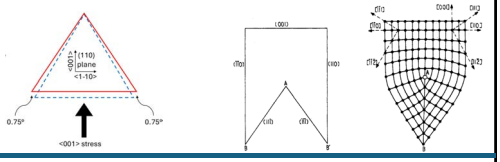
Motivation: How does the gap close?

- Pentatwins are twinned crystals with 5 single crystals around one common axis
- Neighboring grains are linked via a coherent twin grain boundary
- Instrinsic strain has to be present to overcome the 7.35° deficiency



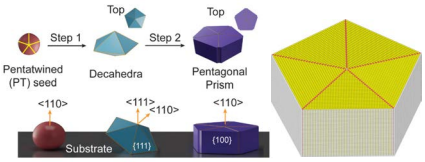
Motivation: Existing theories explain partially

- Homogeneous theory[1]: **"Compress to close"**
- Inhomogeneous theory[2]: **"Bend to close"**
- Explanation of real strain maps: One theory + correction term[3][4]



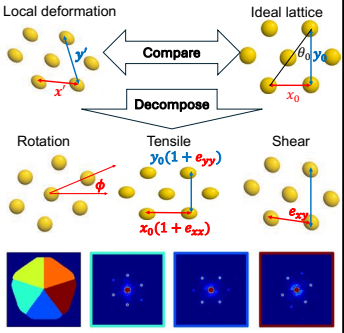
Method: Creation of Pentatwin Prisms

- Aim: Precisely determine atomic positions in real and reciprocal space.
- Easy 5-fold axis alignment enables high-resolution 4D-STEM strain mapping.
- Simulation: geometric construction and MD with a Lennard–Jones potential.



Method: Atomic Strain mapping

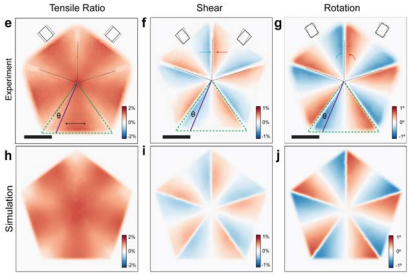
- **Local** determination of strain.
- For each atom in one grain :
  - Strained: $A = [\boldsymbol{x}' \quad \boldsymbol{y}']$
  - Strain-free lattice matrix: $A_0 = \begin{bmatrix} x_0 & 0 \\ 0 & y_0 \end{bmatrix}$
  - Deformation gradient: $D = AA_0^{-1}$
  - Polar decomposition: $D = \begin{bmatrix} cos\phi & sin\phi \\ -sin\phi & cos\phi \end{bmatrix} F$
  - Strain matrix: $e = \begin{bmatrix} e_{xx} & e_{xy} \\ e_{yx} & e_{yy} \end{bmatrix} = F - I$
  - Tensile strain ratio: $ratio = \frac{x_0(1+e_{xx})}{y_0(1+e_{yy})} - \frac{x_0}{y_0}$
- **Separate cartesian coordinate** for each grain



Results: Gap closure

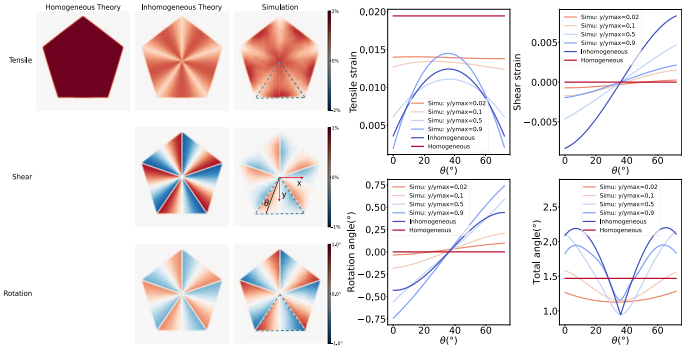
- Experimental and simulated strain maps match closely.
- Averaged angular strain components fully account for the gap closure.

	Tensile	Shear	Rotation	Sum
Experiment	0.66°	0.33°	0.48°	1.47°
Simulation	0.68°	0.30°	0.49°	1.47°



Results: Azimuthal distribution under the unified framework

- Real strain maps deviate from both homogeneous and inhomogeneous theory alone.
- Local strain is too complex to reduce to simple averages.
- Strain shifts from tensile at the center to shear/rotation at the edges.



Conclusions

- The simulation successfully reproduces the experimentally observed strain maps.
- The local strain analysis method accurately reproduces gap closure in an average sense.
- Qualitatively, the strain field evolves from tensile-dominant (homogeneous-like) near the particle center to shear/rotation-dominant (inhomogeneous-like) toward the edges.

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[1] Bagley,B.G. *Nature* **208**, 674–675 (1965)
[2] De Wit, R. *Journal of Physics C: Solid State Physics* 5.5 (1972): 529
[3] Johnson, C. L. *et al. Nat Mater* **7**, 120–124 (2008).
[4] Wu, Hao, et al. *Structural Science* 77.1 (2021): 93-98.

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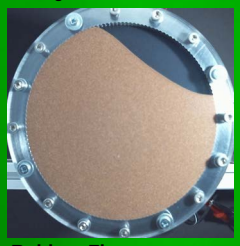
Live Experiment

Strömungslinien in Granularer Materie

Granulare Materialien wie Sand, Zucker oder Reis verhalten sich weder wie klassische Festkörper noch wie Flüssigkeiten. Ihr Verhalten liegt irgendwo dazwischen - abhängig davon, wie stark sie in Bewegung versetzt werden.

Schon in einer einfachen Versuchsanordnung wie einer teilgefüllten, rotierenden Trommel entstehen komplexe Strömungsmuster, die an Phänomene aus der Strömungsmechanik erinnern: vom sanften Gleiten einzelner Körner bis hin zu turbulenten, scheinbar flüssigen Bewegungen. In diesem Experiment können Sie selbst die Drehgeschwindigkeit steuern und beobachten, wie sich mit steigender Rotation völlig unterschiedliche Regime der granularen Strömung ausbilden.

Niedrige Drehzahl

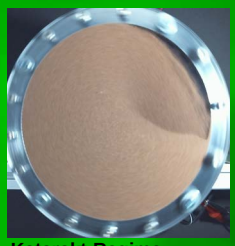


Ruhiger Fluss
Bei niedriger Drehgeschwindigkeit bewegt sich nur eine dünne Schicht an der Oberfläche. Die Körner rollen langsam abwärts, während der Großteil des Materials ruht. Die Oberfläche bleibt dabei nahezu eben - ähnlich wie bei einem Sandhaufen.

Mittlere Drehzahl

S-förmige Oberfläche
Mit zunehmender Geschwindigkeit verformt sich die Oberfläche zu einer charakteristischen S-Form. Ein Teil des Granul-ats gleitet stetig nach unten, während oben neues Material nachrückt. Es entsteht ein statio-näres Strömungsmuster mit klar erkennbarer Umlaufbewegung.

Hohe Drehzahl



Katarakt-Regime
Bei weiterer Erhöhung der Drehzahl verliert das Granulat den Kontakt zur Trommelwand und beginnt frei zu fliegen. Die Körner prallen aufeinander und auf die Wand - ein stark energiegetriebener Zustand, der an einen Partikelregen erinnert.

Sehr hohe Drehzahl

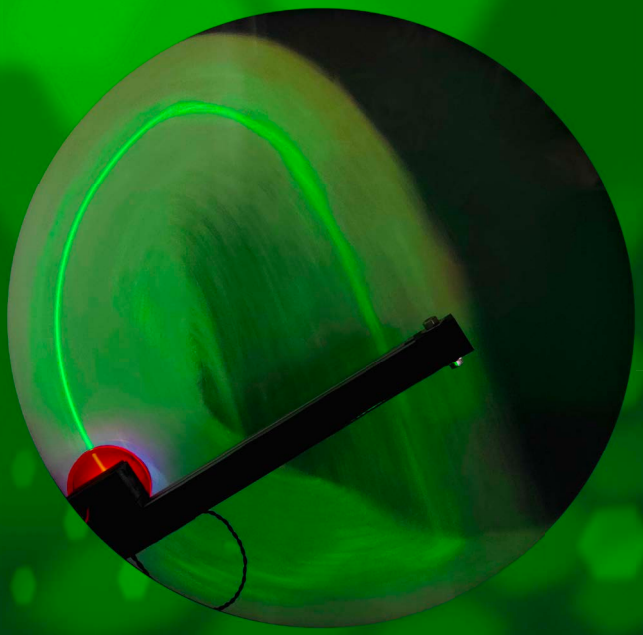
Zentrifugation
Ab einer kritischen Drehzahl haftet das Granulat vollständig an der Wand. Die Zentrifugalkraft überwiegt die Schwerkraft, und die Bewegung friert scheinbar ein. Die Körner rotieren gemeinsam mit der Trommel - ein erstarrtes, rotierendes Festkörperregime.

Granularströmung sichtbar gemacht

Probieren Sie es aus!

In dieser rotierenden Trommel wird das Verhalten granularer Materie direkt erfahrbar. Das leuchtende Granulat zeigt, wie sich die Körner bei unterschiedlichen Drehgeschwindigkeiten bewegen und neu anordnen. Durch die verschiebbare UV-Lichtquelle werden einzelne Partikel zum Nachleuchten angeregt, sodass ihre Bewegung als leuchtende Spur sichtbar bleibt. So lässt sich die Dynamik der Granulatströmung - von ruhigem Fließen bis zum freien Fall - in Echtzeit beobachten und intuitiv verstehen.

Nachleuchtendes Granulat



D04

FP2

Modeling of colloidal interactions and assemblies for optimal functional properties

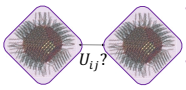
DESIGN OF PARTICULATE PRODUCTS CRC 1411

Harsha Namdeo, Jyoti Pannu, Federico Tomazic, Carlos Lange Bassani, Michael Engel

Mission of the project

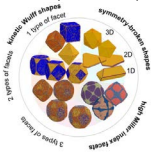
Background and scope

- Optimal nanomaterial design relies on understanding the **interaction-governed structure-property** relationship.
- **Experimental** techniques (e.g., LCTEM, SEM) provide **observational data** but **lack** mechanistic, particle **interaction insights.**
- Computational **simulations** are essential to **extract, manipulate, and understand** the interactions and formation of nanoparticles.
- The goal is to develop reliable **models to corroborate experimental observations** and **guide** experimental **design** protocols.
- Understanding **nanoparticle shape** formation is key to **tailoring** materials for catalytic, optical, and energy applications.
- Specific interest lies in complex structures like **Multiply Twinned Particles (MTPs)** and **highly active high-index facets** for enhanced catalysis.



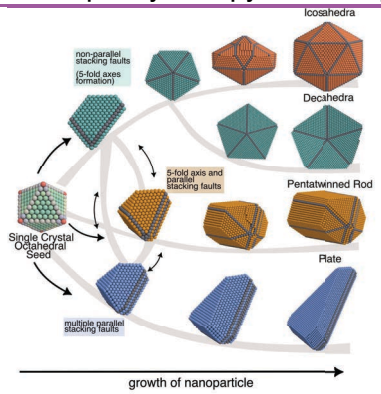
Key research questions

- **WP1:** Developing **2D & 3D interaction potentials** between **complex non-spherical** particles to explain their self-assemblies. **Inverse design** of pair potentials from **observing nanoparticle self-assemblies** of simple and complex nanoparticles.
- **WP2:** How to manipulate defects/disorder to achieve **angle independent structural color**? Quantification, characterization and optimization of disorder in physical parameters for dynamical systems.
- **WP3:** What factors (**polydispersity** and **drying rates**) are responsible for **vacancy formation** in confined colloidal clusters? Which interaction **potential** (soft vs. hard) describes the **observed experimental** findings?
- **WP4:** What processes drive the formation of distinct nanocrystals shapes? What effect do **crystallographic defects**, such as dislocations and stacking faults, have on the **growth and shape** of nanocrystals? How does etching lead to the formation of distinct high-index facets?



Results and ongoing work

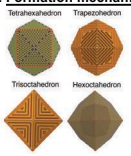
Result 1 Growth pathway of Multiply twinned nanoparticle



- **Monte-Carlo** simulations for the growth of **Multiple Twinned Nanoparticles** (WP4)
- Understanding the mechanism of **shape formations** (A01) starting from a single crystal seed
- Identifying the role of stacking faults in shaping nanoparticle growth and morphology
- Controlling the **formation of stacking faults** during growth can lead to the desired final morphology [6]

Ongoing projects….

1. Formation mechanisms of High Index Facets using KMC



- Systematic study of **four classes** of High Index Facets by etching process using Monte-Carlo simulations (WP4)
- Understanding their formation mechanism
- Studying the effect of temperature and kinetic parameter on the **inclination of the facets**

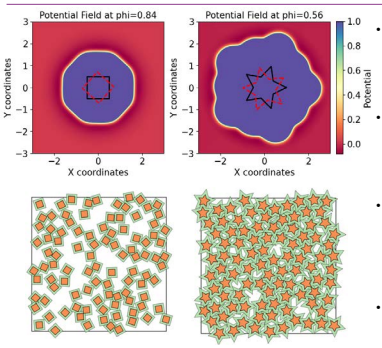
2. Vacancy difference in simulated and experimental colloidal clusters (A05, C01, C05)

- For **100k** confined colloidal hard particles simulated with event-driven MD (WP2, WP3)
- Discrepancy in vacancies between **NanoCT (~4%)** and simulated **cluster (~10⁻⁴)**
- Kinetic trapping of defects? Polydispersity? Better interaction description(soft or hard)?

3. Establishing equivalence between simulated and experimental structures

- Optimized simulated disordered structures by D05 → **Extract features** responsible for structural color D04 → use these features for **fabricating** photonic glasses A05
- Features like average **scatterer spacing**, structure factor (**S(k)**) and form factor (P(k)), packing fraction, average number of different sized neighbours, etc.

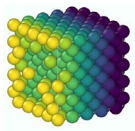
Result 2 Contact surface dominated interactions

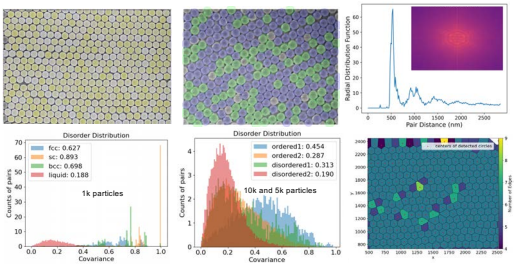


- **Closest contact surface** between nanoparticles **dominants interactions**
- Implemented for 2D particles **tabulated potential** for anisotropic particle shapes (WP1)
- Simulations possible for 2D **convex** and **concave** particle **shapes** (Mercator collaboration Bloomington)
- **Varying ligand** shell **thickness** possible
- Challenging to implement in 3D due to memory issues for large tables
- **Assemblies** of square lattices with square shaped particles, phase transition of liquid crystals for rods, triangular assemblies with triangular particles studied
- Application to **tripod shaped** particles [4], Method development and description [7]

Result 3 Disorder characterization of photonic glasses

- Strategies for **segmenting** SEM and TEM images of photonic crystals and glasses
- Extracted **descriptors**: RDF, Distribution of particle sizes, Voronoi plots for all segmented images
- Simulated broken samples ~ as seen in FIB cut
- **Disorder descriptor** based on neighbourhood comparison to quantify global disorder in the samples





[1] Carlos L. Bassani, Michael Engel. Kinetically Trapped Nanocrystals with Symmetry-Preserving Shapes. *Journal of the American Chemical Society*, 147:9487-9495, **2025**.
[2] Praveen K. Borminieni, Junwei Wang, Nicolas Vogel, Michael Engel. Entropic Trapping of Hard Spheres in Spherical Confinement. *Physical Review Letters* 134, 198201 (**2025**)
[3] Federico Tomazic, Jonathan Martin-Gonzalez, Navid Panchi, Nydia Varela-Rosales, Nicolas Vogel, Michael Engel. Kinetic asymmetry between crystallization and melting in colloidal droplets (In preparation)
[4] Yang Liu, Federico Tomazic, Baixu Zhu, Yi Wang, Chuanliang Huang, Michael Engel, Xingchen Ye. Softness-Directed Symmetry Switching in Nano-tripod Superlattices (In preparation)
[5] Carlos L. Bassani, Kamilla Zaripova, Navid Panchi, Michael Engel. Symmetry Breaking and Shape Yield of Nanocrystals by Defect Dynamics (In preparation)
[6] Jyoti Pannu, Carlos L. Bassani, Michael Engel. Off-Lattice Kinetic Monte Carlo Simulations of Multiply Twinned Nanoparticles (In preparation)
[7] Harsha Namdeo, Navid Panchi, Federico Tomazic, Michael Engel. Close contact surface dominated interactions for complex particles (In preparation)

FAU Friedrich-Alexander-Universität Erlangen-Nürnberg

Funded by: DFG

Efficient numerical integration of rigid body dynamics

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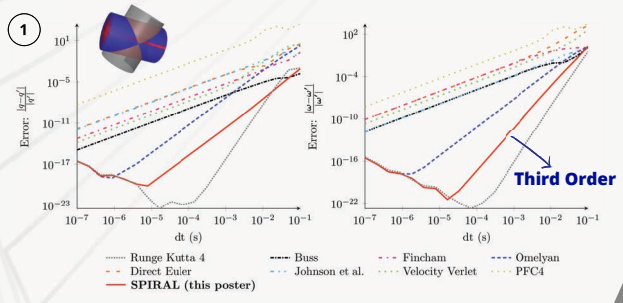
We introduce SPIRAL, a third-order algorithm for integrating rotational motion in particle simulations. It requires only one force calculation per time step, does not require quaternion normalization, and can be formulated for both leapfrog and synchronous integration schemes, making it compatible with many particle simulation codes. The stability and precision of Spiral exceed that of state-of-the-art algorithms. We see potential applications in all simulation techniques that involve 3D rotations, like DEM.

1



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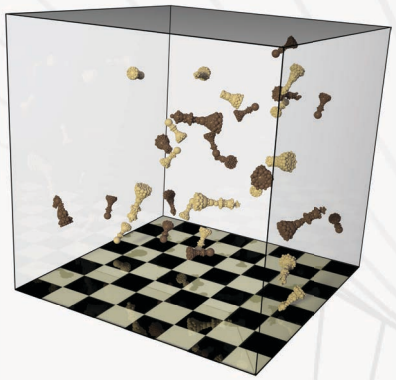


1. Error vs. time step of different algorithms, comparing with an analytical solution: a rotating cylinder under constant torque.
2. Integration algorithms for particle rotations and DEM software that use them. Not necessarily for non-spherical particles.
3. Time relative to Direct Euler to perform a time step.
4. Speedup relative to Direct Euler in the simulation of the rotating cylinder with defined accuracy.
5. Chess pieces modeled as multi-spheres bouncing in a box with rigid boundaries. There's no gravity, damping, or friction.
6. % Energy change throughout the simulation of the chess pieces.

SPIRAL: **Easy to prove!** **PROOF:**

Quaternion update: LeapFrog version

$$q(t+dt) \approx q(t)\, exp\left(\tfrac{dt}{2}\omega\left(t+\tfrac{dt}{2}\right)+O(dt^3)\right), \quad O(dt^3) \approx \tfrac{dt^2}{48}\dot{\omega}\left(t+\tfrac{dt}{2}\right)$$

Quaternion update: Non-LeapFrog version

$$q(t+dt) \approx q(t)\, exp\left(\tfrac{dt}{2}\omega(t)+\tfrac{dt^2}{4}\dot{\omega}(t)+O(dt^3)\right), \text{ with } O(dt^3) \approx \tfrac{dt^3}{12}\dot{\omega}(t)$$

Angular velocity update:

$$\omega(t+dt/2) = \omega(t-dt/2) + \tfrac{1}{6}\left(\boldsymbol{K_1}+\boldsymbol{K_2}+4\boldsymbol{K_3}\right)$$
$$\boldsymbol{K_1} = dt\dot{\omega}\left(\omega, M(t)\right), \quad \boldsymbol{K_2} = dt\dot{\omega}\left(\omega+\boldsymbol{K_1}, M(t)\right)$$
$$\boldsymbol{K_3} = dt\dot{\omega}\left(\omega+\tfrac{1}{4}(\boldsymbol{K_1}+\boldsymbol{K_2}), M(t)\right)$$

This way of updating the angular velocity is similar to a SSPRK3 but with constant torque during the time step.

We start with the norm conserving quaternion derivative:

$$\dot{q} = \frac{dq}{dt} = \tfrac{1}{2}\omega(t)q$$

We integrate the ODE assuming omega depends only on time.

$$q(t+dt) = q(t)\, exp\left(\tfrac{1}{2}\int_t^{t+dt}\omega(t')dt'\right)$$
$$\int_t^{t+dt}\frac{dq}{q} = \tfrac{1}{2}\int_t^{t+dt}\omega(t')dt'$$

Then, expand the unknown omega in a Taylor series.

$$\omega(t') \approx \omega(a) + \dot{\omega}(a)(t'-a) + \tfrac{1}{2}\ddot{\omega}(a)(t'-a)^2 + \ldots$$

Taking a = t + dt/2 for the LeapFrog version and a = t for the Non-Leapfrog, we integrate to obtain the algorithm. To compute the quaternions:

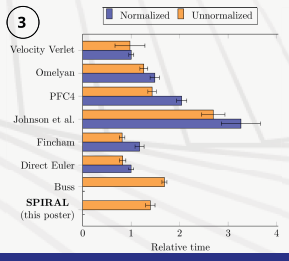
$$e^{\theta\hat{u}} = \cos\theta + \hat{u}\sin\theta$$

û is an unitary vector. It represents the real and vector part of the quaternion.

2

Algorithm	DEM codes using it			
Direct Euler	MFiX	EDEM	BlazeDEMGPU	MUSEN
Velocity Verlet	LIGGGHTS	GranOO	EDEM	MercuryDPM
Fincham	Yade	Esys_Particle	WooDEM	
Buss	PFC7			
Johnson et al.	PFC7			
PFC4	MercuryDPM			
Omelyan	Yade			
SPIRAL	Yade	GeoTaichi	TinyDEM	

3



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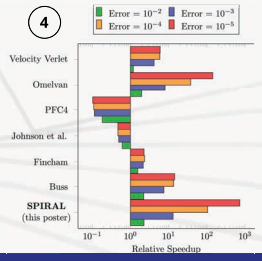

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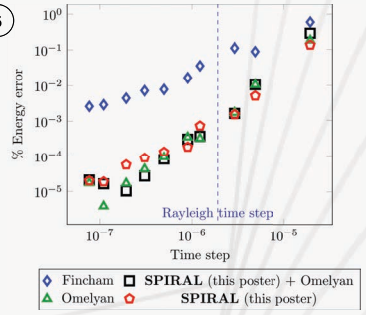


Conclusions:

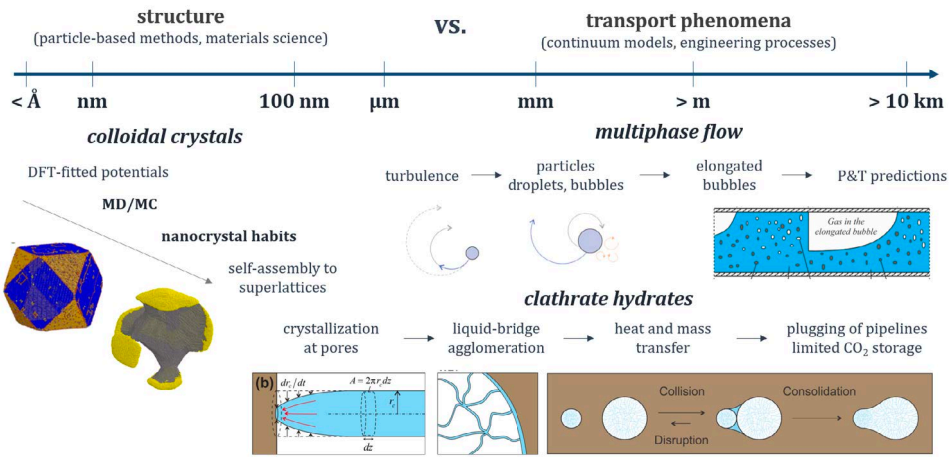
- **A third-order algorithm that only requires one force calculation per time step, and does not require quaternion normalization.**
- **The new algorithm outperforms in accuracy and stability. Does not compromise performance.**
- **This algorithm has already been merged into YADE.**

5. Selected Postdoc Projects

Dr. Carlos L. Bassani

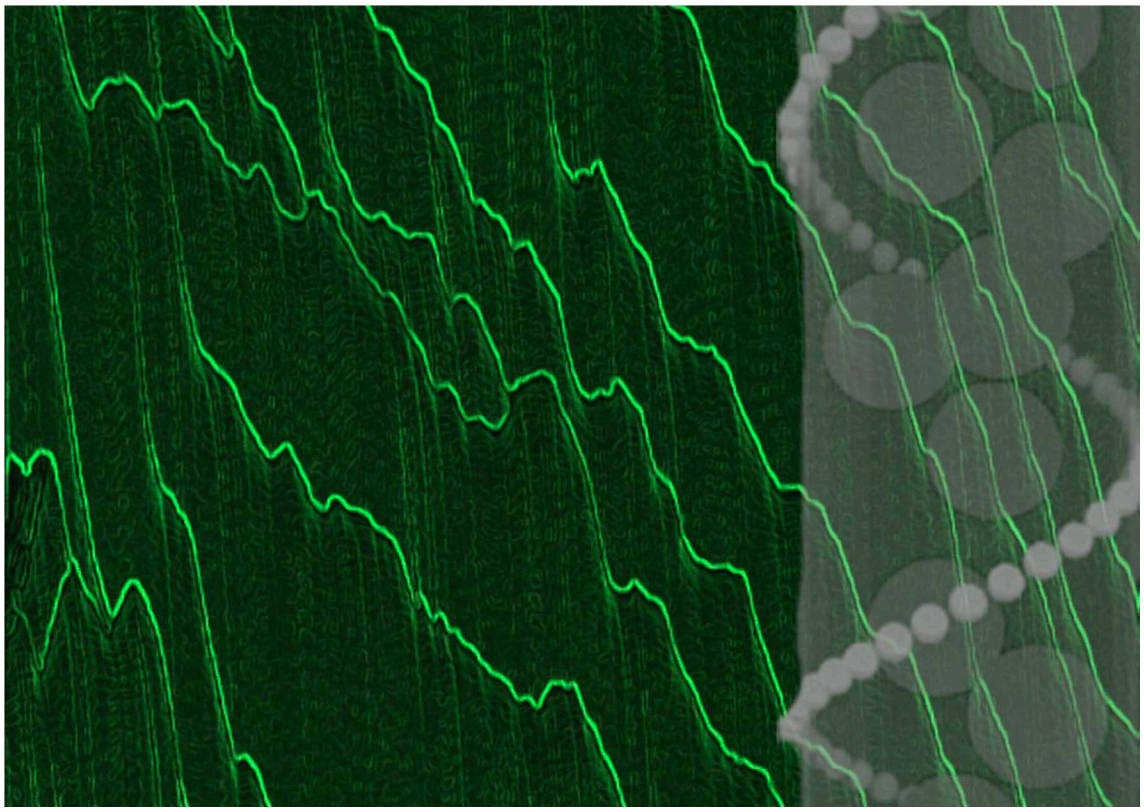
Multiscale modeling of crystals from fundamental science to engineering applications.

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



Priv.-Doz. Dr. Patric Müller
Homogenization of granular pipe flow.

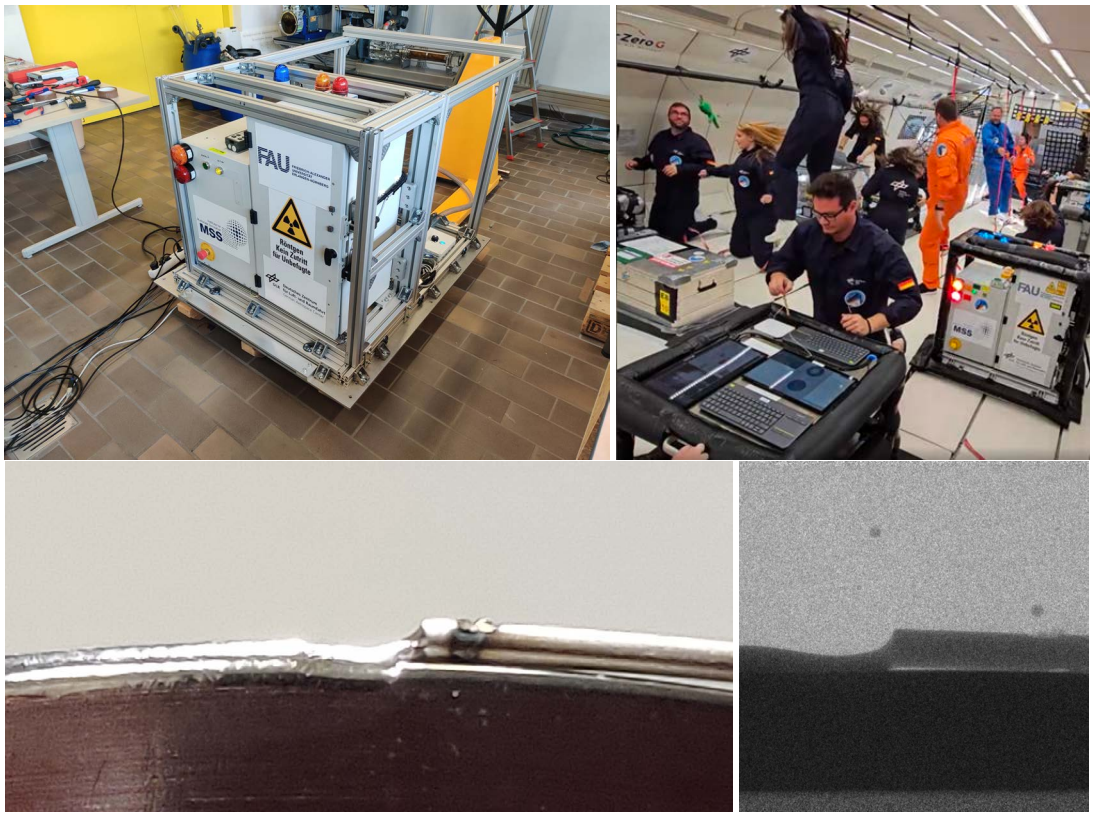
A fundamental problem in granular pipe flows is that they are intrinsically unstable, with the material transport being characterized by large variations in solid fraction (density waves) along the pipe. These waves induce potentially destructive pressure transients on the pipe's inner wall and provide the mechanism responsible for the intermittent behavior of the flow. In this project we will apply particle-based simulations to design rules for combating the cause of flow intermittency that is the triggering mechanism of density waves.



Density waves in gravity driven granular pipe flow.

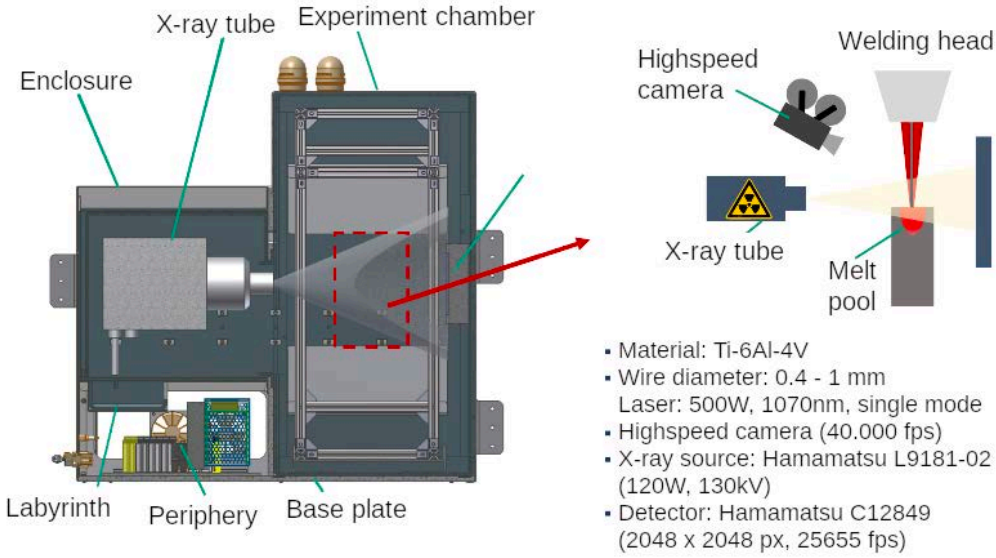
Dr. Achim Sack
LADA: Laser Wire Deposition Welding in Zero Gravity

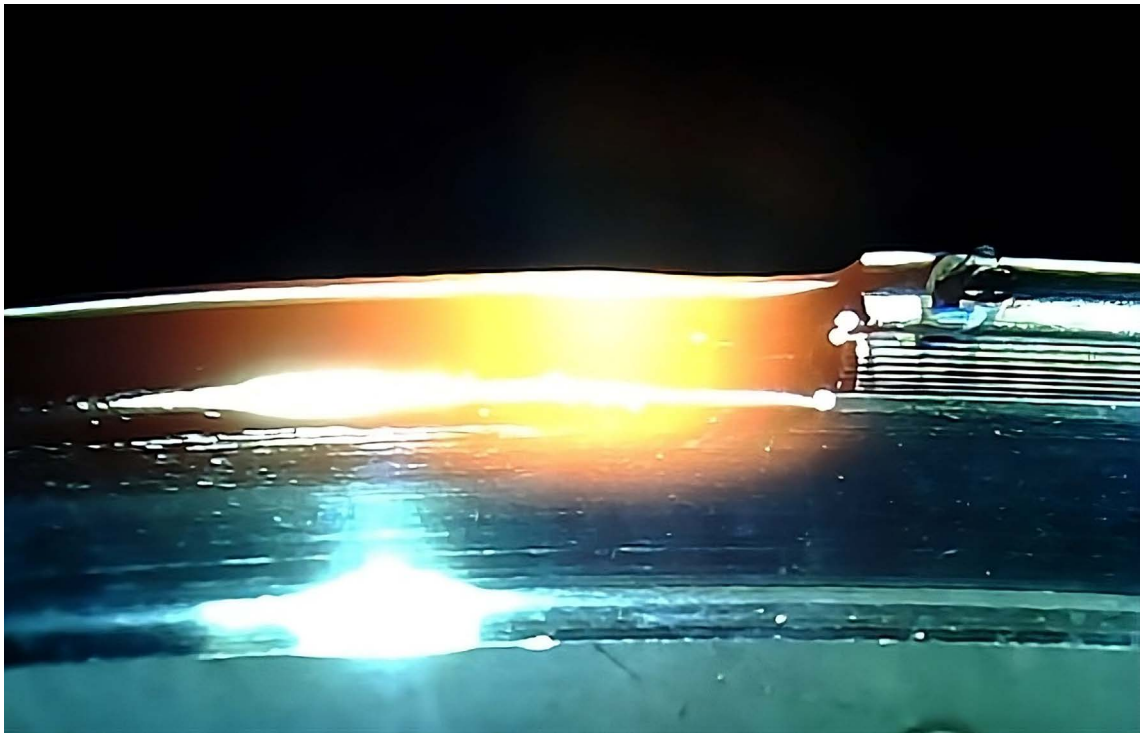
In laser wire welding, a metal wire is melted using a laser and applied to a metallic base, similar to how a 3D printer extrudes plastics. Our project explores how this process could be adapted for space missions in zero gravity, enabling the production of necessary components on-site, such as on space stations or future Moon and Mars missions, reducing the need for spare parts. Key process parameters like laser power, feed rate, and shielding gas flow must be optimized, as their behavior in zero gravity is largely unknown. Initial tests using a 500 W fiber laser, with materials like aluminum and titanium, aim to study the melting behavior. The process is observed in real-time using the HORUS X-ray system, designed for zero gravity, which captures X-ray images of the melt pool. Further experiments involve welding metal wire to the substrate under varying conditions, followed by metallographic analysis. The experimental results will be used to improve a simulation model, which will later be tested in subsequent experiments.



Dr. Achim Sack
Tracer-based radiography of the melt pool dynamics during laser wire welding in weightlessness (ETI)

The aim of the project is to experimentally investigate the process of laser cladding in zero gravity using X-rays. In addition to data on the size and depth, the dynamics of the melt pool will also be recorded using tracers in order to calibrate and verify a ray-tracing coupled Smoothed Particle Hydrodynamics (SPH) method.

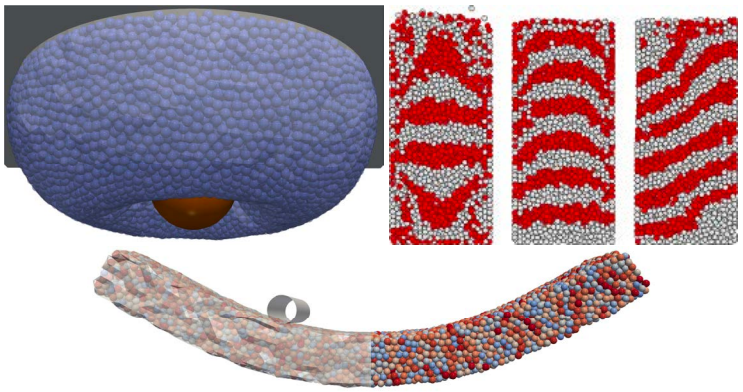




6. Dissertations and Habilitations

Dr. Holger Götz
Jamming and Convection in Granular Media

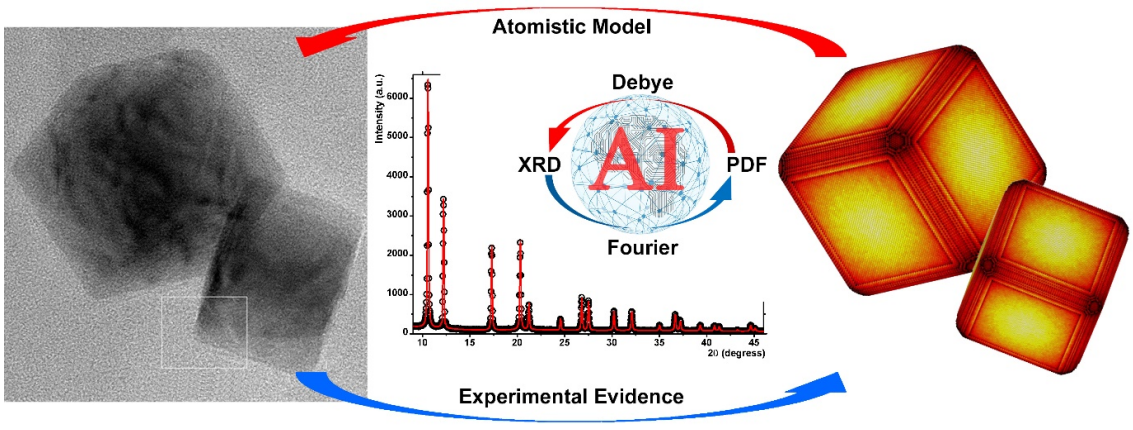
Granular media changes its properties drastically when going through the jamming transition. Technical applications of this transition usually consist of a granulate that is enclosed by a membrane. The jamming transition can then be achieved by applying pressure on the membrane, such that the granulate is compressed. Two such applications are granular grippers and granular metamaterials. To simulate these, I present a method that makes it possible to simulate membranes together with a granulate using the Discrete Element Method (DEM). I use this method to characterize and improve both applications. For the granular gripper, I demonstrate that high holding forces are achieved with granulates composed of soft particles, while low holding forces are achieved with granulates of hard particles. Additionally, I investigate and characterize the deformation behavior of a jammed granular metamaterial and demonstrate that during large deformations of the material, the contact network is reformed, although the granular particles themselves hardly reorganize.
In addition to jammed granular media, I investigate granular convection. Convection forms, for example, when a cylindrical container partially filled with granular material is shaken vertically. In the presence of gravity, a convection pattern is observed, where the material moves upwards in the center and downwards close to the sidewall. In the absence of gravity, the convection has an additional symmetry axis perpendicular to the vibration direction. I find, however, that depending on the vibration parameters, this symmetry is broken and the convection pattern seen under gravity conditions is recovered. I show that this happens when the granulate's volume fraction differs between the collisions of the granulate with the cylinder's two bases.



Exemplary representations of the three investigated systems: the granular gripper (top left), patterns of granular convection (top right), and a beam-shaped granular metamaterial (bottom).

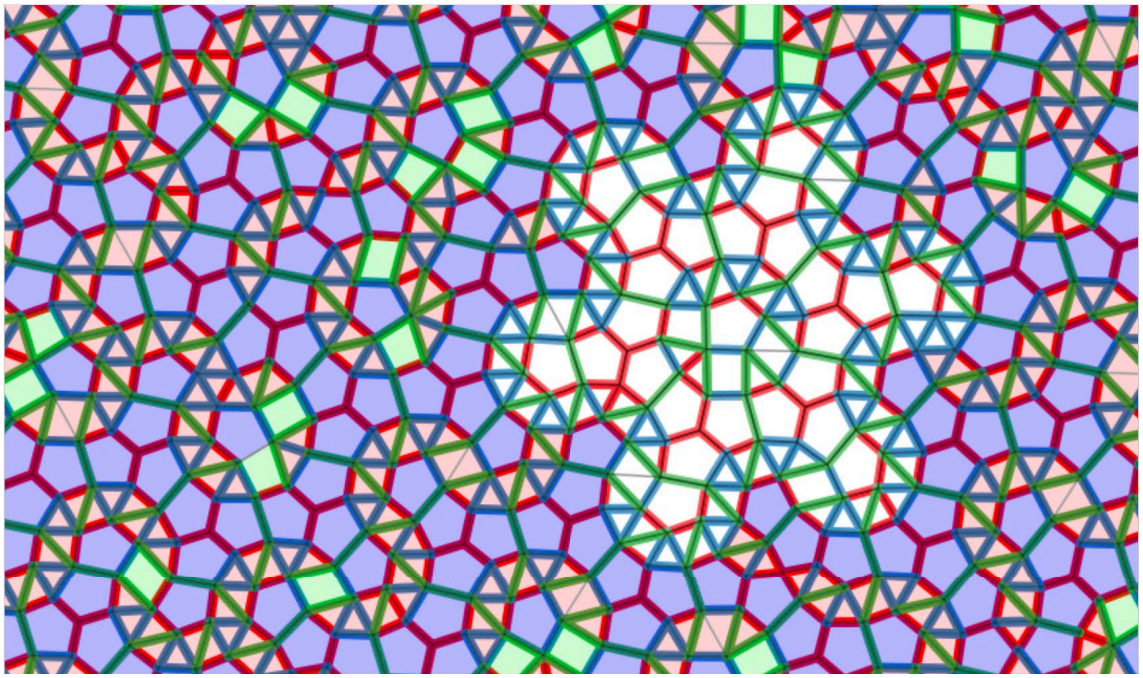
Priv.-Doz. Dr. Alberto Leonardi
Habilitation: Multiscale Simulation of Nanostructured Materials

Materials with nanosized structures hold great promise for energy-sustainable and environmentally responsible processes, where maximizing functionality and efficiency is crucial. Multicomponent nanocrystals (NCs) with limited long-range order are particularly exciting due to their tenable chemistry. Tailored nanoarchitecture can enhance performance in applications such as medicine (e.g., shape memory alloys for implants), aerospace (e.g., high-strength metal alloys), environmental remediation (e.g., filtration of heavy elements), electronics (e.g., semiconductor devices), energy production (e.g., solar cells), and storage (e.g., batteries and supercapacitors). However, these materials present significant characterization challenges: they lack long-range periodicity, precluding standard crystallographic techniques, but are not completely amorphous, making computational approaches expensive. Monodisperse poly-elemental NCs are typically produced through colloidal methods. However, conversion pathways are preferred for achieving sophisticated designs. Reliable chemical design of nanostructure architecture requires an atomic-level understanding of conversion kinetics to fully exploit structure-dependent properties. This work investigates structural disorder and its evolution during physical/chemical reactions to maximize catalyst activity and selectivity. Lattice distortion and structure/composition disorder in nanostructured metal particles were studied using atomistic simulations and experimental evidence. For example, electrochemical processes at the nanoscale revealed galvanic corrosion protection between different metal-species subdomains within a single NC. These insights informed the design of durable nanostructured catalysts with enhanced selectivity and activity for oxygen-reduction reactions and other electrochemical processes. Experimental methods for characterizing nanostructured materials face the challenge of capturing both local structure in ordered regions and information on the microstructure architecture. The complexity of the structure deformation field, linked to physical-chemical properties, necessitates combined experimental and theoretical efforts. Therefore, a core goal of this work is to support both simulation and experimental results. Total scattering approaches are key to understanding disordered nanostructured materials. However, interpreting total scattering data remains challenging. Traditional methods based on Bragg's law cannot address complex disorder scenarios, while modern methods based on the Debye scattering equation fail to capture heterogeneity in multicomponent crystals. To overcome this, Bragg's and Debye's theories are here bridged via the whole pair distribution function modelling (WPDFM) method. The WPDFM method integrates existing and new structure and microstructure models, providing a software tool for 'turn-key' solutions in data analysis. This broadens the work perspective from the focus on metallic nanomaterials to other nanostructured materials such as clay and clay-minerals, which offer diverse applications while providing full environmental compatibility and abundant resources. Here a preliminary work details the contribution to the scattering profile from distinct stacking defects. Although it deals with the sole staking of identical kaolinite layers, it demonstrated that extracting accurate information from the analysis of powder total scattering data is possible.



Dr. Nydia Roxana Varela-Rosales
Computational Design and Thermodynamic Stability of Aperiodic Crystals and their Approximants

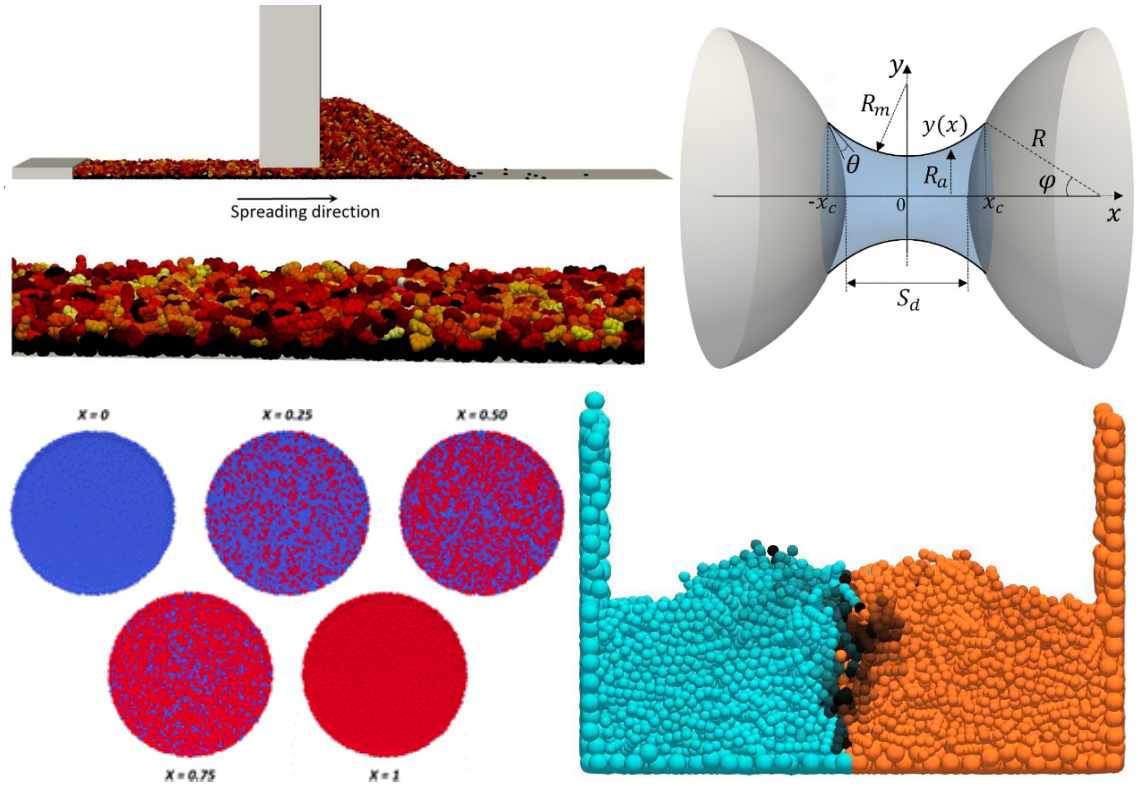
Aperiodic crystals are crystalline structures that lack periodicity (e.g., quasicrystals). These structures revolutionized the field of crystallography just a few years back. We can find them in many classes of substances, from mono/multi-component elements to complex macromolecules formed by polymer networks. Nowadays, we encounter daily applications of these structures in cookware sets, lithium-ion batteries, commercial razors, and others. The applications of these structures are still in their infancy, promising exciting potential across numerous fields. Despite progress in understanding these structures, the answer to how their aperiodic order affects physical properties is still unclear.
Our work aims to advance the understanding of the thermodynamics and stability of aperiodic long-range order structures under circumstances where external constraints, such as external forces and manifold constraints, are in play. We employ advanced free energy methods to analyze the stability of these structures in 2D and 3D systems of spheres. We also use a novel hybrid sampling technique to investigate the self-assembly of a dodecagonal quasicrystal approximant and facilitate its description, which was only possible using quantum mechanical simulation approaches. In summary, this work seeks to further advance the exploration of aperiodic crystals from a theoretical standpoint. We introduce simulation models for 2D and 3D quasicrystals and their approximants and present systematic studies showing their thermodynamic stability.



Tiles of a six-fold aperiodic crystal, with bond connections colored based on distances to nearest neighbors.

Priv.-Doz. Dr. Sudeshna Roy
Habilitation: Multiscale Simulation of Granular Flows: Insights into Additive Manufacturing, Rheology, and Capillary Force

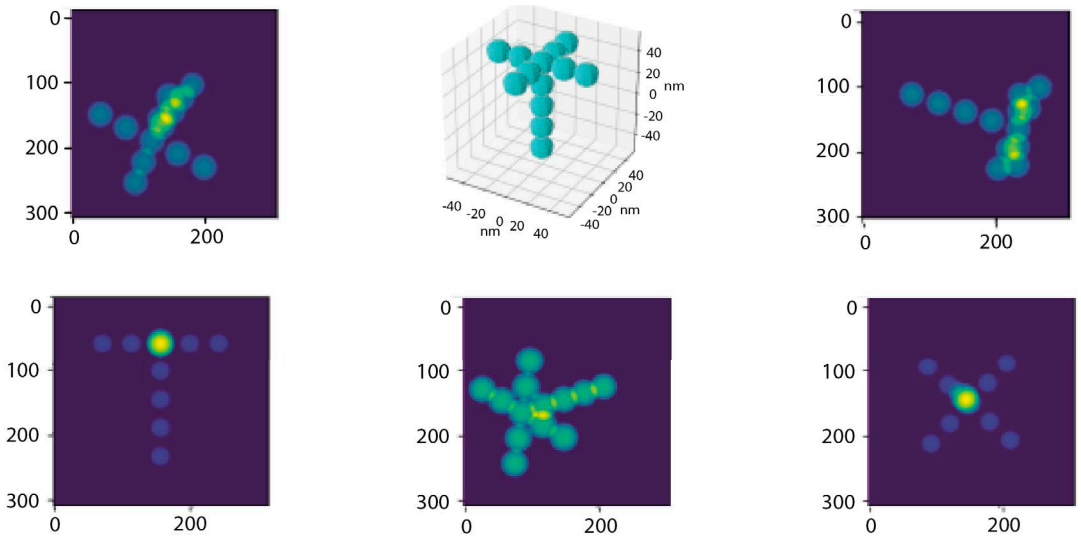
Multiscale modeling approaches for granular materials typically involve coupling different simulation techniques across scales. At the particle level, the Discrete Element Method (DEM) provides detailed information about particle interactions and local structure. At larger scales, continuum methods such as the Finite Element Method (FEM) can capture bulk material behavior. The challenge lies in effectively linking these scales to create a combined multiscale framework. One of the methods of linking the multiscale framework is through volume averaging. Several works on the micro to macro transition of granular materials are based on this method. Recent advancements in multiscale modeling have focused on developing methods to upscale microscopic information to inform macroscopic models. Techniques such as coarse-graining and homogenization have been employed to extract continuum fields from discrete particle data, allowing for a more seamless integration of micro- and macro-scale simulations. Discrete to continuum transition based on coarse graining approaches include several methodologies. These approaches enable researchers to study phenomena such as shear banding, force chains, and particle segregation within the context of larger-scale granular flows. The aim of this thesis is to provide insights into granular flow behaviors across three areas of study using a multiscale approach: (1) powder spreading in additive manufacturing, (2) granular rheology and constitutive modeling, and (3) capillary forces in wet granular systems. Each application demonstrates the utility of multiscale DEM simulations to address unique challenges, while also highlighting common themes such as particle-scale dynamics, bulk-scale outcomes, and the impact of interparticle interactions on flow behavior. By connecting these themes, this work not only advances our understanding of granular systems but also contributes to the development of predictive models for engineering applications.



7. Ongoing PhD Projects

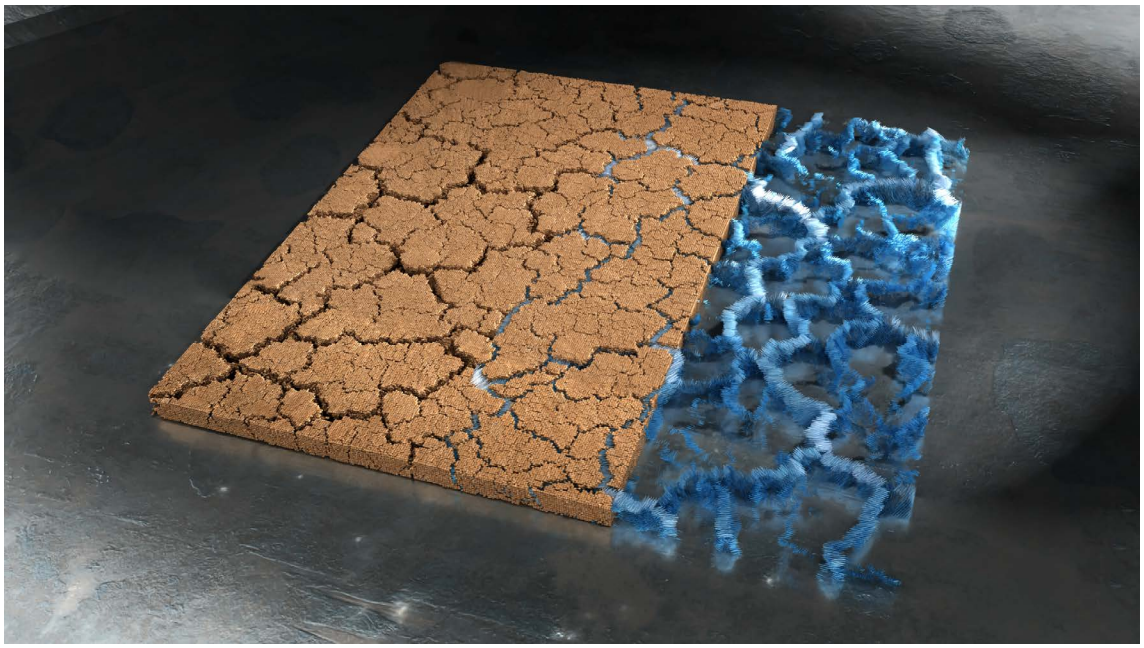
Franziska Anderl
Particle tracking in multi-beam X-ray radiography

To track dynamic particle systems, common x-ray tomography is too slow. To be able to follow the path of a specific particle, multi-beam x-ray tomography can be used instead. By taking five radiographs at a time instead of moving the x-ray source around the object, time-dependent processes become observable. To identify the particles from the reconstructed radiographs, a new algorithm was introduced. It uses a reconstruction – segmentation loop to identify mutually shadowing particles – an artifact that is conditioned by the use of only five instead of a complete angle radiograph. Further more, to ensure consistensy for every time step, a DEM-Simulation of the observed experiement is conducted in parallel. The resulting particle position of the simulation and reconstruction are compared and adjusted. So far, the first part of the algorithm, the identification of the particles, is implemented. In future work, an experiment will be set up to gain real data instead of simulated radiographs and the time tracking will be implemented.



Meysam Bagheri
Physics of Drying Suspensions

Drying suspensions often develop complex networks of cracks as the liquid evaporates. These cracks result from several coupled processes: evaporation causes the particles to pack closely together, and further drying creates liquid bridges between neighboring particles. These bridges generate capillary forces that compress the particle network until it breaks and forms cracks.
The aim of this project is to understand the cracking dynamics in drying suspensions through multiscale simulations. A multiphase model has been developed that represents the coupled motion of particles and the liquid phase. Particle motion is calculated using a force-based molecular dynamics algorithm, while the liquid phase is described as capillary bridges acting between the particles. Closed-form equations for the capillary force and bridge area were derived to avoid solving the full differential equations for the meniscus shape. The model is implemented in an in-house simulation code that can reproduce crack formation during the drying process.



Felix Buchele

Reactive Flow in Porous Media

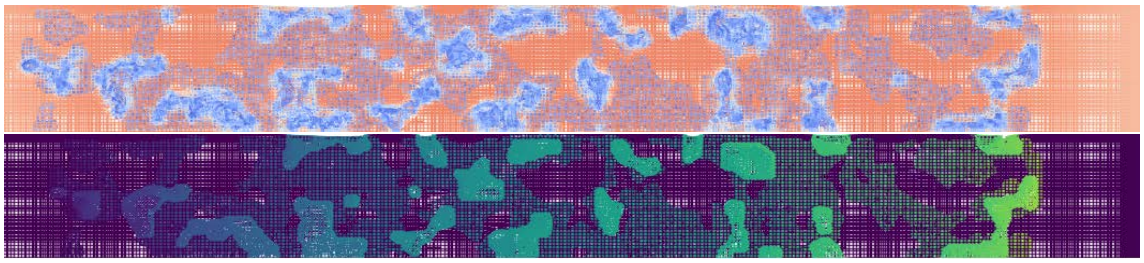
Reactive flow in porous materials involves a complex interplay between chemical kinetics, transport processes, and pore-scale geometry. To address this multiscale coupling, the present work combines three complementary components into a unified modeling framework.

The reactive component builds on a first-principles-based chemistry model that resolves elementary surface reactions using Transition State Theory (TST). Reaction rates are computed from activation enthalpies and entropies obtained through DFT data and thermochemical databases. These quantities are stored as lookup tables to enable efficient evaluation within simulations, eliminating a-priori assumptions about rate-determining steps or global efficiency factors.

The flow component employs a Direct Simulation Monte Carlo (DSMC) solver to capture gas dynamics at the Knudsen scale, where continuum assumptions break down. By resolving molecular collisions and wall interactions explicitly, the method accurately represents rarefied flow behavior in confined geometries, capabilities unattainable with traditional Navier–Stokes solvers. The stochastic formulation allows consistent coupling between microscopic surface reactions and mesoscale mass and energy transport.

The porous media component introduces a method to reconstruct realistic pore geometries for numerical simulation. Various morphologies, such as spherical pores, channel networks, shale-like microstructures, and fibrous or rod-shaped media, can be generated and parameterized based on imaging data [4]. These geometries serve as direct computational domains for DSMC simulations.

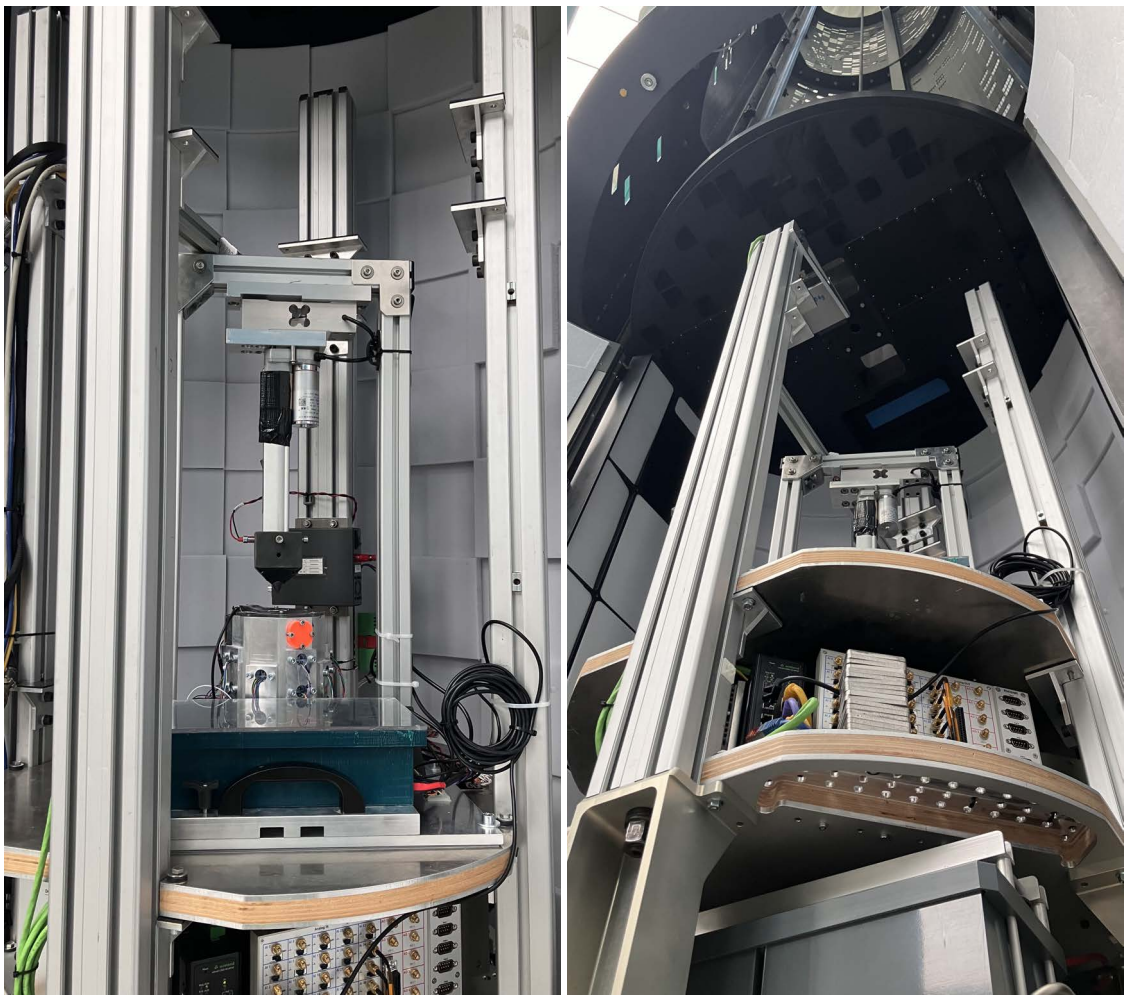
Together, these three components establish a first-principles-based framework for simulating reactive flow through realistic porous structures, bridging the gap between molecular surface chemistry, non-continuum gas dynamics, and microstructural material representation.



Snapshot of a simulation, showing the per-cell occupancy of DSMC samplers and the effect of surface poisoning in a complex geometry.

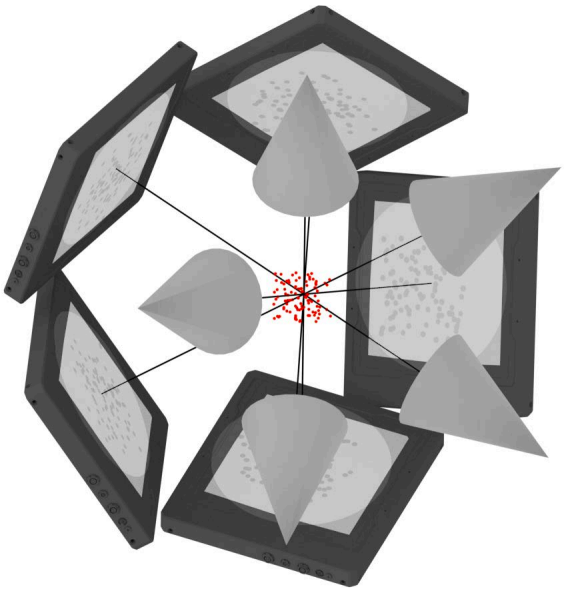
Geovane de Jesus Rodrigues
Granular Rheology in Space

Understanding the mechanics of Lunar soil, named regolith, is crucial to planning future missions. We focused on the effect of gravity on a cone penetration test (CPT), typically used to probe geotechnical soil properties. In our setup for the experiment, we use regolith simulant, as well terrestrial sand. A load cell measures the force acting on the probe, while additional sensors measure the pressure at the bottom and at the wall.
Two different probe geometries were used: a cylinder with a conical tip (typical CPT setup) and a flexible linear probe. As granular material for the experiment, we chose EAC-1 and LHS as regolith simulants and regular sand to serve as reference material. Experiments under hypergravity acceleration levels were performed at the Large Diameter Centrifuge, going from 1 to 20g. Experiments under lunar and microgravity were performed at the Gravity and Drop Tower in Bremen. Additional experiments at 1g were performed in Erlangen at the laboratory. By understanding the influence of gravity on the material flow behavior, we expect to improve existing models for regolith rheological properties description.



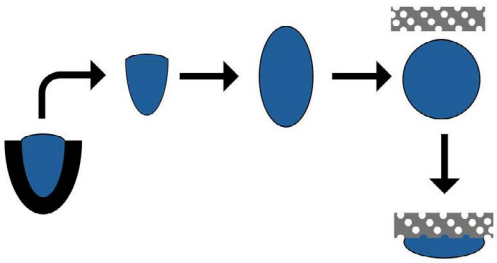
Mark Emmert
Digital Twin for refinment of Particle Tracking Velociometry for multi-ray tomographs.

Particle Tracking Velocioemtry estimates the velocity of specific individual particles based on projections of the particles at different time steps. Difficulties arise from identification of particles over different time steps (mapping) and from particles being shadowed by other particles (due to being mapped on overlying data points in the projection).
Using a multi-ray tomograph, therefor multiple projections per time step, partially tackles shadowing of particles and results in more precise localization of the particles in space. Running a particle simulation coherently to the measured data allows to better estimate particle positions and mapping. Additionally this particle simulation resembles a plausible interpolation for time between time steps.



Kai Ihrig
SPH Simulation of Droplet formation in 0g: influence of the shape on the relaxation time.

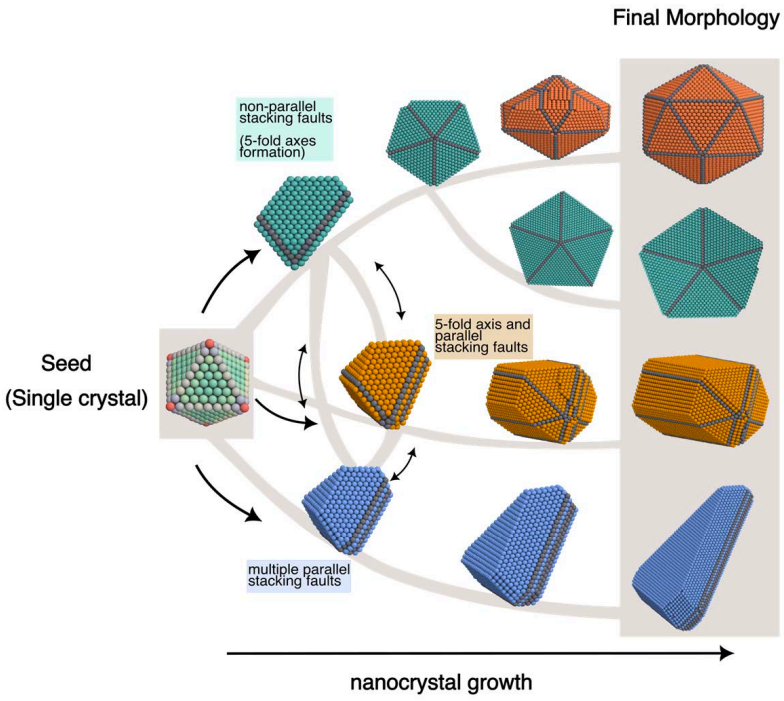
The study of wetting of porous media in zero gravity compels a shape as close as possible to a sphere. In order to achive the desired shape in minimal time, a parameter study was done with Smoothed Particle Hydrodynamics (SPH) method based on the open-source software SPlisHSPlasH.
The main goal of the study was to replicate the "Puddle Jump Experiment" [1] with the center of attention lying on two base shapes. The first beeing a rotational paraboloid and the second one a 3^{rd}-degree rotational paraboloid, or lovingly called 'Gugelhupf'. During over 400 simulations a variety of 'Gugelhupf'-shapes have shown up to 40% faster times in relaxation than the best case rotational paraboloid, hinting at it beeing the best shape for the Puddle-Jump-Experiment. The next step is a validation run with actual experiments collecting data and compare with the simulation results.



Jyoti Pannu

Symmetry Breaking and Growth Mechanism of Multiply Twinned Particles

Achieving precise control over the shapes of metal nanoparticles presents a significant challenge, primarily due to the complex interplay between growth kinetics and surface chemistry at the nanoscale. During the synthesis process, a variety of structures—including single crystals and twinned particles—are formed together [1,2]. This concurrent formation complicates efforts to achieve uniform and reproducible outcomes, as it leads to significant variability in particle morphology. To overcome these challenges, a deep understanding of the mechanisms underlying the formation of different morphologies during growth is essential. This requires advanced techniques, particularly atomistic simulations capable of covering extensive length and time scales. In this project, we introduce a novel off-lattice rejection-free kinetic Monte Carlo (rfkMC) approach. This new methodology captures the intricate growth kinetics of nanoparticles under non-equilibrium conditions and enables the simulation of realistic particle sizes. Our simulations reveal atomic-level growth mechanisms that give rise to various nanoparticle shapes, including decahedra, icosahedra, and penta-twinned rods, all of which develop from single crystal seeds. We have observed that the transformation of shapes and bifurcations in twinned nanoparticles is intricately linked to the emergence of planar defects during their growth. These defects function as critical decision points, significantly influencing the final geometry of the nanoparticles. This research captures the essential factors that govern the shape formation in noble metal nanoparticles, offering valuable insights for developing targeted synthesis strategies.



An octahedron seed can grow into various symmetry-broken shapes due to the kinetic trapping caused by the formation of stacking faults

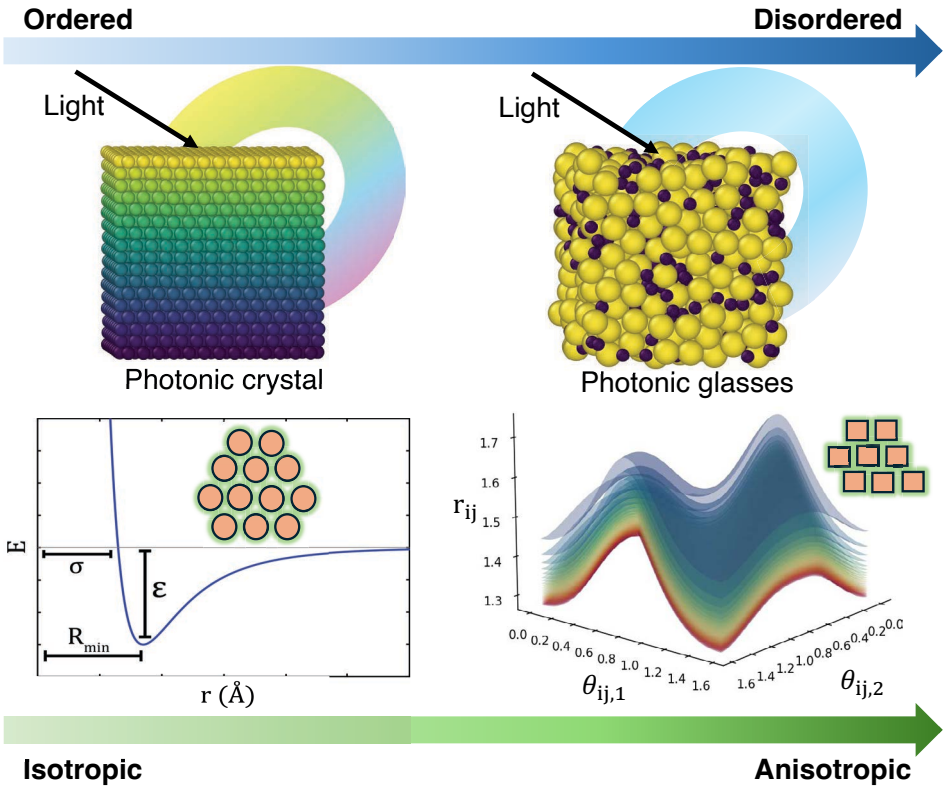
Harsha Namdeo

Modeling of Colloidal Interactions and Assemblies for Optimal Functional Materials

This project aims to develop advanced methods to model colloidal interactions and guide the assembly of particles into optimized, functional materials. By understanding and controlling interparticle forces, we can influence the self-assembly processes that lead to desired material properties. This includes tailoring interactions to achieve specific structural colors or interesting ordered assemblies. The application of machine and deep learning techniques is employed to reconstruct interaction potentials.

The project also investigates how defects and disorder in particle arrangements can influence optical properties of photonic glasses. The aim is to develop angle independent structural colors based on prior simulated disordered structures. The correlation between disorder and color enables the design of materials with tailored optical properties.

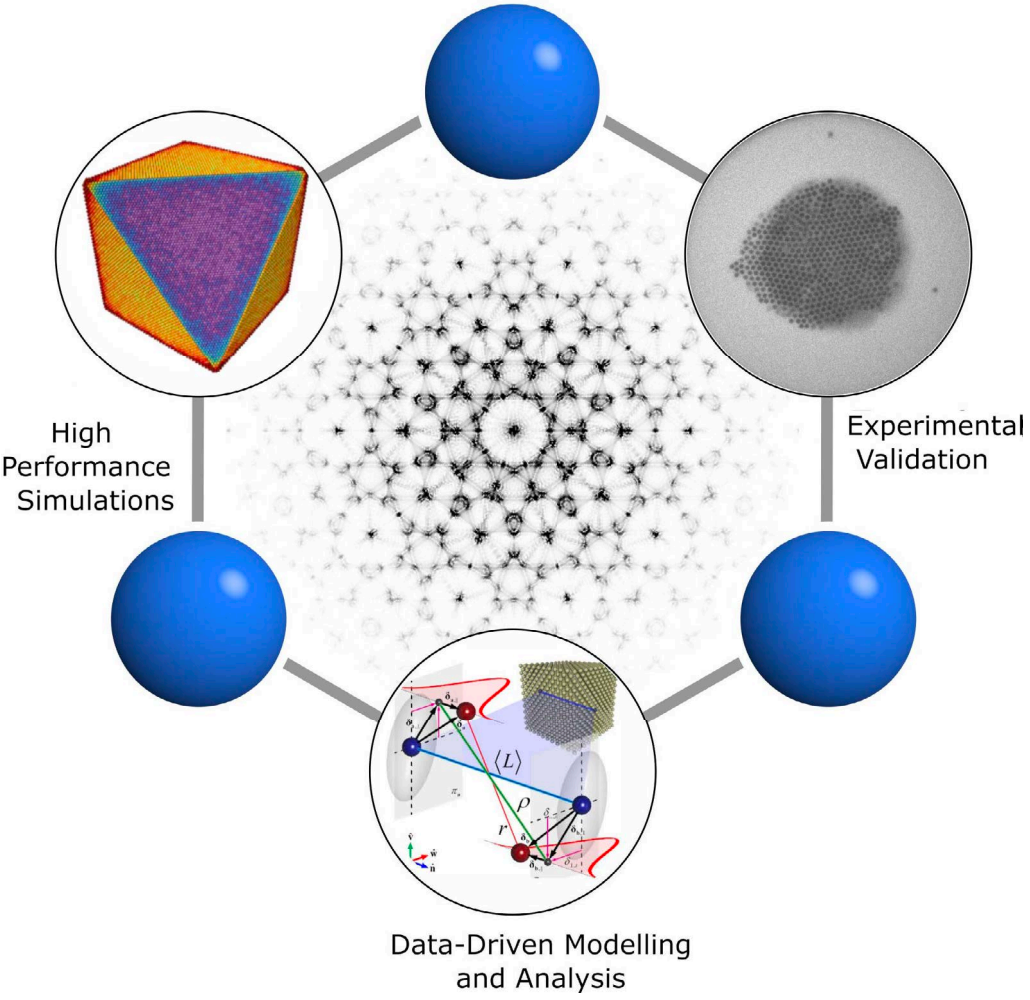
Ultimately, this work seeks to bridge experimental observations with theoretical models, enabling the precise design of materials with targeted functionality.



Navid Panchi

Data-Driven and High-Performance Simulation and Analysis Method for Particle-Based Systems

This research focuses on developing advanced data-driven, high-performance simulation methods and analysis techniques for particle-based systems. It develops algorithms for simulating diffraction patterns, examining system symmetries, and conducting symmetry analysis, with an emphasis on computational efficiency. The research also explores automated extraction of disorder models from simulation data to facilitate the interpretation of complex physical phenomena. Additionally, it addresses the identification and resolution of performance bottlenecks to improve simulation efficiency. Finally, scalable parallelization strategies for heterogeneous hardware architectures are implemented to enhance the speed and scalability of particle-based system simulations and analysis.



Nicolas Pechler

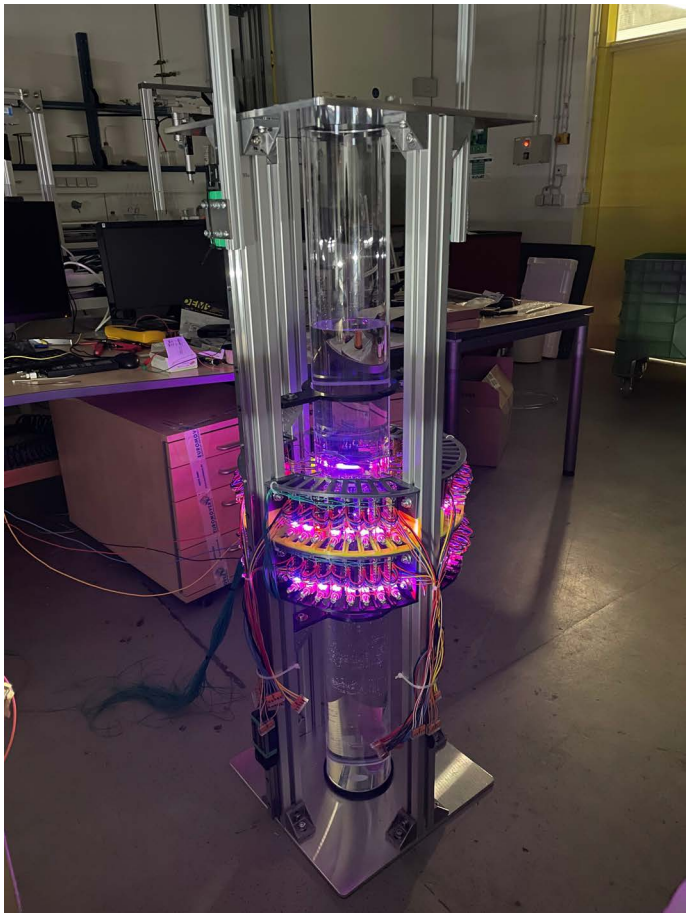
Electrical Impedance Tomography

As part of the ROBIN project, aimed at developing a measurement and imaging method for high-resolution acquisition of thermal-hydraulic parameters in largescale experimental facilities for nuclear safety research, we are developing a sensor based on electrical impedance tomography. This sensor is intended to enable non-intrusive monitoring of two-phase flows in pipelines, allowing for the assessment of flow regimes, fluid velocity fields, and void fields.

Electrical impedance tomography (EIT) is a noninvasive imaging technique used to visualize and monitor the internal conductivity distribution of an object. This is done by placing multiple electrodes on the sample's surface. Current is injected through electrode pairs, leading to an internal potential distribution, which can be measured on the surface by the electrodes. With a change in conductivity, the internal potential shifts, leading to a detection in measurement. For successful reconstruction, measurement data of all injection electrode pairs is processed by a reconstruction algorithm.

One of the significant challenges associated with EIT is its inherently low spatial accuracy. The electrical potential distribution on the surface of the object exhibits only subtle differences, making precise measurements a demanding task. Therefore, the utilization of precise measurement equipment and techniques is important to overcome this limitation and enhance the overall accuracy of the imaging process.

In this context, we utilize frequency multiplexed current excitation to achieve real-time measurement of pipe flow. Alongside determining an improved data evaluation algorithm, the project also aims to optimize the electrode configuration, the geometric design, and the construction of the measurement apparatus.

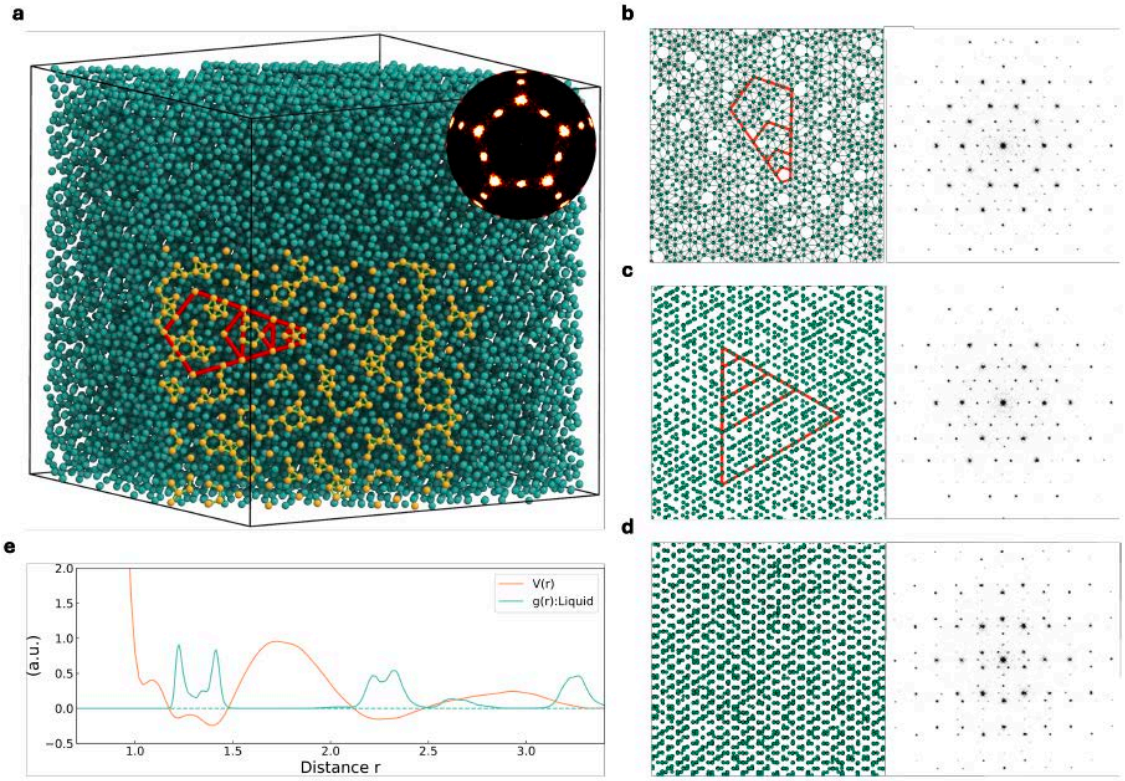


Kaijie Zhao

Simulated Formation of a Primitive Icosahedral Quasicrystal

Quasicrystals exhibit long-range aperiodic order, permitting non-crystallographic symmetries and intrinsic structural flexibility arising from locally adaptive atomic environments. However, direct observation and systematic characterization of such disorder-mediated flexibility remain limited.

In this study, we report the self-assembly of a primitive icosahedral quasicrystal (p-IQC) over an extended range of number densities. Systematic structural analysis reveals that the quasicrystal accommodates significant density variations through local rearrangements associated with phasonic degrees of freedom. Comparison with idealized model structures demonstrates consistent thermodynamic stability and close structural correspondence across densities. These findings offer evidence to the intrinsic local structural flexibility of the pIQC, and highlight the potential of structural adaptability of quasicrystals to external stimuli.



Simulation of the self-assembly of a primitive icosahedral quasicrystal in a one-component system. (a) Isotropic particles in a cubic box with periodic boundary conditions. Particles align in columns (top surface), and one layer is highlighted (yellow) to present the local sparsity of the structure. The bond-orientational order diagram is depicted in the corner. (b–d) Simulation snapshots and diffraction patterns from the (b) fivefold, (c) threefold, and (d) twofold directions. Scaling of polygons with respect to the factor τ and the clear Bragg peaks with subtle diffuse scattering in the diffraction patterns reveal the underlying quasiperiodic characteristic. (e) Pair potential $V(r)$ and radial distribution function (RDF) of the low-density icosahedral quasicrystal phase. The system is simulated at low pressure ($p = 0.5$) and contains 32 000 particles.

Wing To Ku

Homogenization of Granular Pipe Flow

The transport of particulate matter through narrow pipes is intrinsically unstable, with large variations in solid fraction (density waves) and the potential for clogging. These issues can lead to destructive pressure transients on the pipe walls. Previously, introducing a helical texture on the pipe wall was found to help homogenize the flow. Building on this idea, we developed an improved system called the helical spine wall geometry. We tested the system using the discrete element method (DEM) and investigated the effect of different modulations on the efficiency and homogeneity of granular pipe flow. We also compared the new geometry with the previous helical wall texture and observed superior performance. Finally, the concept was extended to fluid-driven granular pipe flow, where a similar enhancement was observed.

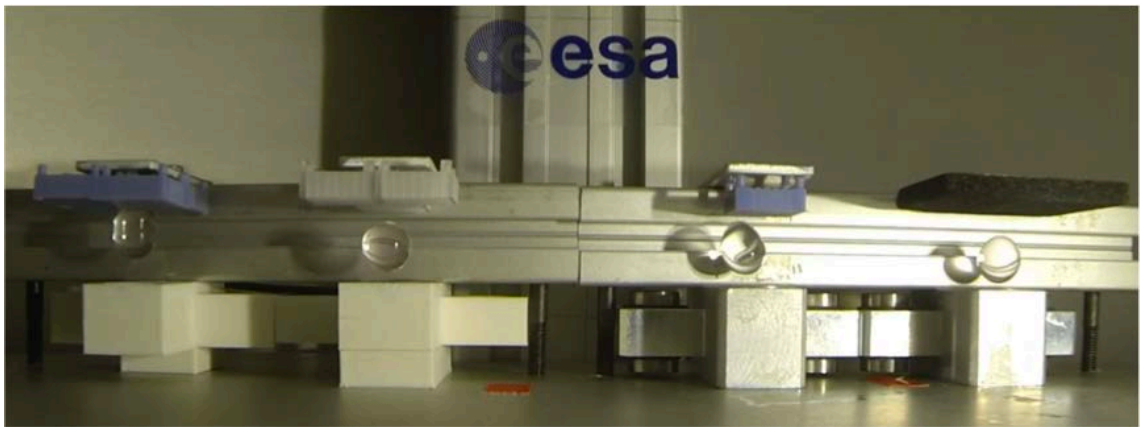
Granular flow in a pipe under gravity,influenced by a helical spine wall geometry.From left to right, the period of the helical spine wall increases from 50R (where R is the particle radius),to 500R with the last image showing a straight pipe. The colors indicate particle velocity: red represents slower flow, and blue represents faster flow. The figure is compressed vertically by a factor of three for better visualization.

8. Students Projects

Master theses

Kai Ihrig
SPH simulation of drop formation in zero gravity: Influence of the initial shape on relaxation behavior

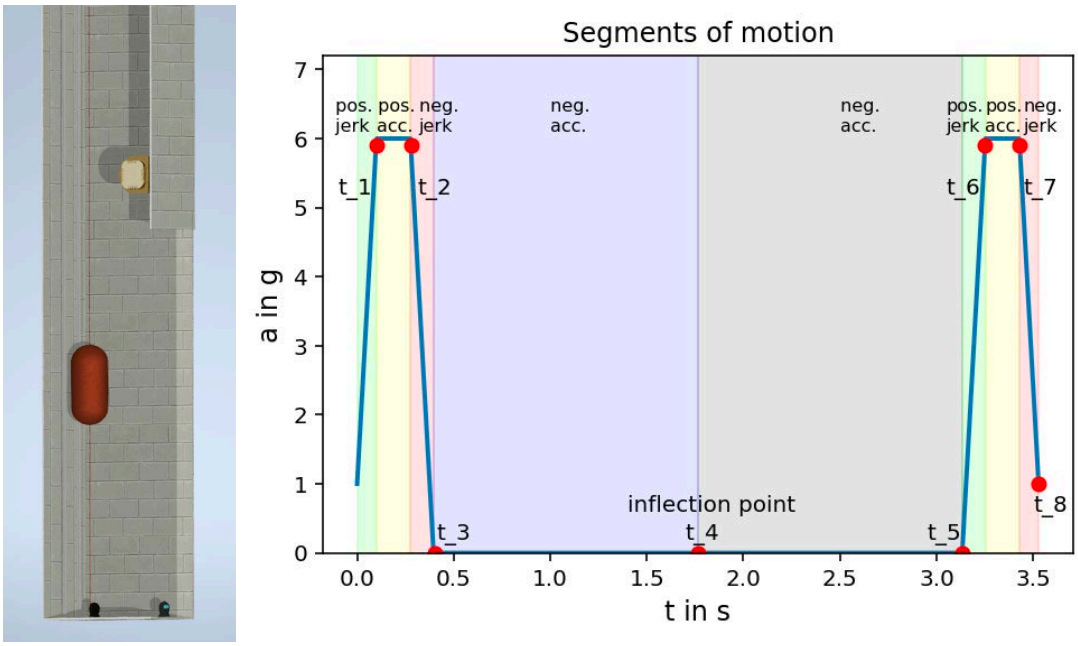
We investigate capillary auto-ejection (puddle jumping) as a mechanism for producing centimetric droplets within seconds. By analyzing how trough geometry controls the conversion of surface energy into translational and vibrational modes, this work provides design principles for reliable, on demand droplet formation in limited duration microgravity experiments.



Laura Steub

Gravitational Force Research Elevator – G FREE

The experimental gondola is actuated by a high-torque synchronous motor via an endless toothed belt, allowing precise control of its motion. By following a customizable acceleration profile, the system can reproduce a variety of gravitational environments. To prevent lateral deflection, the gondola is mounted on a double strand of linear guides, ensuring stable and accurate motion. Over the available 12-meter height, the tower is capable of generating up to three seconds of weightlessness, as well as various hypo- and hypergravity conditions with corresponding experimental durations.

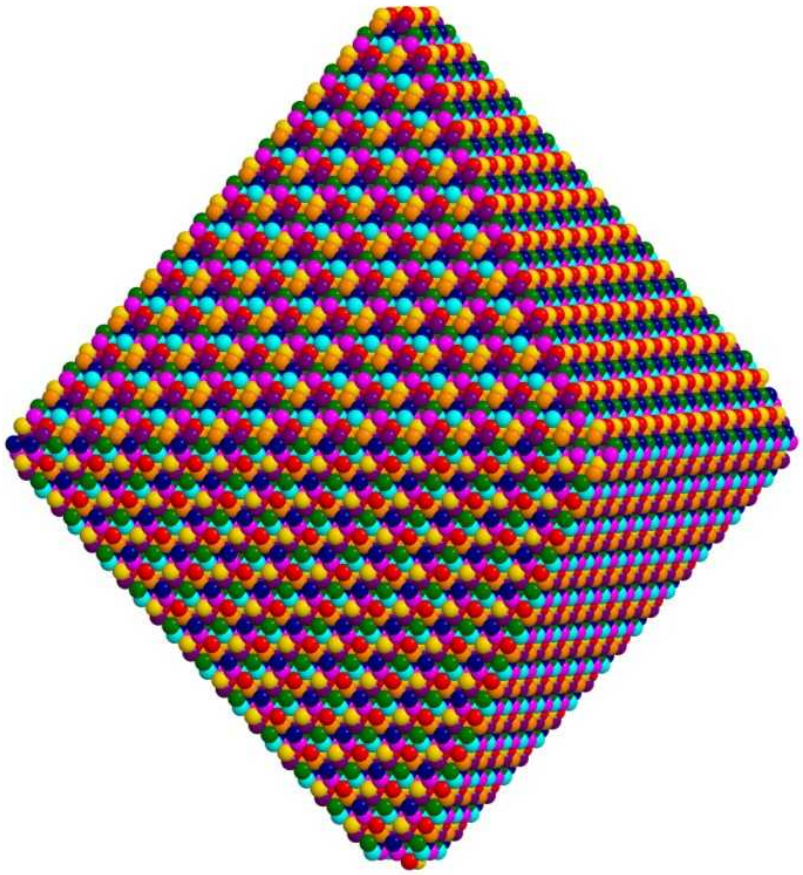


Left: Planned setup of the G-FREE; right: Segments of the planned motionequation for a zero-g profile

Arne Bringewatt

Data-Driven Optimization of Nanocrystals Simulated by Kinetic Monte Carlo

The shape of nanocrystals is a fundamental determinant of their functional properties, yet the vast "shape-space" for many crystal lattices remains unexplored due to the limitations of manual investigation. While the growth mechanisms of face-centered cubic (fcc) systems are well-documented, a systematic understanding of body-centered cubic (bcc), hexagonal close-packed (hcp), and complex binary systems is still lacking. This thesis presents an automated, systematic framework designed to bridge this gap by coupling rejection-free kinetic Monte-Carlo (rfKMC) simulations with advanced optimization techniques. Central to this approach is the use of a broken-bond model to simulate crystal growth at scales exceeding the capabilities of traditional molecular dynamics. To navigate the high-dimensional parameter space of these models, a shape-recognition algorithm based on spherical harmonics is implemented to mathematically classify resulting morphologies. This classification is integrated into a genetic algorithm that iteratively optimizes bond energy levels to converge upon desired target shapes. By automating the discovery process, this method eliminates the need for labor-intensive visual inspection and provides a high-throughput means of mapping the relationship between energy parameters and crystal habits. The utility of this framework is demonstrated through its application to bcc and hcp lattices, as well as the industrial semiconductor Cadmium Telluride (CdTe), offering new insights into the synthesis routes of complex nanocrystalline structures.

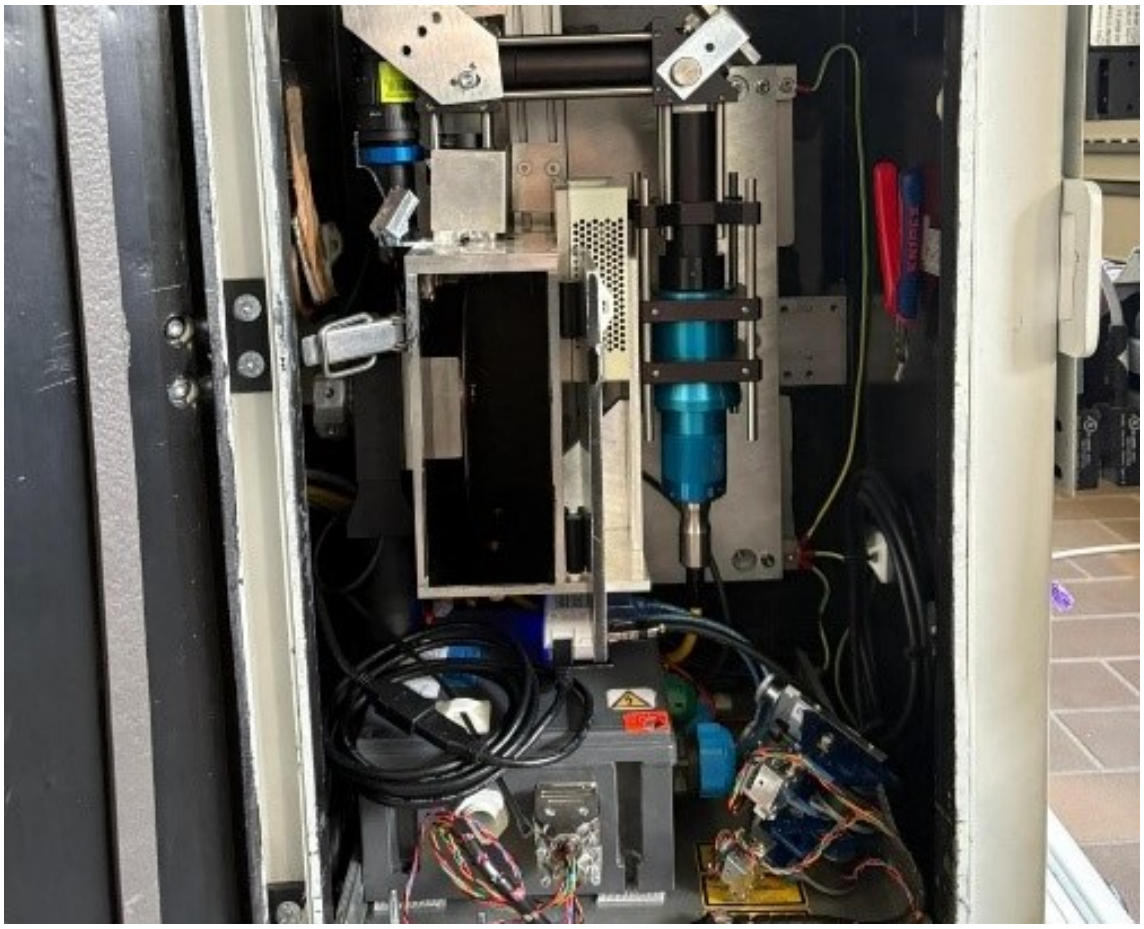


Bachelor theses

Felix Böhmer
Development of a wire feeder for LASER metal deposition in microgravity

The objective of this thesis is to develop, build, and commission a functional wire feeder for the LADA project. LADA is a project focused on laser metal deposition welding under microgravity conditions and regularly participates in parabolic flight campaigns in Bordeaux.
During the most recent campaign, an outdated wire feeder was used, which did not operate reliably. This made it necessary to develop a new wire feeding system. Key challenges include the very limited space inside the experimental setup and the high stiffness of the titanium wire. In previous designs, the wire was difficult to unwind and tended to tangle easily.

The aim of this work is therefore to develop and test a smooth-running wire feeder that can be used in the next measurement campaign in May.



Quirin Beckh

Perpetual Focault Pendulum

The work focuses on a continuously driven Foucault pendulum, which can be used to construct a clock based on the Earth's rotation. Since the exact angular velocity at which the Earth rotates beneath the pendulum is known when taking the latitude of the location into account, and since the pendulum oscillates undisturbed in its plane of oscillation, the deviation of the pendulum bob relative to the previous oscillation can be measured. From this deviation, a method of time measurement can be derived, although it is not directly coupled to conventional clock time. The principle of this pendulum was already developed in 1851 by the French physicist Léon Foucault, thereby providing experimental proof of the Earth's rotation about its own axis. A disadvantage of a conventional pendulum, however, is that due to energy losses such as air resistance, the oscillation gradually decays and the pendulum must be re-energized after a certain time. To ensure continuous and undisturbed operation for time measurement, an external energy input is required. In conventional pendulums, this energy is typically supplied via magnetic coils embedded in a plate at the bottom, accelerating the pendulum as it passes through the equilibrium position.
In this project, however, the energy input is achieved by pulling on the suspension string. In order to avoid the use of a motor and additional visible components in the apparatus, a Nitinol wire is used. When heated, this wire undergoes a reversible phase transition within its crystal structure, resulting in a contraction of the wire. The heating of the wire is accomplished by passing an electric current through it. A crucial aspect of this type of drive is the correct timing for lifting and lowering the pendulum bob. The lifting of the pendulum bob, and thus the energizing of the wire, must occur at the moment of zero crossing, since the system works against the centrifugal force in order to produce an additional acceleration in the direction of the plane of oscillation. The lowering of the pendulum bob, and thus the cooling of the wire, must take place at the point of maximum deflection, where no centrifugal force is present because the velocity of the pendulum bob is zero.
The control of the wire is intended to be implemented using an Arduino in order to ensure uniform oscillation. The position of the pendulum bob at maximum deflection is to be detected from above using a camera and compared with the position from the previous oscillation. Using a Raspberry Pi, the resulting time difference can then be calculated.

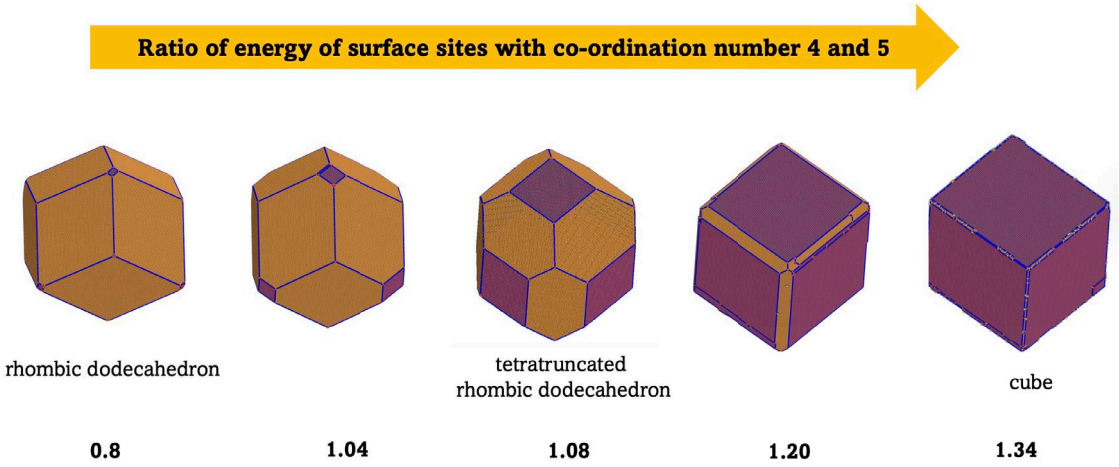
Foucault pendulum at the Kirchhoff Institute for Physics at the University of Heidelberg

Other projects

Sanjukta Chowdhury

Shape Diagram of Body-Centered Cubic Crystals

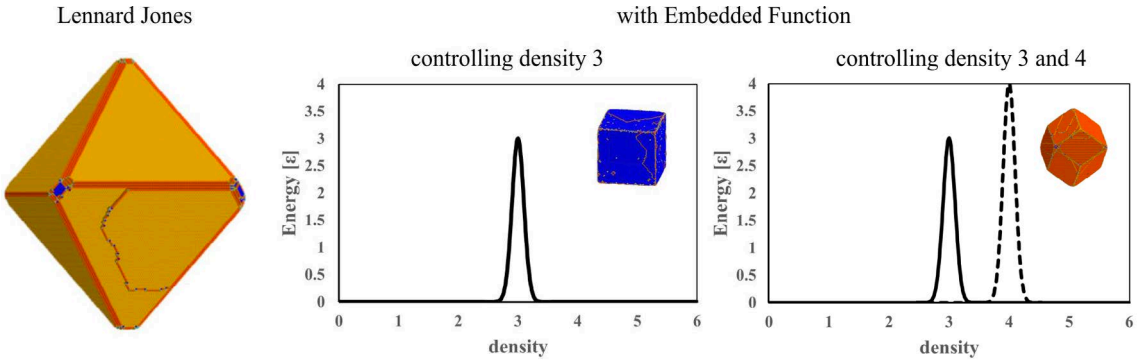
Nanocrystal research has accelerated in recent years because their properties differ markedly from those of bulk materials, finding applications in electronics, medicine, catalysis, photonics, and others. The nanocrystal shape plays a pivotal role in properties. Traditionally studied by empirical methods, shape formation mechanisms yet require a systematic analysis based on a theoretical approach. To address this, we use kinetic Monte Carlo simulations to predict body-centered cubic (BCC) nanocrystal shapes. The simulations consider atom-by-atom growth, enabling energy tracking and shape transformation. This far exceeds the spatial and temporal resolution of traditional measurement techniques, such as microscopy and tomography. Simulations reveal nanocrystal shape control by altering relative growth rates between facets with different crystallographic [directions. Experimentally, these rates are modulated by the addition of ligands and ions that adsorb to specific surface sites. This study pinpoints the surface sites (adatoms) that play a major role on shape transformations from rhombic dodecahedron (equilibrium shape of BCC) to cubes (metastable). By defining the coordination number of BCC as the number of first and second neighbor atoms, which present minimal separation 2.4, we find that the surface sites controlling shape transformation occur at coordination numbers 4 and 5 (see graphical abstract). Future directions of this study will tackle transformations to octahedra, with the aim of predicting the full shape diagram of symmetry-preserving polyhedral shapes of BCC nanocrystals bound by low Miller index facets. The establishment of shape diagrams will transfer the scientific knowledge to engineering of nanomaterials in a similar fashion phase diagrams made for classic materials.



Yaopeng Liu

Energy Model for Surface-Site Adsorption using Embedded Functions

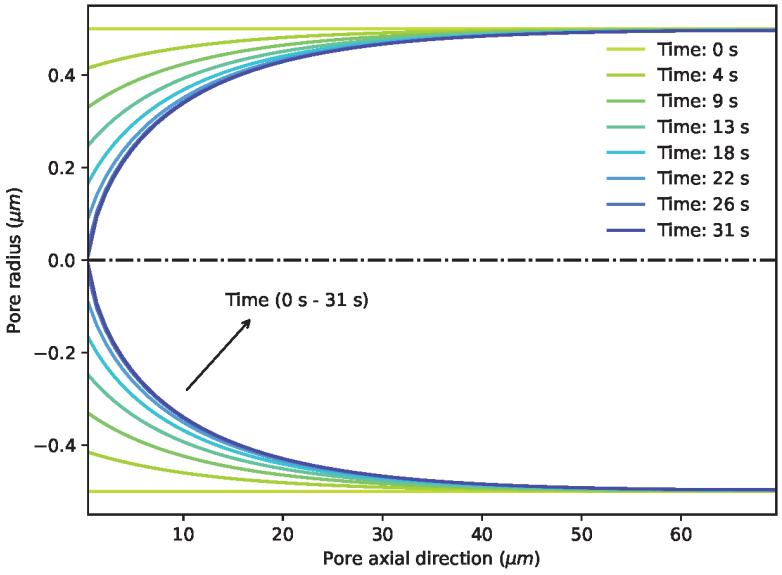
We introduce a continuous, coarse-grained potential-energy model for surface-site adsorption that enables nanocrystal shape control. A Lennard–Jones (LJ) pair potential is augmented with an embedded function for the local density, using a sigmoid to select sites by their coordination number (CN). This embedded-density term imposes an energy bias on selected CN ranges, selectively lowering or raising the energy of those surface sites to steer facet-specific growth and, in turn, overall nanocrystal morphology. Targeted tests that bias CN ≈ 3 and CN ≈ 4 reproducibly shift relative facet growth rates to yield the expected shapes—octahedra (dominant $\{111\}$), cubes ($\{100\}$), and rhombic dodecahedra ($\{110\}$). Implemented in an on-lattice kinetic Monte Carlo framework, the model produces deterministic transitions among these shape families via continuous parameter tuning, while retaining the simplicity, speed, and transferability of pair-potential descriptions. Because the embedded term is continuous and depends only on a local-density descriptor, it can be transferred to off-lattice models required for studying symmetry-broken morphologies and defect-mediated shapes inaccessible to rigid lattice models, to be tested in future work. Nanocrystal morphology governs plasmonic resonances and active-site distributions central to plasmonics-enabled photocatalysis, cancer phototherapies, and sensing applications such as Raman spectroscopy.



Isabella Schneider

Pore Sealing of Clathrate Hydrates from Finite Volume Simulations

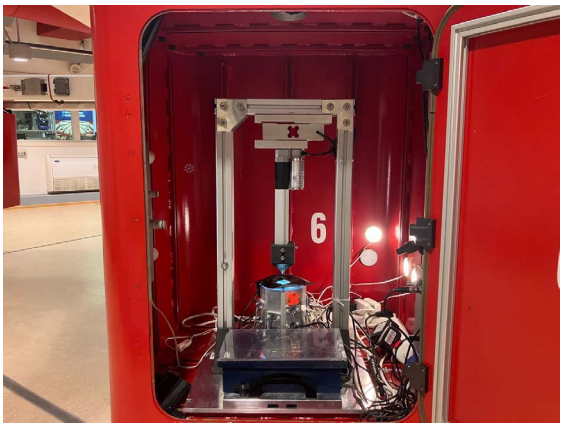
This work presents the first transient numerical investigation of pore sealing in methane clathrate hydrates using a finite volume formulation that concurrently resolves coupled mass and heat transfer. The model captures the spatiotemporal evolution of methane concentration, temperature, and pore geometry within a single micrometer-sized hydrate pore, enabling a detailed analysis of the dynamic interplay between diffusion and crystallization. The pore is represented as a cylindrical, water-filled microchannel where dissolved methane diffuses axially and crystallizes on the hydrophilic walls. Governing equations for mass and heat transfer are derived from Fick's second law and the transient heat equation, in which source terms represent the local effects of crystallization — namely, gas consumption in the mass balance and heat release in the energy balance. A fugacity-based first-order kinetic law links local concentration to the crystallization rate, while the progressive accumulation of hydrate continuously reduces the pore radius over time, dynamically coupling transport and geometry. The one-dimensional (pseudo–two-dimensional) finite volume formulation ensures strict conservation of mass and energy, and verification against the analytical steady-state solution of Bassani et al. confirms the numerical accuracy of the implemented scheme. The temporal discretization employs a semi-implicit (Crank–Nicolson) scheme that is second-order accurate and unconditionally stable; boundedness and consistency are maintained, and convergence is guaranteed by the Lax equivalence theorem. Under typical conditions, pore closure occurs on the order of tens of seconds. Transient simulations reveal that, beyond the classical steady-state diffusion limitation, a new, time-dependent mechanism arises due to progressive pore constriction, which hinders diffusive inflow and thus limits hydrate growth. This pore-sealing–induced mass transfer limitation leads to an asymptotic trend in the amount of gas consumed and reduces the total gas converted per pore by up to 45 % compared to steady-state predictions, demonstrating that unsteady diffusion–crystallization coupling plays a critical role in pore-scale kinetics. In contrast, heat transfer effects are found to be negligible at the pore scale: temperature variations along the pore remain below 0.012 K and do not significantly influence local properties or crystallization rates. A sensitivity analysis spanning pressure, temperature, initial pore radius, and the constant of proportionality of crystal integration, k_i, shows that higher pressure, lower temperature, and larger initial radii accelerate pore shrinkage and increase total gas consumption, whereas k_i exerts dominant control over closure timescales and overall gas conversion — underscoring the need for its precise determination in realistic porous-medium evolution. The model establishes a mechanistic link between pore-level transport phenomena and macroscopic hydrate behavior, providing insights relevant to safer and greener flow assurance in natural-gas production and to carbon-sequestration strategies.



9. Experimental Campaigns

Centrifuge campaign at ESA/ESTEC in the Netherlands

Olfa D'Angelo, Geovane de Jesus Rodrigues and Nadja Al Akkam were at the Large Diameter Centrifuge (LDC) for testing the effect of hypergravity on the behavior of granular materials similar to the soil found on the Moon surface.
During the LDC campaign at the Large Diameter Centrifuge in the ESA/ESTEC in Nordwijk, Netherlands, we brought our experiment, a penetration test, to observe the behaviour of two lunar regolith simulants under hypergravity. Using LHS and EAC-1 as probe materials, and regular earth sand as reference material, we conducted the tests during 10 days. The tests were performed under gravity accelerations up to 20 times Earth's gravity. We used two experimental setups: one with a cylindrical probe containing a conical tip, and a second setup with a linear probe. The idea was to observe the difference in the resistance force experienced by the probe as it was inserted. Also, we observed how the pressure within the materials was transmitted to the wall of the recipient where it was contained. With these results, we expect to increase our knowledge about the influence of gravity in the mechanical and rheological response of these types of granular materials. This campaign is part of the GRIS project, financed by the German Aerospace Center.



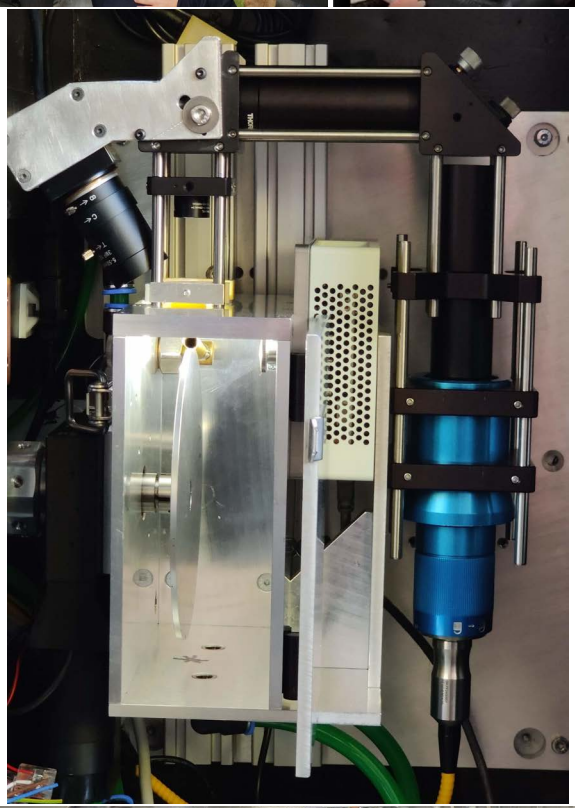
43rd DLR parabolic flight campaign

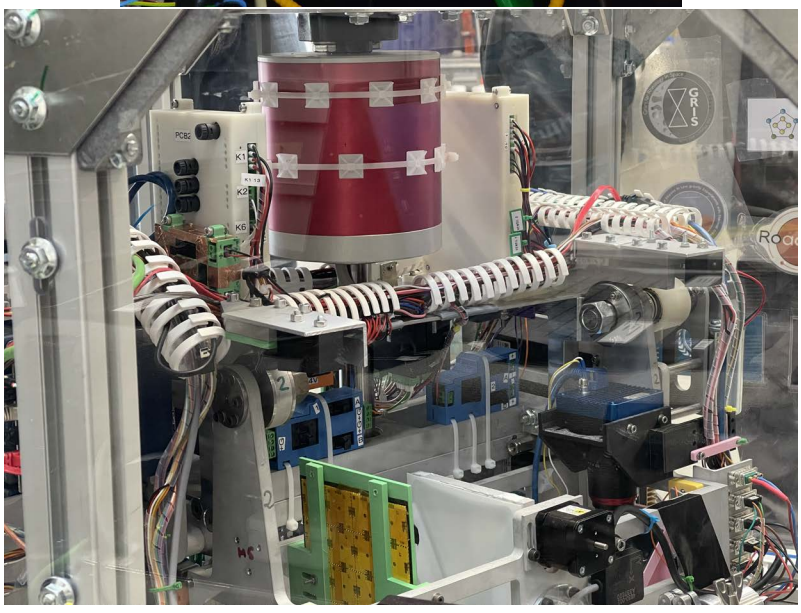
In September, the MSS had the special opportunity to take part in a parabolic flight campaign to conduct two innovative experiments in weightlessness and under reduced gravity. Preparations began with an integration week from September 9 to 13, during which the experiments were installed and tested in the aircraft, the Airbus A310 ZERO-G. On the flight days from September 17 to 19, 31 parabolas were flown per day. Each of these parabolas provided around 22 seconds of weightlessness, during which we were able to collect valuable data. The flights were carried out from Bordeaux Mérignac in France and organized by the company Novespace. Funding was provided by the German Aerospace Center (DLR).
Our chair was represented with two experiments. The first experiment, Granular Rheology in Space (GRIS), investigated the flow behavior of lunar regolith simulants under reduced gravity. This experiment is of central importance for future lunar missions, such as NASA's Artemis mission, as lunar regolith could potentially be used as a construction material or raw material. The aim of GRIS was to analyze how regolith flows through an opening, when blockages occur and how the angle of repose correlates with the material properties. With the help of a centrifuge, the experiment could be carried out at different gravities between zero gravity and 1g in order to investigate these questions under realistic conditions.
The second experiment, LASER wire welding in zero gravity (LADA), dealt with the additive manufacturing of metal components using laser wire cladding. The process could be used in future space missions to manufacture spare parts directly on site, e.g. on space stations or moon bases. As part of the parabolic flight, initial tests were carried out using a 500 W fiber laser and the materials aluminum and titanium. The processes were observed using the specially developed HORUS X-ray system in order to analyze the behavior of the melt in zero gravity.
Despite the intensive and demanding flight days, many of the planned experiments were carried out successfully. The results of these experiments will provide important findings for the development of future space missions.
On board:

Name	**Experiment**
(right figure from left to right)	
Vadim Medvedev	LADA (Lehrstuhl Photonische Technologien)
Felix Boehmer	LADA (MSS, student)
Prof. Thorsten Pöschel	LADA
Walter Pucheanu	(MSS, master technician)
Dr. Achim Sack	LADA
(left figure 2 and 4 from left)	
Geovane de Jesus Rodrigues	GRIS
Dr. Olfa D'Angelo	GRIS


Air Zero G
FAU
MSS


Zero G
FAU
MSS




PCB2
K1
K2
K6
GRIS

First Lunar gravity campaign at the new generation drop tower in Bremen

Olfa D'Angelo and Geovane de Jesus Rodrigues used the new generation drop tower, the Gravity Tower Bremen (GTB) at ZARM in Bremen, for the first ever commercial campaign simulating Moon's gravity. Their experiments will help future space missions planning by better understanding the effect of low gravity on granular flows, in particular Moon sand, known as Lunar regolith.
During the Drop and Gravity Tower campaign, performed at the ZARM in Bremen, Germany, we conducted the penetration test under low gravity. LHS and EAC-1 were used as lunar regolith simulants, and regular Earth sand was used as reference material. The tests were performed under lunar and microgravity. It was also the first time that the Gravity Tower was used for experiments under lunar gravity. Using two experimental setups, we observed the resistance force experienced by a cylindrical probe with a conical tip, and a linear probe. We also observed the pressure distribution transmitted within the materials to the container walls. Understanding the behaviour of granular materials under other gravitational accelerations will help the planning of future missions to our moon. This campaign is part of the GRIS project, financed by the German Aerospace Center.

10. Funding

Research funding

“Kinetic pathways to control nanocrystal shapes”
ERC Starting Grant 2025
Applicant: Dr. Carlos L. Bassani

“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

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

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

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

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

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

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

"NSF-DFG MISSION: Aufklärung der Dynamik von Nanokristallbildung und -umwandlung durch multimodale In-situ-Elektronenmikroskopie"
German Science Foundation (DFG)
Applicant: Prof. Michael Engel

"NSF-DFG Confine: Erzeugung funktionaler Suprapartikel durch gezielte Anordnung nichtsphärischer Nanopartikel unter Einschluss"
German Science Foundation (DFG)
Applicant: Prof. Michael Engel

"Kontrollierte Unordnung in nanostrukturierten Materialien: Kopplung von Experimenten und Simulationen"
German Science Foundation (DFG)
Applicant: Prof. Michael Engel

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

"Whole Pair Distribution Function Modelling of Layered Materials"
Ada Lovelace Centre (UK)
Applicant: Priv.-Doz. Dr. Alberto Leonardi

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

"Behaviour of Granular Matter under Vibrations (SPACE GRAINS)"
European Space Agency (ESA)
Applicants: Prof. Joseph Anthony (Leeds, UK), Dr. Sebastien Aumaitre (Saclay, France), Dr. Michael Berhanu (Paris, France), Prof. Eric Clément (Paris, France), Prof. Douglas Durian (U. Pennsylvania, USA),

Dr. Eric Falcon (Paris, France), Prof. Stéphan Fauve (Paris, France), Prof. Angel Garcimartin (Pamplona, Spain), Dr. Yves Garrabos (Bordeaux, France), Prof. Meiying Hou (Beijing, China), Prof. Xiaoping Jia (Marne, France), Carole Lecoutre (Bordeaux, France), Prof. Stefan Luding (Twente, Netherlands), Prof. Diego Maza Ozcodi (Pamplona, Spain), Prof. Thorsten Pöschel (Erlangen, Germany), Prof. Matthias Sperl (Cologne, Germany), Prof. Nicolas Vandewalle (Liege, Belgium)

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

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

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

"Tracergestützte Radiografie der Schmelzpooldynamik beim Laser-Draht-Auftragsschweißen in Schwerelosigkeit"
Emerging Talents Initiative (ETI)
Applicant: Dr. Achim Sack

11. Publications

Scientific Papers Published by the MSS in Peer-Reviewed Journals in 2025

1. M. Bagheri, T. Pöschel, Cascade crack in chain of beads. *Physical Review E* **112**, 045414, DOI: 10.1103/hzs3-8ffk (2025).
2. M. Bagheri, S. Roy, T. Pöschel, Comparison of bulk properties of wet granular materials using different capillary force approximations. *EPJ Web of Conferences* **334**, 01002, DOI: 10.1051/epjconf/202533401002 (2025).
3. M. Bagheri, S. Roy, T. Pöschel, Discrete Element Simulations of particles interacting via capillary forces using MercuryDPM. *SoftwareX* **29**, 101987, DOI: 10.1016/j.softx.2024.101987 (2025).
4. C. L. Bassani, M. Engel, Kinetically Trapped Nanocrystals with Symmetry-Preserving Shapes. *Journal of the American Chemical Society* **147**, 9487–9495, DOI: 10.1021/jacs.4c17157 (2025).
5. M. W. Beims, P. G. Lind, T. Pöschel, T. Tél, M. Vince, D. E. Wolf, Imre M. Jánosi (1963–2023). *Chaos* **35**, 060401, DOI: 10.1063/5.0274421 (2025).
6. M. W. Beims, T. Pöschel, P. G. Lind, Special Issue: From Sand to Shrimps: In Honor of Professor Jason A. C. Gallas. *CHAOS* **35**, 070401, DOI: 10.1063/5.0285515 (2025).
7. A. Bezold, G. de Jesus Rodrigues, J. Vollhüter, O. Nagel, M. Köbrich, A. Stark, M. Mills, S. Neumeier, Influence of Fe additions on the property profile of high-strength CoNi-based superalloys. *Journal of Applied Physics* **137**, 195102, DOI: 10.1063/5.0268680 (2025).
8. P. K. Bommineni, J. Wang, N. Vogel, M. Engel, Entropic Trapping of Hard Spheres in Spherical Confinement. *Physical Review Letters* **134**, 198201, DOI: 10.1103/PhysRevLett.134.198201 (2025).
9. Z. Cheng, C. Shi, K. Zhao, M. Engel, M. R. Jones, Y. Han, Precision mapping of equilibrium disclination strain in pentagonally twinned nanostructures. *Science Advances* **11**, eaea9781, DOI: 10.1126/sciadv.aea9781 (2025).
10. O. D'Angelo, Q. Yu, T. Pöschel, Granular jamming and rheology in microgravity. *Soft Condensed Matter* **(in press)**, DOI: 10.48550/arXiv.2507.08674 (2025).
11. H. Götz, T. Pöschel, Shaping Softness from Hard Elements. *American Journal of Physics* **(in press)** (2025).

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13. W. Luo, E. Parteli, T. Pöschel, F. Fan, Inertial migration regimes of a neutrally buoyant sphere in pipe Poiseuille flow. *Journal of Fluid Mechanics* **(in press)**, DOI: 10.1017/jfm.2026.11211 (2025).
14. S. Mühlbauer, S. Strobl, T. Pöschel, Particle-based simulation of reactive open-boundary flows. *Results in Engineering* **(in press)**, DOI: 10.2139/ssrn.5732799 (2025).
15. S. Mühlbauer, S. Strobl, T. Pöschel, Particle-based simulation of reactive open-boundary flows. *Results in Engineering* **(in press)**, DOI: 10.2139/ssrn.5732799 (2025).
16. P. Müller, A. Panchenko, W. T. Ku, T. Pöschel, Particle size segregation in granular pipe flow. *Chaos* **35**, 043137, DOI: 10.1063/5.0239010 (2025).
17. L. Ortellado, A. Abate, A. Santarossa, L. R. Gómez, T. Pöschel, Principle of local symmetry in mixed-mode fracture. *Communications Physics* **8**, 252, DOI: 10.1038/s42005-025-02151-9 (2025).
18. A. N. Rayavarapu, N. Panchi, M. Engel, P. K. Bommineni, Formation of hexagonal binary crystals in additive hard disk mixtures. *Journal of Chemical Physics* **163**, 154503, DOI: 10.1063/5.0293041 (2025).
19. A. Santarossa, O. D'Angelo, A. Sack, T. Pöschel, All-terrain granular gripper. *Particuology* **104**, 283–288, DOI: 10.1016/j.partic.2025.07.006 (2025).
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21. C. A. del Valle, V. Angelidakis, S. Roy, J. D. Muñoz, T. Pöschel, SPIRAL: An efficient algorithm for the integration of the equation of rotational motion. *Computer Physics Communications* **297**, 109077, DOI: 10.1016/j.cpc.2023.109077 (2024).
22. C. A. del Valle, V. Angelidakis, S. Roy, J. D. Muñoz, T. Pöschel, Efficient numerical integration of rigid body dynamics. *EPJ Web of Conferences* **340**, 09017, DOI: 10.1051/epjconf/202534009017 (2025).
23. N. R. Varela-Rosales, M. Engel, Computational self-assembly of a six-fold chiral quasicrystal. *Soft Matter* **21**, 596–603, DOI: 10.1039/D4SM00933A (2025).
24. N. R. Varela-Rosales, M. Engel, Solid-angle nearest-neighbor method for size-disperse systems of spheres. *Journal of Chemical Physics* **163**, 224128, DOI: 10.1063/5.0295910 (2025).
25. J. Wang, J. Martín-González, L. J. Römling, S. Englisch, C. F. Mbah, P. Bommineni, E. Spiecker, M. Engel, N. Vogel, Breakdown of Magic Numbers in Spherical Confinement. *ACS Nano* **19**, 11702–11711, DOI: 10.1021/acsnano.4c11099 (2025).
26. T. Wen, S. Roy, T. Pöschel, G. Xu, X. Zeng, Froude scaling of rotating intrusion drag in microgravity regolith. *Physical Review E* **(in press)** (2025).
27. H. Xiao, H. Torres, A. Sack, T. Pöschel, Locomotion of a scallop-inspired swimmer in granular matter. *Physical Review Applied* **24**, 034049, DOI: 10.1103/52rv-8mpz (2025).

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28. V. Angelidakis, M. Blank, E. J. R. Parteli, S. Roy, D. S. Nasato, H. Xiao, T. Pöschel, in *Progress in Powder Based Additive Manufacturing*, ed. by D. Drummer, M. Schmidt (Springer, Cham, 2025), pp. 263–283, DOI: 10.1007/978-3-031-78350-0_13.
29. C.-J. Hsieh, *Formation of Nanocrystals with High-Index Facets using Kinetic Monte Carlo Simulations*, Master's thesis at Friedrich-Alexander-Universität Erlangen-Nürnberg (openFAU, Proceedings of the Institute for Multiscale Simulation, Vol. 47, 2025), DOI: 10.25593/open-fau-1600.
30. J. Pollet, *Mechanical properties of jammed granulate metamaterials*, Master's thesis at Friedrich-Alexander-Universität Erlangen-Nürnberg (openFAU, Proceedings of the Institute for Multiscale Simulation, Vol. 49, 2025), DOI: 10.25593/open-fau-1775.
31. S. Roy, *Simulation of Granular Flows: Insights into Additive Manufacturing, Rheology, and Capillary Force*, Habilitation thesis at Friedrich-Alexander-Universität Erlangen-Nürnberg (openFAU, Proceedings of the Institute for Multiscale Simulation, Vol. 50, 2025), DOI: 10.25593/open-fau-2401.

32. A. A. Santarossa, *Experimental Research and Enhancement of Granular Gripping Systems*, PhD thesis at Friedrich-Alexander-Universität Erlangen-Nürnberg (openFAU, Proceedings of the Institute for Multiscale Simulation, Vol. 53, 2025), DOI: 10.25593/open-fau-2015.

33. F. Tomazic, *Particle Self-Assembly into Complex Suprastructures: The Role of Shape and Interaction*, PhD thesis at Friedrich-Alexander-Universität Erlangen-Nürnberg (openFAU, Proceedings of the Institute for Multiscale Simulation, Vol. 54 (in press), 2025), DOI: 10.25593/open-fau-2091.

34. D. E. Wolf, T. Pöschel, *Fractal packing of nanomaterials*, In: *Packing Problems in Soft Matter Physics: Fundamentals and Applications*, Chan, Ho-Kei Chan (Eds.), Hutzler, Stefan, (Eds.), Mughal, Adil, (Eds.), O'Hern, Corey S., (Eds.), Wang, Yujie, (Eds.), Weaire, Denis, (Eds.), pp. 517–541, 2025, DOI: 10.1039/9781837673940-00517

Submitted manuscripts

35. V. Marzulli, M. A. Velasco, A. Sack, F. Cafaro, T. Pöschel, Quasi-static cyclic penetration process in granular materials: A comparative study. *International Journal for Numerical and Analytical Methods in Geomechanics* **(submitted)** (2025).

36. S. Mühlbauer, T. Pöschel, Geometry Optimization of Open-Cell Metal Foam Catalytic Carriers. *Chemical Engineering Science* **(submitted)** (2025).

37. S. Mühlbauer, T. Pöschel, Multiscale Simulation of Optimized Open-cell Metal Foam Catalysts. **(submitted)** (2025).

38. S. Mühlbauer, S. Strobl, M. Coleman, T. Pöschel, Simulation of Catalytic Reactions in Open-cell Foam Structures. *Chemical Engineering Science* **(submitted)**, DOI: 10.1016/j.ces.2026.123489 (2025).

39. H. Rahim, T. Pöschel, S. Roy, Dilatancy-induced surface deformation in dense cohesive granular media. *Physics of Fluids* **(submitted)**, 033305, DOI: 10.48550/arXiv.2601.01172 (2025).

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42. H. Xiao, J. Wang, A. Sack, R. Stannarius, T. Pöschel, Reciprocal swimming in viscoelastic granular hydrogels. *Journal of Fluid Mechanics* **(submitted)**, DOI: 10.48550/arXiv.2510.16586 (2025).

Book Series: Proceedings of the Institute for Multiscale Simulation

The Institute for Multiscale Simulation (MSS) has launched the book series *Proceedings of the Institute for Multiscale Simulation* with FAU's publishing house openFAU. The series is dedicated to publishing doctoral dissertations, habilitation theses, outstanding selected student works–including Bachelor's and Master's theses–as well as further scholarly contributions originating from the Institute.

The central aim of this initiative is to make these works accessible to a broader audience and to provide them with the visibility they deserve in recognition of their scientific quality. In particular, the series highlights exceptional student research, demonstrating the high academic standards and innovative spirit cultivated at MSS. At the same time, it serves as an inspiration and point of reference for prospective Bachelor's and Master's students, offering concrete examples of excellent theses and showcasing the diverse research opportunities available at the Institute. By presenting these works in a professional and openly accessible format, the series seeks not only to disseminate knowledge, but also to attract and motivate talented students to pursue their own research projects, e.g. Master's theses, at MSS.

The volumes published to date are listed below.

Simon Renard: *Kritische Parameter der vertikalen Oszillation für das Einsetzen granularer Konvektion.*
Staatsexamensarbeit
Proceedings of the Institute for Multiscale Simulation, Vol. 1 (2000)
DOI: 10.25593/open-fau-766

Gregor Mückl: *Molekulardynamik dichter Granulate.*
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Dominik Krengel: *Pattern formation in a horizontally vibrated granular submonolayer.*
Diploma thesis
Proceedings of the Institute for Multiscale Simulation, Vol. 3 (2012)
DOI: 10.25593/open-fau-720

Britt Michelsen: *Validation of Dune Simulations using OpenFOAM.*
Bachelor's thesis
Proceedings of the Institute for Multiscale Simulation, Vol. 4 (2012)
DOI: 10.25593/open-fau-788

Laura Steub: *Hysteretischer Übergang zwischen Fluidisierungsmoden in horizontal angeregtem Granulat.*
Bachelor's thesis
Proceedings of the Institute for Multiscale Simulation, Vol. 5 (2014)
DOI: 10.25593/open-fau-772

Felix Verbücheln: *Optimierung der Textur granulatdurchströmter Röhren hinsichtlich des Massenflusses.*
Master's thesis
Proceedings of the Institute for Multiscale Simulation, Vol. 6 (2014)
DOI: 10.25593/open-fau-767

Jonas Rathke: *Damping an oscillation with granular dampers.*
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Mohammad Hassan Nadjafabadi Farahani: *Simulation based optimization of granular damping devices.*
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Dominik Werner: *Bestimmung der Eigenschaften eines selbstoptimierenden granularen Dämpfers mittels numerischer Simulation.*
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Daniel Kreitmeir: *Statistische Untersuchung der Fairness einer Münze bei asymmetrischer Massenverteilung.*
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Nydia Roxana Varela Rosales: *Classification of Particle Environments in Simulation Data with Machine Learning.*
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Carina Rabe: *Einfluss der Partikelform auf die elektrische Leitfähigkeit granularer Packungen.*
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Niklas Tobie: *Kann man die Temperatur von Wasser hören?*
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Abeer Al-Ani: *Homogenization of Fluid Driven Granular Pipe Flow.*
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Kamilia Gabaidullina: *Coarse-grained computational modeling of the spray-drying process for the fabrication of colloidal supraparticles.*
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Navid Panchi: *Bayesian Optimization for Diffraction Profile Modeling.*
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Deniz Fakioglu: *Automatisierung eines Elektroimpedanz Tomographen unter Verwendung von Robotik und Digitaler Bildverarbeitung.*
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Bijohn Chandrew Aseervatham: *The Dzhanibekov-Effect - an intuitive theoretical and practical approach to understand the rotation of rigid bodies about their intermediate axis.*
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Frederik Keil: *A Tool to Analyze Random Packings of Meissner Tetrahedra.*
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Yasmin Gerlach: *Tomographische Analyse von Pigmentsuspensionen in porösen Strukturen für kosmetische Anwendungen.*
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Prashanth Prakash Kamath: *Simulation of Critical Settling Velocity of Gas Hydrate Slurries.*
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Qing Yu: *Granular Jamming Transition versus Gravitational Acceleration.*
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Valentin Hartinger: *Kann man die Temperatur von Wasser hören?*
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Harsha Namdeo: *Reconstruction of Pair Potentials from Nanoparticle Configurational Data.*
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Nadja Al Akkam: *The Rheology of Lunar Regolith and its Simulants.*
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Daniel Adam: *Implementation of a 3D phantom generator for the acquisition of validation data for EIT image reconstruction.*
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Chia-Jui Hsieh: *Formation of Nanocrystals with High-Index Facets using Kinetic Monte Carlo Simulations.*
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Julian Pollet: *Mechanical properties of jammed granulate metamaterials.*
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Sudeshna Roy: *Simulation of Granular Flows: Insights into Additive Manufacturing, Rheology, and Capillary Force.*
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Manuel Baur: *Röntgen Radiographie granularer Systeme - Dichte und Dynamik der Teilchen.*
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Theresa Rogge: *Simulation des Ablagerungsprozesses von Metallpulver für SLM Prozesse.*
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Angel Santarossa: *Experimental research and enhancement of granular gripping systems.*
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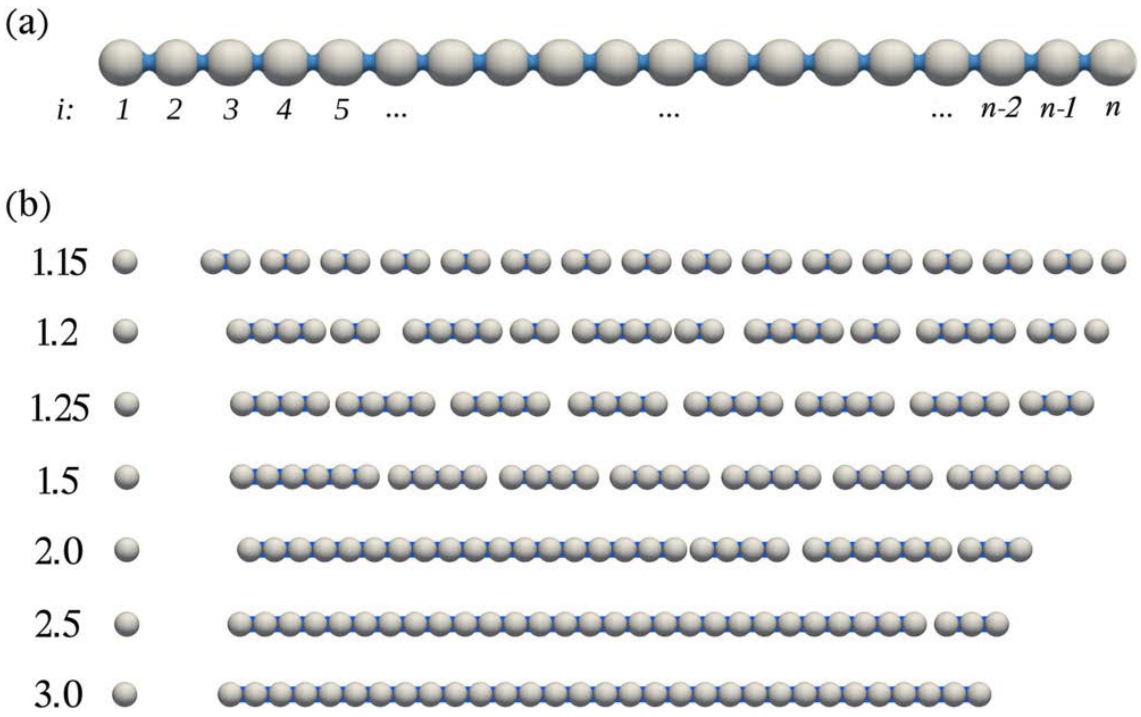
Federico Tomazic: *The Role of Shape and Interaction*
PhD thesis
Proceedings of the Institute for Multiscale Simulation, Vol. 54 (2025)
DOI: 10.25593/open-fau-2091

Cascade crack in chain of beads

Meysam Bagheri, Thorsten Pöschel

Abstract:
We consider a homogeneous chain of spheres linked by liquid bridges under tension. The rupture of a single liquid bridge leads to a fragmentation cascade driven by the inverse relation between the capillary force and the sphere distances. The initial length of the liquid bridges determines the number and size of the fragments and the velocity of the fragmentation front.



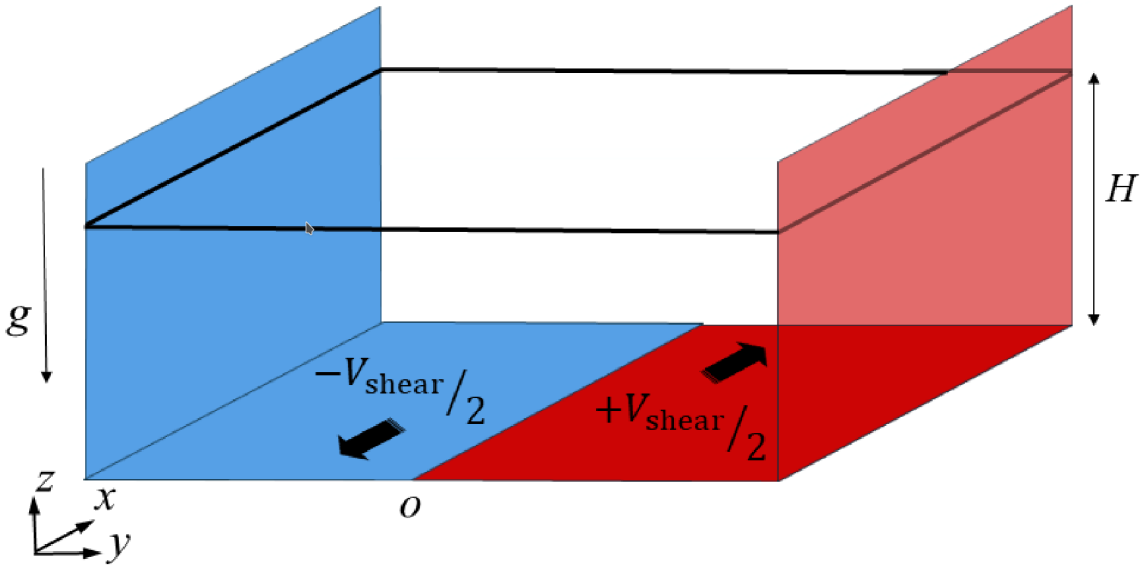
(a) Initial configuration of the chain; (b) final configurations obtained for a chain of $n = 32$ spheres for $\alpha \in \{1.15, 1.2, 1.25, 1.5, 2, 2.5, 3\}$.

M. Bagheri, T. Pöschel, Cascade crack in chain of beads. *Physical Review E* **112**, 045414, DOI: 10.1103/hzs3-8ffk (2025).

Comparison of bulk properties of wet granular materials using different capillary force approximations

Meysam Bagheri, Sudeshna Roy, Thorsten Pöschel

Abstract:
We perform Discrete Element Method simulations of wet granular matter in a split-bottom shear cell. To calculate the capillary forces from the liquid bridges between the grains, we used three different approximations. The simulations of the shear cell showed a linear increase in bulk cohesion with the surface tension of the liquid, consistently for all approximations. However, the macroscopic friction coefficient shows only a weak dependence on surface tension.



Linear split-bottom shear cell.

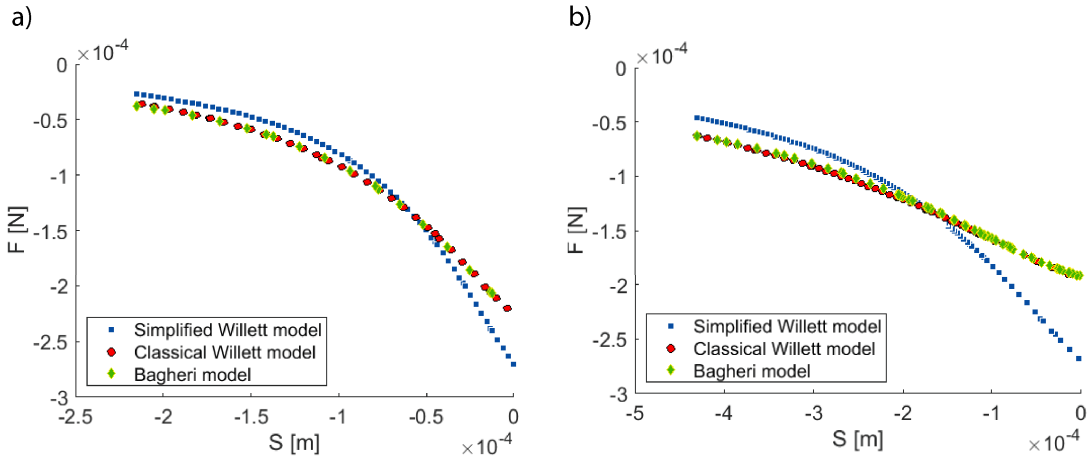
M. Bagheri, S. Roy, T. Pöschel, Comparison of bulk properties of wet granular materials using different capillary force approximations. *EPJ Web of Conferences* **334**, 01002, DOI: 10.1051/epjconf/202533401002 (2025).

Discrete element simulations of particles interacting via capillary forces using MercuryDPM

Meysam Bagheri, Sudeshna Roy, Thorsten Pöschel

Abstract:

We present the implementation of two advanced capillary bridge approximations within the Discrete Element Method (DEM) framework of the open-source code MercuryDPM. While MercuryDPM already includes a simplified version of the Willett approximation, our work involves implementing both the classical Willett approximation and the recently published Bagheri approximation in MercuryDPM. Through detailed descriptions and illustrative simulations using a two-particle collision model, we demonstrate the enhanced accuracy and capabilities of these approximations in capturing the complex dynamics of wet granular matter.



Capillary force, F_c, exerted by a liquid bridge as a function of the particle distance for solutions obtained from the fitted equations of the simplified Willett approximation, the classical Willett approximation, and the Bagheri approximation for liquid bridge volumes (a) $V = 10\,\text{nl}$ and (b) $V = 80\,\text{nl}$, for particle sizes of $0.5\,\text{mm}$ and $1\,\text{mm}$.

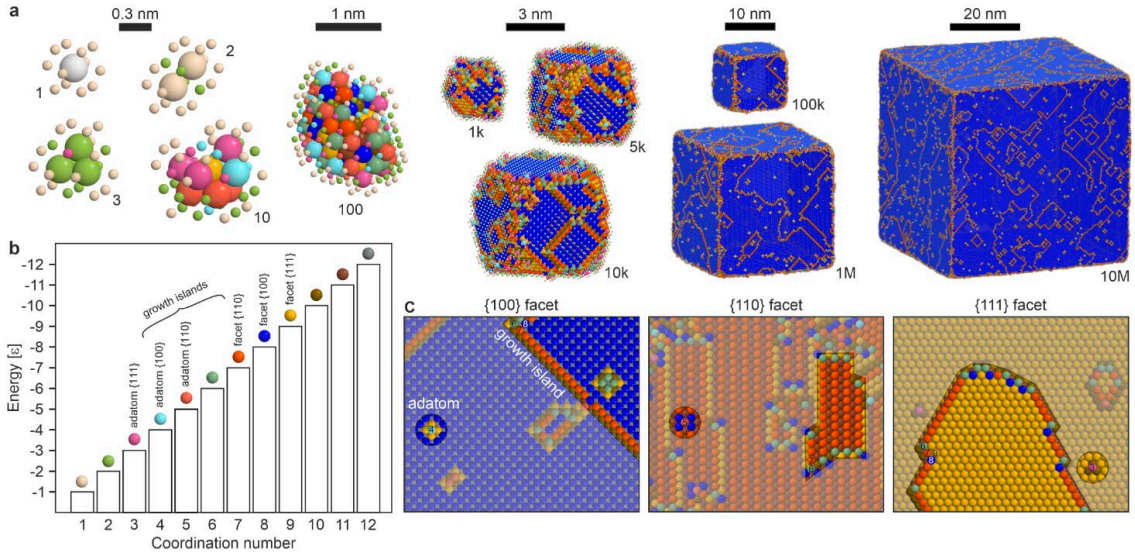
M. Bagheri, S. Roy, T. Pöschel, Discrete Element Simulations of particles interacting via capillary forces using MercuryDPM. *SoftwareX* **29**, 101987, DOI: 10.1016/j.softx.2024.101987 (2025).

Kinetically trapped nanocrystals with symmetry-preserving shapes

Carlos L. Bassani, Michael Engel

Abstract:

The shape of nanocrystals is crucial in determining their surface area, reactivity, optical properties, and self-assembly behavior. Traditionally, shape control has been achieved through empirical methods, highlighting the need for a more refined theoretical framework. A comprehensive model should account for the kinetic factors at distinct stages of the shape formation process to identify the key determinants of nanocrystal morphology. By modulating kinetics at terraces, ledges, and kinks, we reveal that the primary factors are the adatom nucleation energies and the geometry of growth islands. Transient sites dominate the growth process, leading to kinetically trapped, metastable shapes. We illustrate these concepts with face-centered cubic nanocrystals, demonstrating diverse shape evolutions, including surface roughening and the preservation of crystal symmetry in cubes, octahedra, rhombic dodecahedra, and their truncated variants. This study reveals the mechanisms driving the formation of cubic nanocrystal shapes and offers guidance for their precise synthesis.



Kinetic Monte Carlo simulation to predict nanocrystal shapes. (a) Exemplary growth trajectory of fcc NC into a cube. Large spheres represent atoms and small spheres represent growth sites. The inset numbers represent the numbers of atoms composing the NC. The scale bars are for a lattice parameter of 0.4 nm, representative of noble metals. (b) Energy scales with coordination number. Coordination numbers relate to NC surface topology features, including adatoms, growth islands, facets, and bulk atoms. (c) Exemplary adatoms and growth islands in primary facets. Number insets represent coordination numbers.

C. L. Bassani, M. Engel, Kinetically Trapped Nanocrystals with Symmetry-Preserving Shapes. *Journal of the American Chemical Society* **147**, 9487–9495, DOI: 10.1021/jacs.4c17157 (2025).

Imre M. Jánosi (1963–2023)

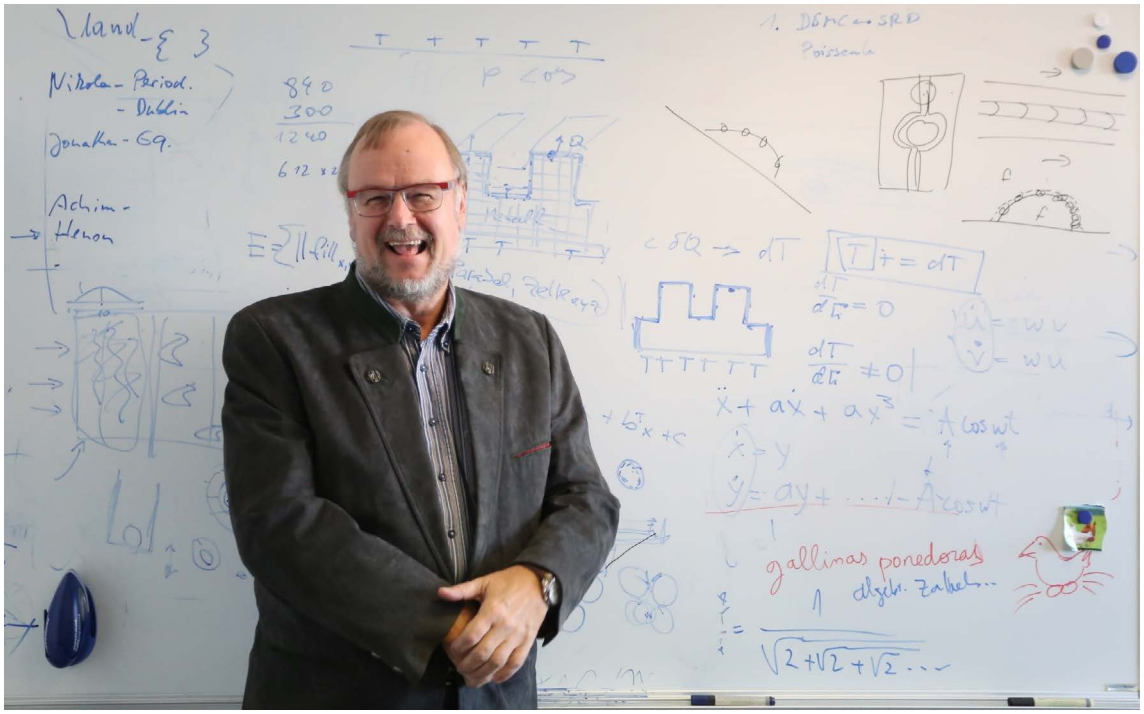
Marcus W. Beims, Pedro G. Lind, Thorsten Pöschel, Támas Tél, Miklós Vincze, Dietrich E. Wolf

Imre Jánosi and Jason Gallas in February 2019 at the Max-Planck-Institute for the Physics of Complex Systems in Dresden. Photo: ©Marcia Gallas

M. W. Beims, P. G. Lind, T. Pöschel, T. Tél, M. Vince, D. E. Wolf, Imre M. Jánosi (1963–2023). *Chaos* **35**, 060401, DOI: 10.1063/5.0274421 (2025).

From Sand to Shrimps: In Honor of Professor Jason A. C. Gallas
Special Issue - Chaos 35
Marcus Beims, Thorsten Pöschel, Pedro G. Lind as Guest Editors

This Focus Issue is a tribute to Jason A. C. Gallas and his outstanding career as a scientist. Gallas coined the term “shrimps” to name ubiquitous structures he found in parameter space, and which are now known to exist in many nonlinear systems. His work impacted several fields, ranging from climate and geophysics to quantum optics and medicine. The contributions to the issue will include both the theoretical topics Gallas worked on, as well as the different applied fields he approached during his scientific career.



Professor Jason A. C. Gallas, during one of his visits to Germany (Erlangen, 2014).

M. W. Beims, T. Pöschel, P. G. Lind, Special Issue: From Sand to Shrimps: In Honor of Professor Jason A. C. Gallas. *CHAOS* **35**, 070401, DOI: 10.1063/5.0285515 (2025).

Influence of Fe additions on the property profile of high-strength CoNi-based superalloys

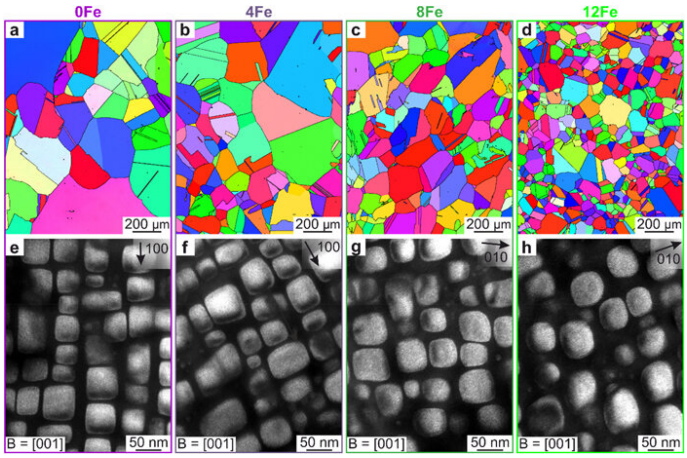
Andreas Bezold, Geovane de Jesus Rodrigues, Jan Vollhüter, Oliver Nagel, Manuel Köbrich, Andreas Stark, Michael J. Mills, Steffen Neumeier

Abstract:

CoNi-based superalloys offer excellent high-temperature properties; yet Co is also a strategic alloying element, and its content should only be as high as necessary. This study investigates Fe as a partial substitute for Co to reduce costs while evaluating its impact on mechanical properties. To this end, we systematically examine the effect of Fe substitution on thermophysical properties, microstructure, partitioning behavior, lattice misfit, yield strength, and creep performance of three polycrystalline CoNi-based superalloys derived from CoWAlloy1 (Co–32Ni–12Cr–6Al–3W–2.5Ti–1.5Ta–0.4Si–0.1Hf–0.08B, all in at. %). In these alloys, 4, 8, and 12 at. % Co is replaced by Fe.

Increasing Fe content results in a gradual reduction of the solvus, solidus, and liquidus temperatures by 3.0, 1.9, and 1.4 °C per at. % Fe, respectively. The γ' volume fraction and the lattice misfit decrease by approximately 0.7 % and 0.01 %, respectively, per at. % Fe substitution for Co. Fe predominantly partitions to the γ matrix, enhancing the partitioning of Co and Ni while reducing that of Al, Cr, and Ta, with no significant effect on Ti and W.

Substituting Co with Fe moderately reduces yield and creep strength, primarily due to the decreasing γ' volume fraction and a transition in the dominant deformation mechanisms from stacking-fault shearing and microtwinning to matrix-based deformation with increasing Fe content. Beneficial elemental segregation behavior and localized phase transformations along creep-induced stacking faults remain active in alloys with high Fe content. These findings highlight the potential of Fe alloying to reduce costs while maintaining high-temperature strength in CoNi-based superalloys.



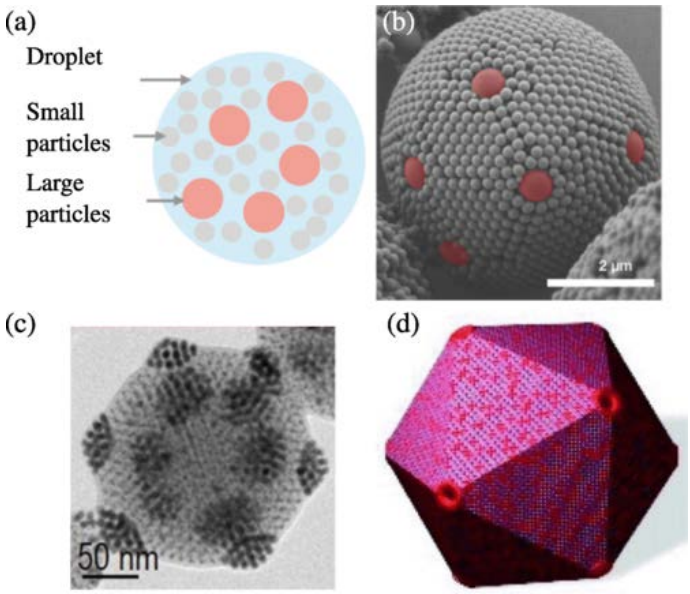
Microstructures of (a) and (e) 0Fe, (b) and (f) 4Fe, (c) and (g) 8Fe, and (d) and (h) 12Fe. (a)–(d) EBSD maps of the grain structure and (e)–(h) dark-field TEM images of the γ/γ'microstructure taken in two-beam conditions with g=100 and 010.

A. Bezold, G. de Jesus Rodrigues, J. Vollhüter, O. Nagel, M. Köbrich, A. Stark, M. Mills, S. Neumeier, Influence of Fe additions on the property profile of high-strength CoNi-based superalloys. *Journal of Applied Physics* **137**, 195102, DOI: 10.1063/5.0268680 (2025).

Entropic Trapping of Hard Spheres in Spherical Confinement

Praveen K. Bommineni, Junwei Wang, Nicolas Vogel, Michael Engel

Abstract:
Monodisperse spherical colloidal particles confined within emulsion droplets can crystallize into icosahedral clusters. Experimentally, it was observed that a few large colloidal particles added as defects preferentially migrate to the vertices of the icosahedral clusters. To understand this structure formation phenomenon, we simulate the confined self-assembly of hard spheres in the presence of a small number of larger particles. The results demonstrate that large spheres are significantly influenced by concentric shells of small spheres near the crystallization transition. Entropic forces drive the large spheres to the cluster surface, where they settle into free-energy minima at the icosahedron vertices. Notably, the addition of twelve large spheres results in the formation of a perfect icosahedral frame.
Free-energy calculations via umbrella sampling are used to quantify this process and show that both the migration to the cluster surface and the trapping at the vertices, with trapping strengths of multiple $k_{\mathrm{B}}T$, result from free-energy minimization. Moreover, our study reveals that the crystallization pathway and dynamics of large spheres are consistent across different systems, suggesting the robustness of entropic trapping.



Examples demonstrating templating of icosahedral clusters. (a) Schematic representation of a mixture of many small particles and a few large particles in an emulsion droplet. (b) Scanning electron microscopy observation of the successful diffusion of five large polystyrene colloidal particles (red) into the vertices of the icosahedral cluster. (c) Coassembly of two types of grafted nanoparticles into a patchy icosahedron in a drying emulsion droplet. Reprinted with permission from AAAS. (d) Molecular crystallization and segregation of anionic and cationic surfactants. Copyright 2004 by the National Academy of Sciences.

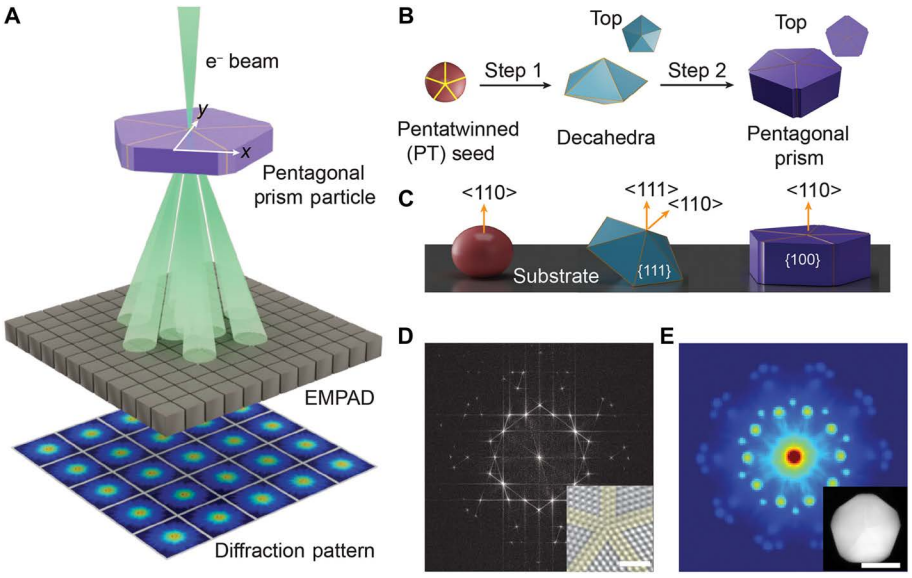
P. K. Bommineni, J. Wang, N. Vogel, M. Engel, Entropic Trapping of Hard Spheres in Spherical Confinement. *Physical Review Letters* **134**, 198201, DOI: 10.1103/PhysRevLett.134.198201 (2025).

Precision mapping of equilibrium disclination strain in pentagonally twinned nanostructures

Zhihua Cheng, Chuqiao Shi, Kaijie Zhao, Michael Engel, Matthew R. Jones, Yimo Han

Abstract:

Pentatwinned nanostructures are key to understanding the mechanical, chemical, and structural behavior of nanomaterials owing to their unique fivefold symmetry and lattice strain from a 7.35° disclination gap between 111 twin boundaries. However, the precise equilibrium strain distributions have remained unclear because of heterogeneity among individual particles, requiring statistical analysis across large sample populations. Here, we use nanobeam four-dimensional scanning transmission electron microscopy (4D-STEM) to extract averaged strain profiles from uniformly sized, shape-identical particles, achieving high-resolution, statistically robust insights beyond single-particle noise. The strain profiles reveal how tensile, shear, and rotational components collectively compensate for the angular deficit, with particle shape–dependent local variations highlighting the importance of morphological control in synthesis. By integrating in situ heating with 4D-STEM, we captured a previously unobserved strain relaxation pathway involving the formation of periodic partial dislocations that stabilizes the strain-relieved equilibrium state. This study establishes a quantitative framework for equilibrium strain in fivefold-twinned nanostructures and offers strain engineering strategies for tailored properties. Precision mapping of pentatwinned nanostructures reveals equilibrium strain distribution across fivefold twin boundaries.



Experimental design for precise mapping of strain with 4D-STEM. (A) Schematic illustration of 4D-STEM with x and y axes marked by white arrows. The x axis is parallel to the edge of the domain, whereas the y axis is perpendicular to it. A similar choice of axes is applied to all domains. (B) Schematic illustration of the synthesis of pentagonal prism particles from PT seeds, with decahedron particles as an intermediate product. (C) Possible orientations of particles on the substrate after drop-casting them on the TEM grid, showing that small PT seeds and pentagonal prism particles are more likely to orient along the $\langle 110 \rangle$ zone axis, whereas decahedron particles are more likely to align along the $\langle 111 \rangle$ zone axis. (D) FFT image and atomic-resolution image (inset) and (E) the cepstrum image of corresponding pentagonal prism NPs (inset), showing that the alignment of the $\langle 110 \rangle$ zone axis can substantially increase the precision of our analyses in both real and reciprocal spaces. Scale bars: 5 nm (D) and 50 nm (E).

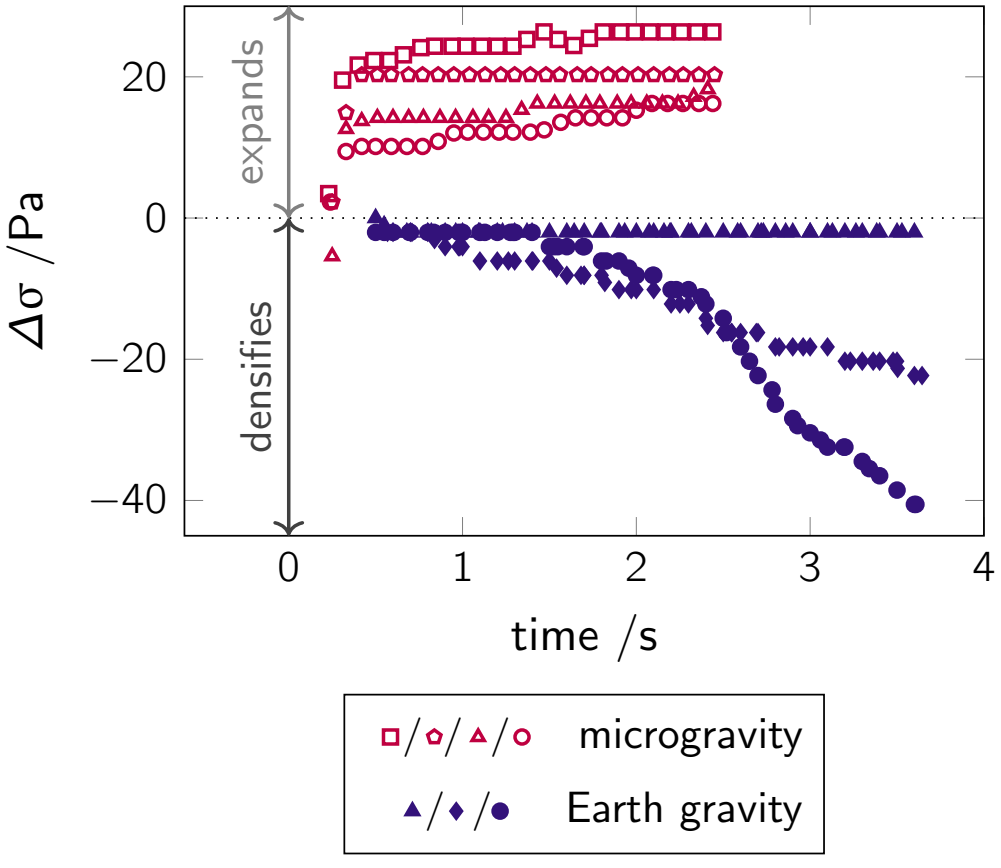
Z. Cheng, C. Shi, K. Zhao, M. Engel, M. R. Jones, Y. Han, Precision mapping of equilibrium disclination strain in pentagonally twinned nanostructures. *Science Advances* **11**, eaea9781, DOI: 10.1126/sciadv.aea9781 (2025).

Granular jamming and rheology in microgravity

Olfa D'Angelo, Qing Yu, Thorsten Pöschel

Abstract:

Understanding how granular materials behave in low gravity is crucial for planetary science and space exploration. It can also help us understand granular phenomena usually hidden by gravity. On Earth, gravity dominates granular behavior, but disentangling its role from intrinsic particle interactions is challenging. We present a series of compression and shear experiments conducted in microgravity using the Center of Applied Space Technology and Microgravity (ZARM) drop tower and GraviTower Bremen (GTB). Our in-house developed experimental setup enables precise measurement of packing density and in-situ shear stress via a Taylor-Couette rheometer. We find that the jamming transition occurs at lower packing density in microgravity than on Earth, confirming that gravity promotes densification. Rheological measurements further reveal that in microgravity, the lack of a secondary force field and predominance of cohesive interparticle forces increase the stress needed for granular media to flow. These findings highlight gravity's dual role in enhancing both compaction and flow, and demonstrate the need for tailored granular models, valid in low- and microgravity environments.



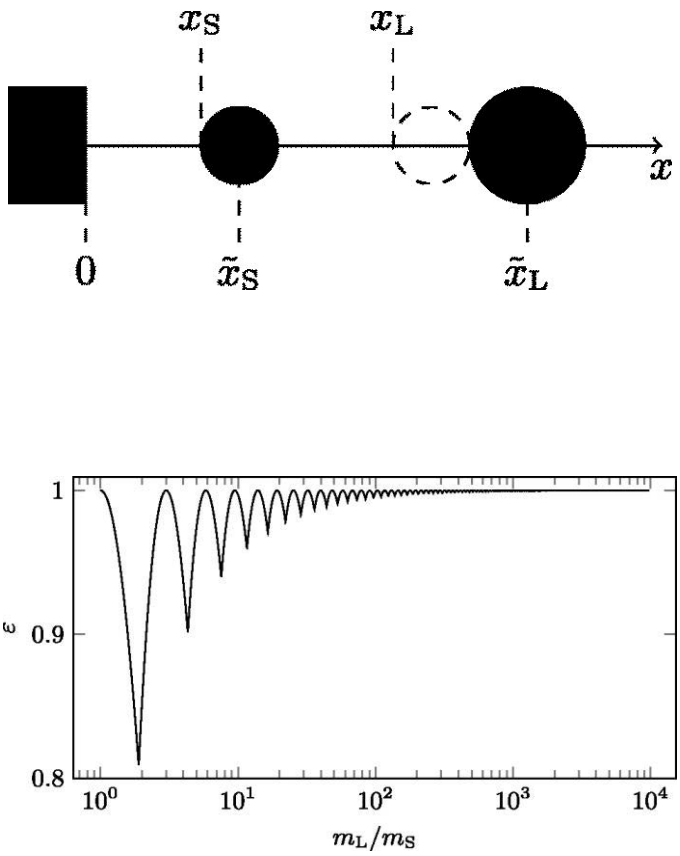
Evolution of relative normal pressure in Earth- and microgravity. The normal pressure change, $\Delta\sigma$, applied by the granular media to the piston, is plotted as a function of time for all experiments with small particles (d = 80 μm). Microgravity experiments were conducted in the GTB. Different symbols represent the different repetitions of the experiment.

O. D'Angelo, Q. Yu, T. Pöschel, Granular jamming and rheology in microgravity. *Soft Condensed Matter* **(in press)**, DOI: 10.48550/arXiv.2507.08674 (2025).

Shaping Softness from Hard Elements

Holger Götz, Thorsten Pöschel

Abstract:
We consider a particle moving toward a solid wall, with a second particle of much smaller mass positioned between them. Although both the particle and the wall are perfectly rigid—implying instantaneous elastic collisions—the trajectory of the larger particle follows that of motion in a soft repulsive potential.



Upper figure: Sketch of the system and introduction of the variables. The larger particle with radius R_L at position $\tilde{x}_L$ moves toward the solid wall and hits the small sphere with radius R_S, which rests at $\tilde{x}_S$. The transformation in Eq. (1) significantly simplifies the notation, as the collision criteria for R_L and R_S no longer involve the radii. Diagram: The coefficient of restitution as a function of the mas ratio m_L/R_S. For particular values, $\varepsilon = 1$ is achieved, due to complete momentum transfer in the last collision, n, i.e., $\dot{x}_S^{(n)} = 0$.

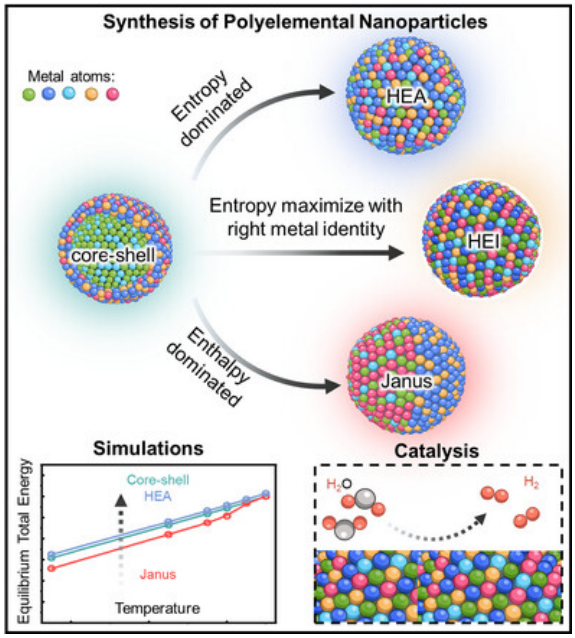
H. Götz, T. Pöschel, Shaping Softness from Hard Elements. *American Journal of Physics* **(in press)** (2025).

A Programmable Nanoparticle Conversion Pathway to Monodisperse Polyelemental High Entropy Alloy, Intermetallic, and Multiphase Nanoparticles

Nabojit Kar, Alberto Leonardi, Maximilian McCoy, Rukshanthan Selvaraj, Sara E. Skrabalak

Abstract:

Polyelemental nanoparticles (PE NPs), those consisting of four or more elements, exhibit unique properties from synergistic compositional effects. Examples include high entropy alloys, high entropy intermetallics, and multiphase types, including Janus and core-shell architectures. Although colloidal syntheses offer excellent structural control for mono- and bi-elemental compositions, achieving the same control for PE NPs remains challenging. Here, this challenge is addressed with a NP conversion strategy wherein different types of PE NPs – including high entropy alloy, high entropy intermetallic, and multiphase Janus nanoparticles – are achieved through thermal transformation of readily synthesized colloidal core-shell NPs. Through systematic variations in stoichiometry and metal identity to the core-shell precursor NPs, along with atomistic simulations that probe phase stabilities, we deduce that the final mixing states of the various NPs are governed by the balance between the enthalpy and entropy of mixing. Moreover, our annealing method allows us to trap NPs at intermediate states of mixing, creating distinct surface ensembles that were evaluated as catalysts for the hydrogen evolution reaction. This study is the first, to our knowledge, to report colloidally derived precursor NPs enabling the synthesis of all types of PE NPs in a single process. This NP conversion strategy offers a general route to diverse PE NPs.



Polyelemental nanoparticles, composed of four or more elements, encompass high-entropy alloys, high-entropy intermetallics, and multiphase structures such as Janus and core-shell architectures. These nanoparticles were obtained through the thermal transformation of colloidally synthesized core-shell nanoparticles. Systematic variations in stoichiometry and metal identity of the precursor nanoparticles, combined with atomistic simulations evaluating phase stability, reveal that the final mixing states of these nanoparticles are dictated by the interplay between enthalpy and entropy of mixing.

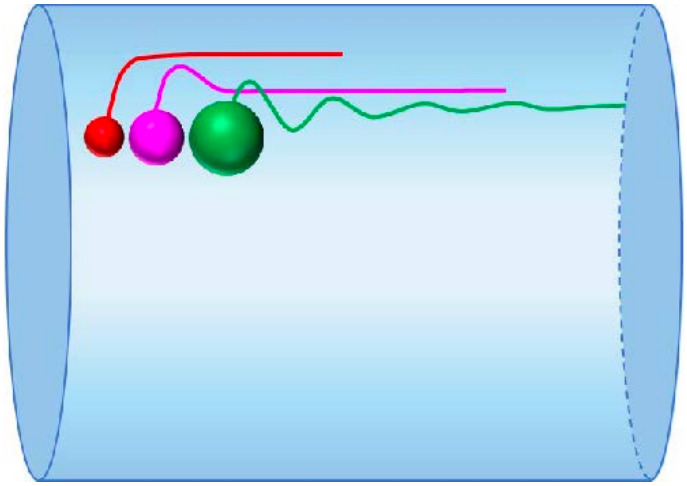
N. Kar, A. Leonardi, M. McCoy, R. Selvaraj, S. E. Skrabalak, A Programmable Nanoparticle Conversion Pathway to Monodisperse Polyelemental High Entropy Alloy, Intermetallic, and Multiphase Nanoparticles. *Angewandte Chemie - International Edition* **64**, e202505523, DOI: 10.1002/anie.202505523 (2025).

Inertial migration regimes of a neutrally buoyant sphere in pipe Poiseuille flow

Weile Luo, Eric J.R. Parteli, Thorsten Pöschel, Fengxian Fan

Abstract:

The inertial migration of a neutrally buoyant sphere in pipe Poiseuille flow is examined using numerical simulations. Three migration regimes are observed with increasing Reynolds number (Re): monotonic convergence to the equilibrium position, overshooting convergence and damped oscillations. The critical Reynolds numbers separating these regimes decrease with the sphere-to-pipe diameter ratio, d/D. The axial entry length, L_p , required for the sphere to reach equilibrium decreases with both Re and d/D in the monotonic regime, but increases in the oscillatory regime. These results elucidate the dynamics of inertial migration and inform strategies for manipulating particles in confined, particle-laden flows.

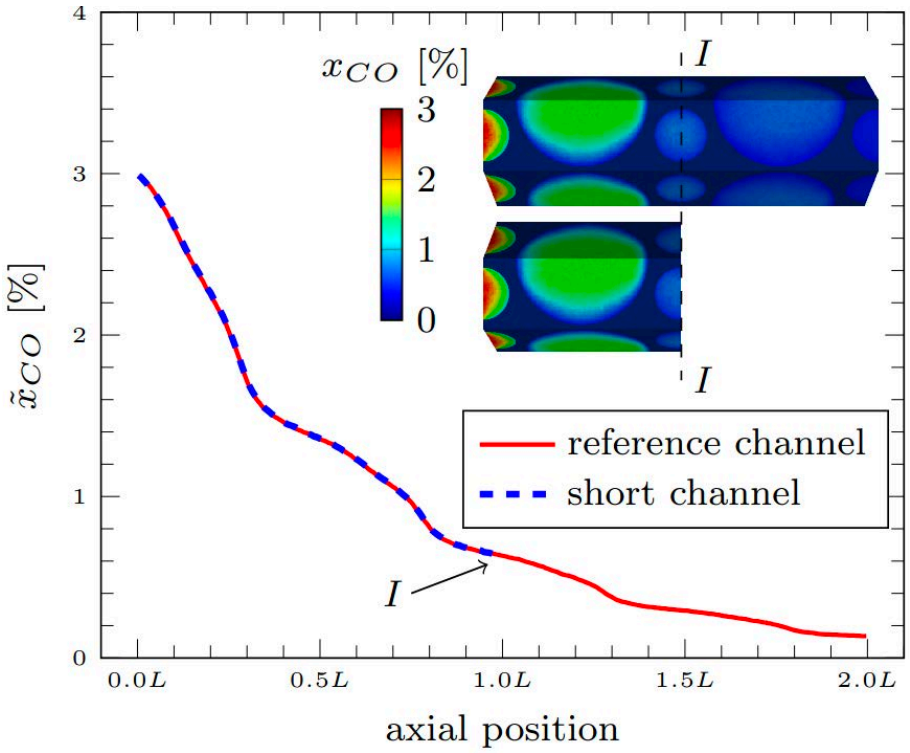


W. Luo, E. Parteli, T. Pöschel, F. Fan, Inertial migration regimes of a neutrally buoyant sphere in pipe Poiseuille flow. *Journal of Fluid Mechanics* **(in press)**, DOI: 10.1017/jfm.2026.11211 (2025).

Particle-based simulation of reactive open-boundary flows

Sebastian Mühlbauer, Severin Strobl, Thorsten Pöschel

Abstract:
A particle-based method is introduced for numerically stable simulations of open-boundary flows involving volume-conserving chemical reactions. The method reproduces the behavior of heteroge- neous catalytic systems with high accuracy when validated against high-fidelity reference simulations and delivers identical results at significantly higher computational e!ciency. Owing to its general formulation, the approach is readily applicable to a wide range of reactive flow problems, including catalytic processes, electrochemical systems, and microreactor simulations.



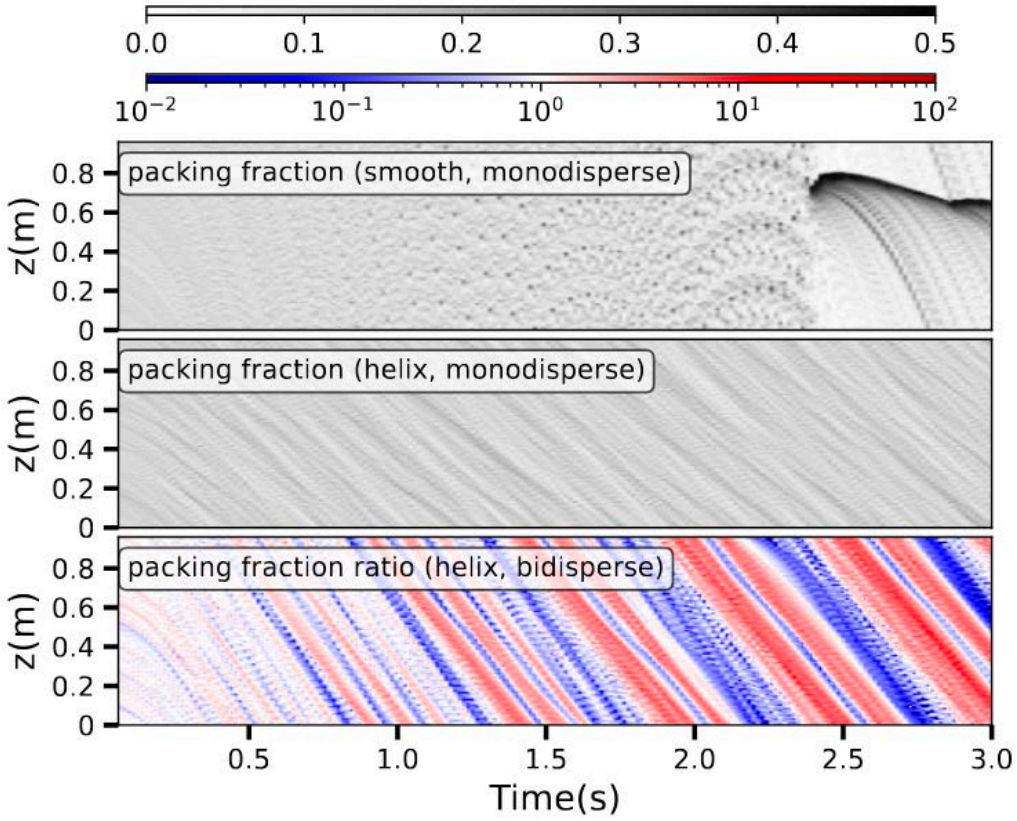
Particle flow rate of CO normalized by the total particle flow rate for an open-cell porous foam structure. The inset shows the CO mole fraction for the two systems considered.

S. Mühlbauer, S. Strobl, T. Pöschel, Particle-based simulation of reactive open-boundary flows. *Results in Engineering* **(in press)**, DOI: 10.2139/ssrn.5732799 (2025).

Particle size segregation in granular pipe flow

Patric Müller, Artem Panchenko, Wing To Ku, Thorsten Pöschel

Abstract:
The flow of particles through pipes is relevant in many in- dustrial applications. This type of granular flow is natu- rally unstable, causing density waves and pressure fluctu- ations that can damage the pipe walls. Traditional meth- ods to stabilize the flow typically require external energy inputs. Recently a passive solution has been suggested, where helical textures on the inner wall of the pipe homog- enize the flow and prevent the formation of particle plugs without external energy. So far, this idea has only been developed for the flow of monodisperse granulates (uni- form particle sizes). Utilizing numerical simulations, the current study extends these findings to bidisperse granu- lates (varying particle sizes), examines effects of particle size segregation and, thus, brings the research idea closer to practical application.



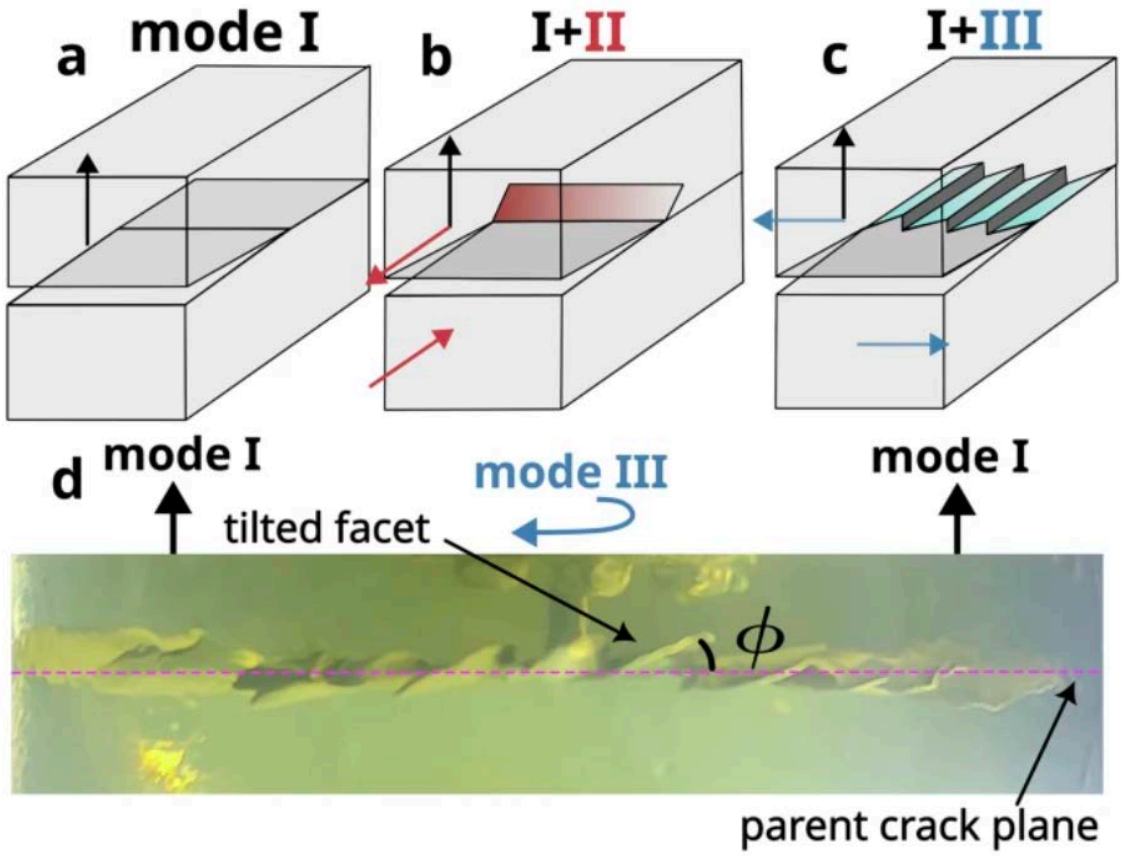
Spatio-temporal plots of the packing fraction along the pipe. Upper panel: formation of plugs in a smooth pipe; mid panel: homogenization due to helical inner wall texture; lower panel: particle size segregation in the flow of a binary mixture in case of a helical inner wall texture; The gray value in the upper and mid panel indicates the packing fraction, the color in the lower panel displays the ratio of the packing fraction of the large and the small particles

P. Müller, A. Panchenko, W. T. Ku, T. Pöschel, Particle size segregation in granular pipe flow. *Chaos* **35**, 043137, DOI: 10.1063/5.0239010 (2025).

Principle of local symmetry in mixed-mode fracture

Laureano Ortellado, Anabella Abate, Angel Santarossa, Leopoldo R. Gómez, Thorsten Pöschel

Abstract:
A particle-based method is introduced for numerically stable simulations of open-boundary flows involving volume-conserving chemical reactions. The method reproduces the behavior of heteroge- neous catalytic systems with high accuracy when validated against high-fidelity reference simulations and delivers identical results at significantly higher computational e!ciency. Owing to its general formulation, the approach is readily applicable to a wide range of reactive flow problems, including catalytic processes, electrochemical systems, and microreactor simulations.



The opening mode I (a), the deviation of fractures in mixed-mode I+II, where in-plane shear is applied to a planar fracture generated by the first mode (b), and fracture fragmentation during mixed-mode I+III, where out-of-plane shear is superimposed on the opening mode (c). (d) Mixed-mode I+III fracture in a hydrogel, where the initial fracture tip/front becomes segmented into facets, which are tilted at an angle ϕ with respect to the parent planar crack.

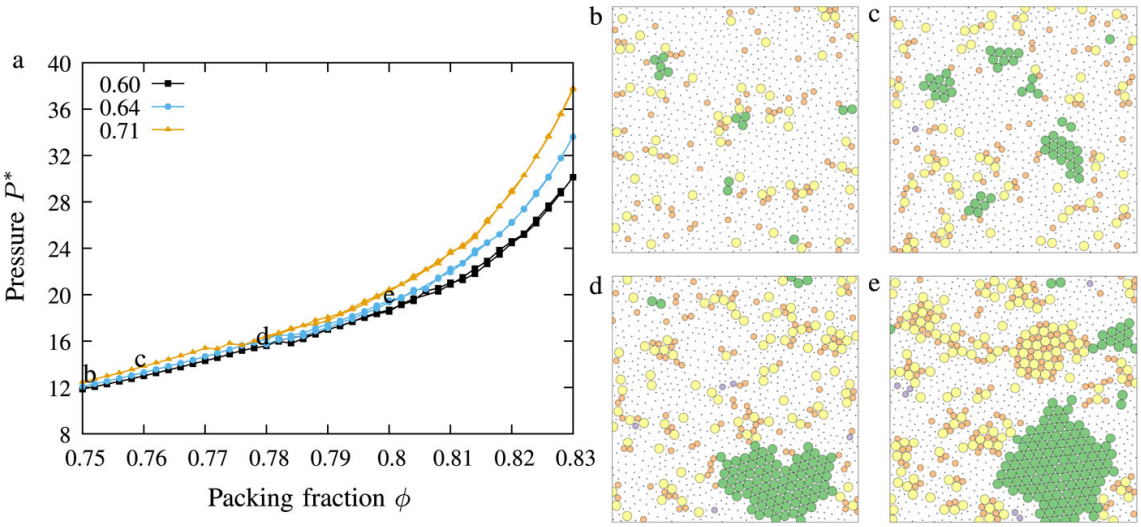
L. Ortellado, A. Abate, A. Santarossa, L. R. Gómez, T. Pöschel, Principle of local symmetry in mixed-mode fracture. *Communications Physics* **8**, 252, DOI: 10.1038/s42005-025-02151-9 (2025).

Formation of hexagonal binary crystals in additive hard disk mixtures

Appala Naidu Rayavarapu, Navid Panchi, Michael Engel, Praveen K. Bommineni

Abstract:

The hard disk model is a foundational system for understanding two-dimensional phase behavior. Its extension to binary mixtures introduces additional structural complexity and kinetic constraints that hinder the formation of ordered phases. Although geometric constructions predict a variety of binary crystals at high densities, these phases often fail to self-assemble in simulations due to slow dynamics and competing phase separation. Here, we investigate the spontaneous formation of the H2 hexagonal binary hard disk crystal in additive mixtures using event-driven molecular dynamics. We show that crystallization is highly sensitive to thermodynamic conditions, requires long equilibration, and is facilitated by particle swap moves. Despite its high packing fraction, the H2 crystal forms spontaneously at equimolar composition and near-ideal size ratio but is kinetically hindered at intermediate densities by the formation of competing one-component hexagonal phases. Our results identify the conditions under which H2 binary crystals spontaneously form and show that their emergence can proceed through non-classical nucleation pathways involving metastable intermediates. These findings offer new insights into entropy-driven self-assembly in two-dimensional mixtures and inform strategies for realizing complex order in colloidal and granular materials.



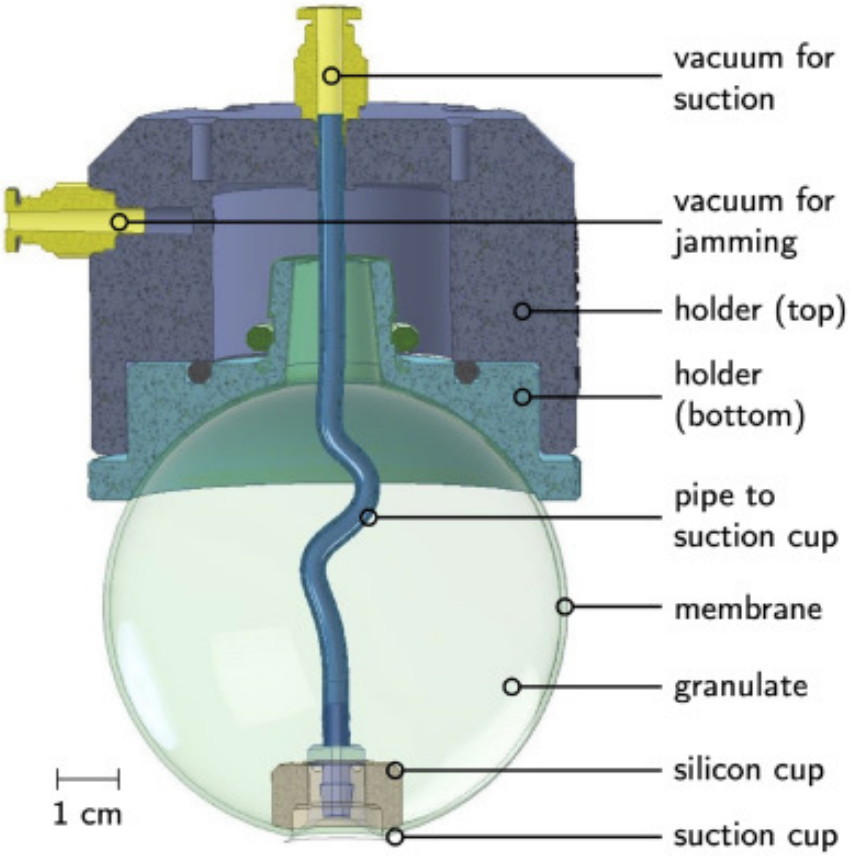
Crystallization of binary hard-disk mixtures without swap moves. (a) Packing fraction versus pressure equation of state at size ratios $\alpha = 0.60$, 0.64, and 0.71. Snapshots show (b) a disordered fluid mixture at the beginning of the simulation, (c) the emergence of precritical nuclei composed of large particles (shown in green), (d) growth of a stable HEXL crystal alongside the appearance of binary crystal precritical nuclei, and (e) the emergence of multiple H_2 nuclei (large particles in yellow and small particles in orange) from the phase-separated fluid.

A. N. Rayavarapu, N. Panchi, M. Engel, P. K. Bommineni, Formation of hexagonal binary crystals in additive hard disk mixtures. *Journal of Chemical Physics* **163**, 154503, DOI: 10.1063/5.0293041 (2025).

All-terrain granular gripper

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

Abstract:
Granular grippers can manipulate a wide variety of objects, but need to be pressed against the object to conform to it. If the object is placed on unstable ground, e.g., on sand or water, this step might cause the object to sink or move away from the gripper, hindering proper operation. We introduce a granular gripper with an integrated suction cup, where suction and jamming are controlled independently. We demonstrate the system's robust and enhanced gripping capabilities by comparing its grasping performance with a typical granular gripper design. We show that the proposed device can grip objects that are challenging for typical granular grippers, including those placed on unstable ground, as the suction cup stabilizes the object, allowing the gripper to conform.



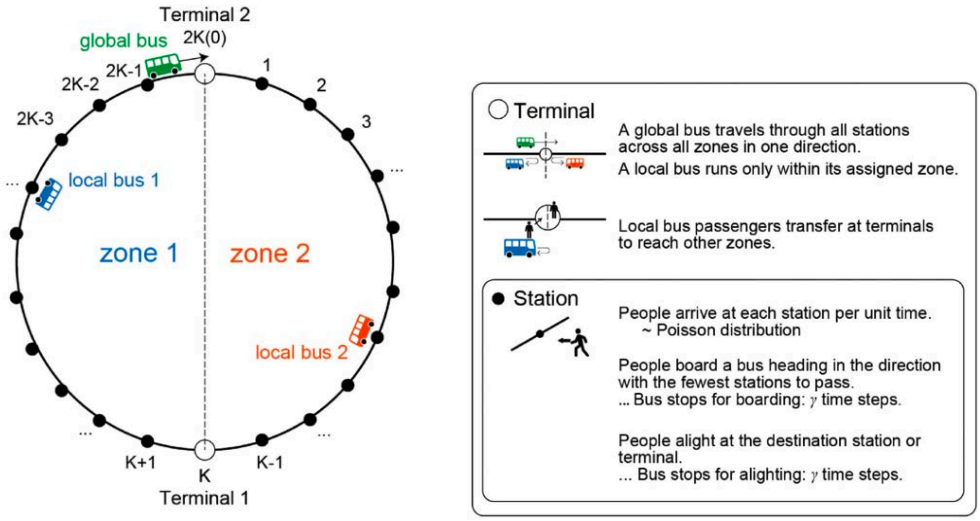
Cross section of the gripper with suction mechanism.

A. Santarossa, O. D'Angelo, A. Sack, T. Pöschel, All-terrain granular gripper. *Particuology* **104**, 283–288, DOI: 10.1016/j.partic.2025.07.006 (2025).

Synchronization in bus systems with partially overlapping routes

Sakurako Tanida, Thorsten Pöschel

Abstract:
In an increasingly interconnected world, understanding congestion-related phenomena in transportation and their underlying mechanisms is crucial for improving efficiency. As the transportation system becomes denser, different modes of transportation have more opportunities to interact with each other, giving rise to emergent dynamics that simple models cannot explain. In this study, we investigate the synchronized motion of indirectly coupled transportation modes. We develop a numerical simulation model on a one-dimensional periodic lattice, where each point represents a bus station. In this system, two types of buses operate: multiple local buses with nonoverlapping routes, each serving a specific zone, and a single global bus that partially overlaps with the routes of the local buses. We perform numerical simulations to examine how close the arrival times of these buses are to each other—that is, how synchronized their motions are. When the number of zones is two, three, or five, robust synchronization occurs not only between the global bus and the local buses but also among the local buses themselves. In contrast, no synchronization is found for other numbers of zones. We developed a mathematical model using self-consistent equations and found that two distinct arrival patterns at the terminals must be considered. A stability analysis reveals which pattern is ultimately realized in the simulations. Our results show that transportation modes can exhibit coherent motion even when sharing only partial or no direct route overlaps. This outcome highlights that emergent behavior depends not only on local interactions but is also strongly shaped by the system's overall structural configuration.



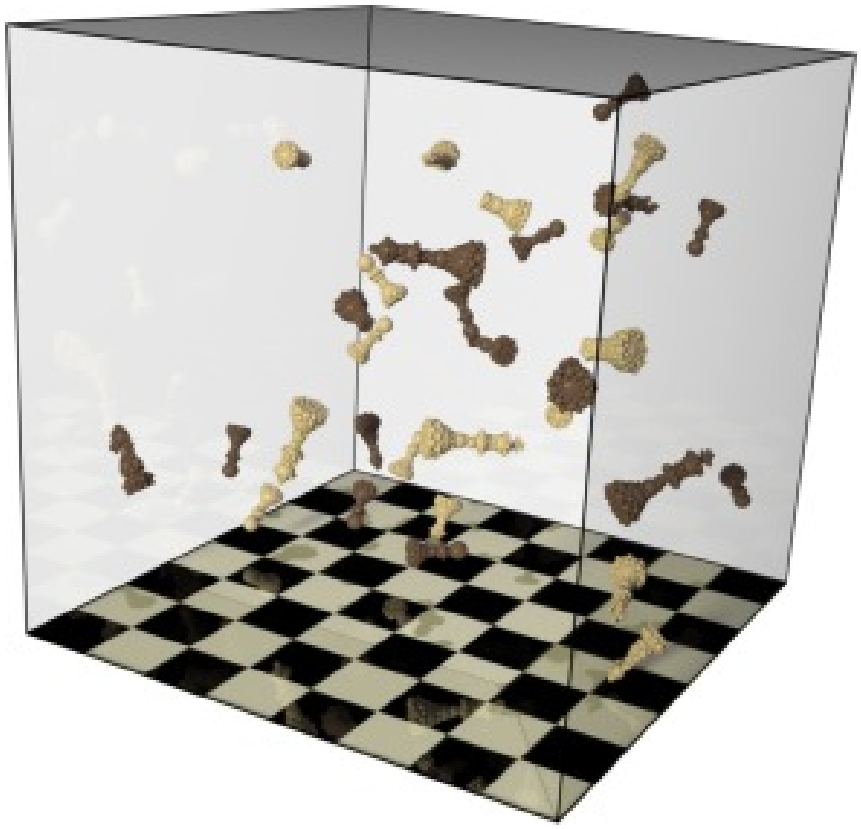
Schematic and summary table of the formulated problem. The upside shows a one-dimensional system with periodic boundary conditions, illustrating an example with two zones. Each zone is serviced by a local bus (blue for zone 1 and orange for zone 2), while the global bus (green) traverses both zones continuously without changing direction. The system operates on a circular route, with stations represented by black circles and labeled by their index. The bottom side summarizes bus and passenger behaviors at both terminals and regular stations.

S. Tanida, T. Pöschel, Synchronization in bus systems with partially overlapping routes. *Physical Review E* **112**, 044307, DOI: 10.1103/39cy-mztc (2025).

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

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

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



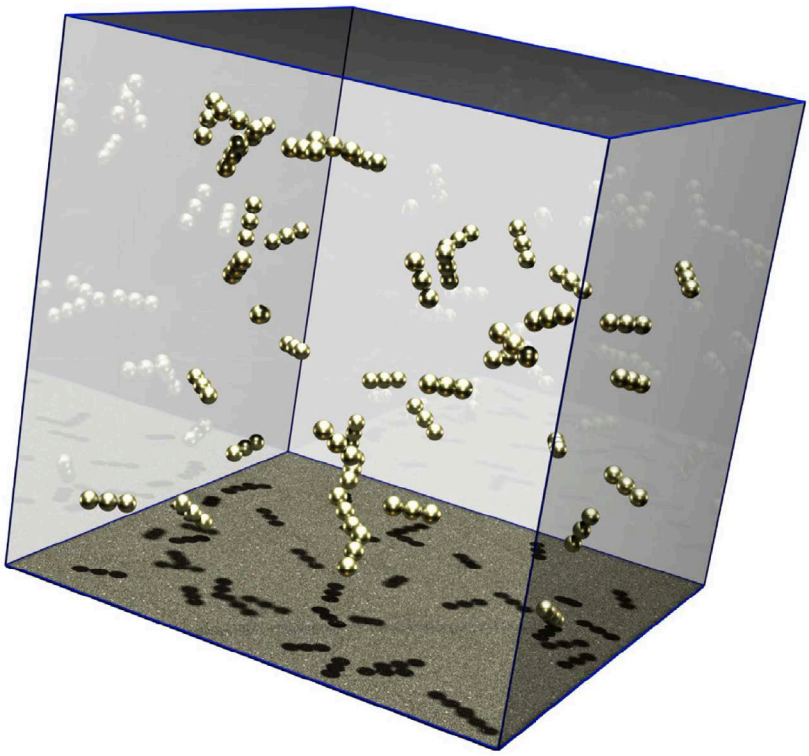
Snapshot of a simulation of non-spherical particles (chess pieces modeled as multi-spheres) bouncing in a box. The elastic Hertz contact force describes particle-particle and particle-wall collisions.

C. A. del Valle, V. Angelidakis, S. Roy, J. D. Muñoz, T. Pöschel, SPIRAL: An efficient algorithm for the integration of the equation of rotational motion. *Computer Physics Communications* **297**, 109077, DOI: 10.1016/j.cpc.2023.109077 (2024).

Efficient numerical integration of rigid body dynamics

Carlos Andrés del Valle, Vasileios Angelidakis, Sudeshna Roy, José Daniel Muñoz, Thorsten Pöschel

Abstract:
Integrating equations of motion is a crucial aspect of discrete element method (DEM) simulations. However, this integration can be particularly challenging when dealing with rigid body dynamics. In this work, we review Spiral, a third-order integration algorithm designed for the rotational motion of extended bodies. Spiral offers stability and precision, surpassing commonly used algorithms. Furthermore, Spiral addresses many challenges associated with rotation dynamics in leading DEM codes, such as YADE, MERCURY DPM, LIGGGHTS, and PFC, without compromising performance. This algorithm eliminates the need for quaternion normalization at each time step, requires only one force calculation per time step, and is compatible with both leapfrog and synchronous integration methods.



Simulation snapshot of rod-like particles modeled as multi-spheres bouncing within a box.

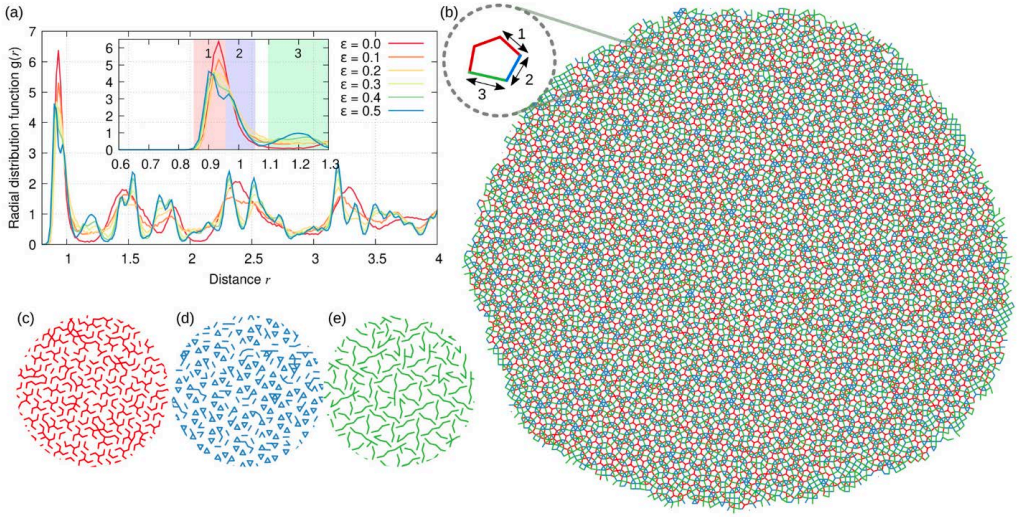
C. A. del Valle, V. Angelidakis, S. Roy, J. D. Muñoz, T. Pöschel, Efficient numerical integration of rigid body dynamics. *EPJ Web of Conferences* **340**, 09017, DOI: 10.1051/epjconf/202534009017 (2025).

Computational self-assembly of a six-fold chiral quasicrystal

Nydia Roxana Varela-Rosales, Michael Engel

Abstract:

Quasicrystals and their periodic approximants are complex crystalline phases. They have now been observed in many metallic alloys, soft matter systems, and particle simulations. In recent experiments of thin-film perovskites on solid substrates, the type of complex phase was found to change depending on thermodynamic conditions and the type of substrate used. Here, we investigate the effect of a substrate on the relative thermodynamic stability of a two-dimensional model quasicrystal and its approximants. Our simulation model consists of particles interacting via the Lennard-Jones–Gauss potential. Our numerical methods are molecular dynamics simulations and free energy calculations that take into account phason flips explicitly. For substrates interacting weakly with the particles, we observe an incommensurate–commensurate transition, in which a continuous series of quasicrystal approximants locks into a small number of approximants. Interestingly, we observe that the 3/2 approximant exhibits phason mode fluctuations in thermodynamic equilibrium. Such fluctuations are reminiscent of random tiling and a phenomenon usually associated only with quasiperiodic order. For stronger substrates, we find an enhancement of the stability of the dodecagonal quasicrystal and variants of square lattices. We explain all observed phenomena by the interplay of the model system with the substrate. Our results demonstrate that designing novel complex periodic and quasiperiodic structures by choice of suitable substrates is a promising strategy.



(a) RDFs averaged from MD trajectories at various ε values with $T = 0.2$. The inset provides a detailed view of the short-distance range. Shaded areas indicate the cutoffs used to construct bond networks, highlighting short nearest-neighbor bonds (red), long nearest-neighbor bonds (blue), and secondary-peak bonds (green). (b) A simulation snapshot at $\varepsilon = 0.5$, illustrating the three types of bonds identified in the RDF. In pentagon tiles, there are typically three red bonds, one green bond, and one blue bond. (c)–(e) The same snapshot as in (b), with each panel displaying only one type of bond: (c) short nearest-neighbor bonds (red), (d) long nearest-neighbor bonds (blue), and (e) secondary-peak bonds (green).

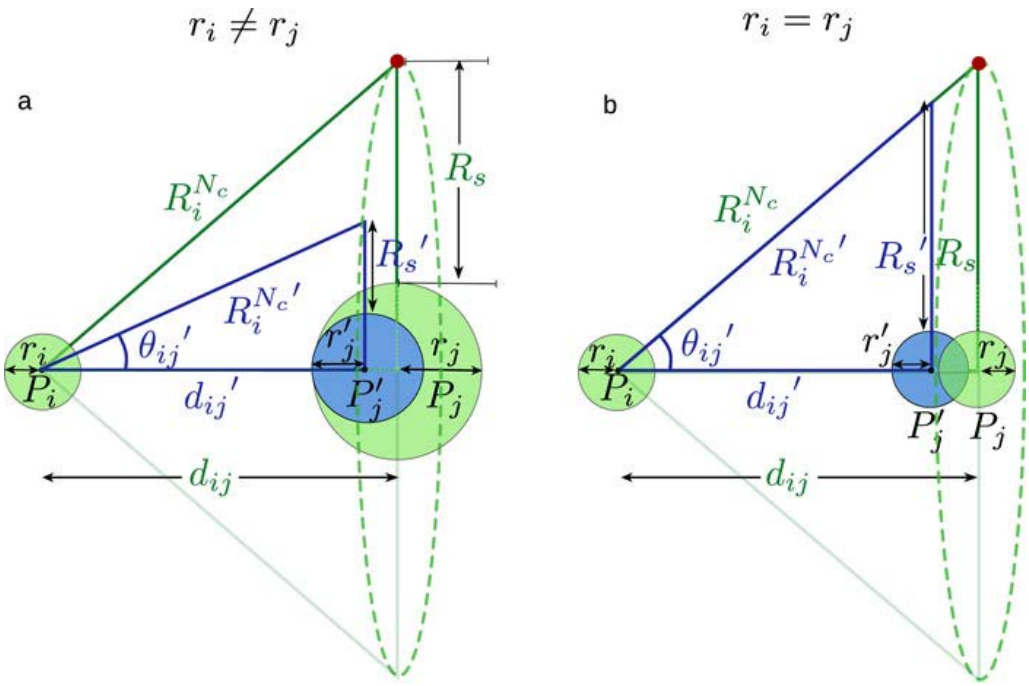
N. R. Varela-Rosales, M. Engel, Computational self-assembly of a six-fold chiral quasicrystal. *Soft Matter* **21**, 596–603, DOI: 10.1039/D4SM00933A (2025).

Solid-angle nearest-neighbor method for size-disperse systems of spheres

Nydia Roxana Varela-Rosales, Michael Engel

Abstract:

Identifying nearest neighbors accurately is essential in particle-based simulations, from analyzing local structure to detecting phase transitions. While parameter-free methods, such as Voronoi tessellation and the solid-angle nearest-neighbor (SANN) algorithm, are effective in monodisperse systems, they become less reliable in mixtures with large size disparities. We introduce SANNR, a generalization of SANN that incorporates particle radii into the solid-angle criterion for robust, size-sensitive neighbor detection. We compare SANNR against Voronoi, Laguerre, and SANN in binary and size-disperse sphere mixtures. Using Wasserstein distance metrics, we show that SANNR closely matches size-aware Laguerre tessellation while preserving the geometric continuity of SANN. Applied to the crystallization of the complex AB13 phase, SANNR improves detection of local bond-orientational order and better captures the emergence of global symmetry. SANNR, thus, offers a smooth, parameter-free, and extensible framework for neighbor detection in polydisperse and multicomponent systems.



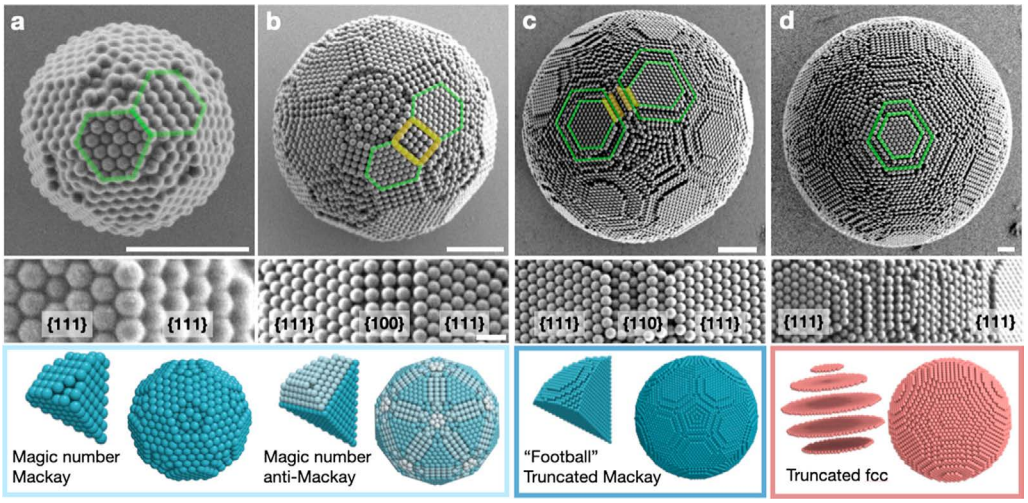
Effect of perturbations on solid-angle blocking in SANN and SANNR. (a) Radius rescaling: increasing r_j enlarges the blocked angle (blue to green). (b) Displacement: moving P_j closer increases the solid angle. In both cases, SANN overestimates the neighbor count, while SANNR compensates via radius-aware regularization.

N. R. Varela-Rosales, M. Engel, Solid-angle nearest-neighbor method for size-disperse systems of spheres. *Journal of Chemical Physics* **163**, 224128, DOI: 10.1063/5.0295910 (2025).

Breakdown of Magic Numbers in Spherical Confinement

Junwei Wang, Jonathan Martín-González Lukas J. Römling, Silvan Englisch, Chrameh Fru Mbah, Praveen Bommineni, Erdmann Spiecker, Michael Engel, Nicolas Vogel

Abstract:
Magic numbers in finite particle systems correspond to specific system sizes that allow configurations with low free energy, often exhibiting closed surface shells to maximize the number of nearest neighbors. Since their discovery in atomic nuclei, magic numbers have been essential for understanding the number-structure–property relationships in finite clusters across different scales. However, as the system size increases, the significance of magic numbers diminishes, and the precise system size at which magic number phenomena disappear remains uncertain. In this study, we investigate colloidal clusters formed through confined self-assembly. Small magic number clusters display icosahedral symmetry with closed surface shells, corresponding to pronounced free energy minima. Our findings reveal that beyond a critical system size, closed surface shells disappear, and free energy minima become less pronounced. Instead, we observe a distinct type of colloidal cluster, termed a football cluster, which retains icosahedral symmetry but features lower-coordinated facets disconnected by terraces. A sphere packing model demonstrates that forming closed surface shells becomes impossible beyond a critical system size, explaining the breakdown of magic numbers in large confined systems.



Four types of colloidal clusters observed via electron microscopy for increasing system size. (a) Mackay clusters are small-sized, spherically truncated Mackay icosahedra, exposing a closed surface shell with hexagonal $\{111\}$ facets (green) around five-fold axes. (b) Anti-Mackay clusters are medium-sized, spherically truncated Mackay cores with anti-Mackay shells, exposing a closed surface shell with hexagonal $\{111\}$ facets (green) sharing edges with rectangular $\{100\}$ facets (yellow). (c) Football clusters are large-sized, spherically truncated Mackay icosahedra, exposing a nonclosed surface shell, in which hexagonal $\{111\}$ terraces (green) are separated by corrugated $\{110\}$ facets (yellow). (d) fcc clusters are even larger-sized, spherically truncated fcc crystals, exposing a nonclosed surface shell, in which eight hexagonal $\{111\}$ facets (green) and six square $\{100\}$ facets are separated by terraces and steps. Insets below show magnified views of the closed surface shells (a,b), nonclosed surface shells (c,d), and the ideal sphere-packing models together with one of the 20 constituent tetrahedral grains with Mackay structure (a), additional anti-Mackay surface termination (light blue in b), surface terraces (dark blue in c), and stacked layers of the fcc lattice (red in d). Scale bars: $2\,\mu$m.

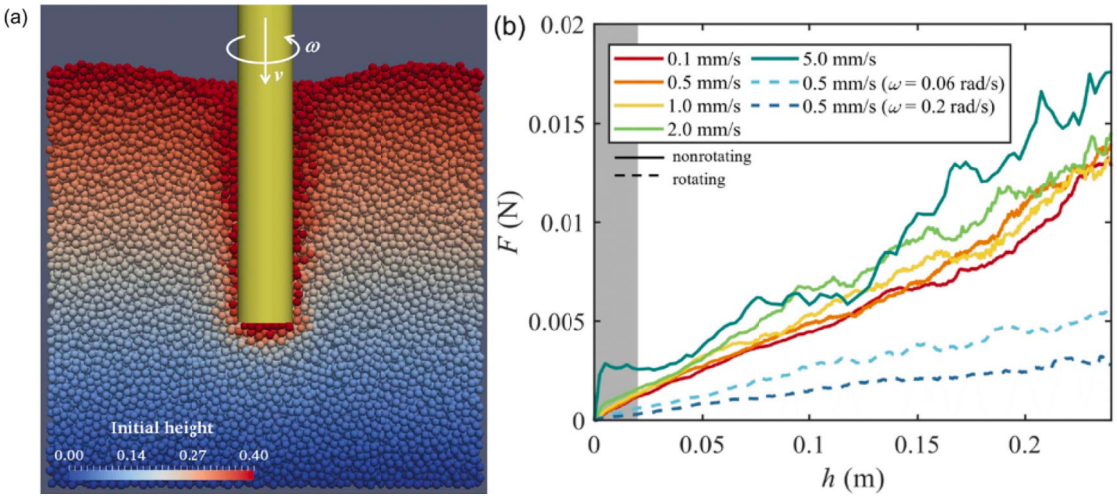
J. Wang, J. Martín-González, L. J. Römling, S. Englisch, C. F. Mbah, P. Bommineni, E. Spiecker, M. Engel, N. Vogel, Breakdown of Magic Numbers in Spherical Confinement. *ACS Nano* **19**, 11702–11711, DOI: 10.1021/acsnano.4c11099 (2025).

Froude scaling of rotating intrusion drag in microgravity regolith

Tongge Wen, Sudeshna Roy, Thorsten Pöschel, Guangkui Xu, Xiangyuan Zeng

Abstract:

Rotational intrusion into granular media is crucial for small body sampling but remains less studied than its non-rotational counterpart. Using a GPU-accelerated discrete element method, we investigate the resistance of a rotating cylindrical penetrometer as a function of the Froude number. Unlike quasi-static intrusion, which creates a stagnant zone ahead of the intruder, rotation disrupts this structure, inducing shear dilation both in front of and around the intruder. This results in a thin, highly mobilized layer of particles, causing the slope of the force-depth to decrease following a negative power-law relationship with increasing Froude number. As rotation intensifies, the rate of resistance reduction slows, and sliding friction becomes negligible, while rolling and torsional resistances remain significant. Furthermore, introducing cohesion shifts the granular medium's response from plastic to elasto-plastic, significantly altering the force-depth relationship and leading to resistance saturation. A brief gravity scan shows that weaker gravity modestly increases the depth-dependence of relative resistance and amplifies the influence of rotation. These findings enhance the understanding of rotational intrusion mechanisms under micro-gravity.



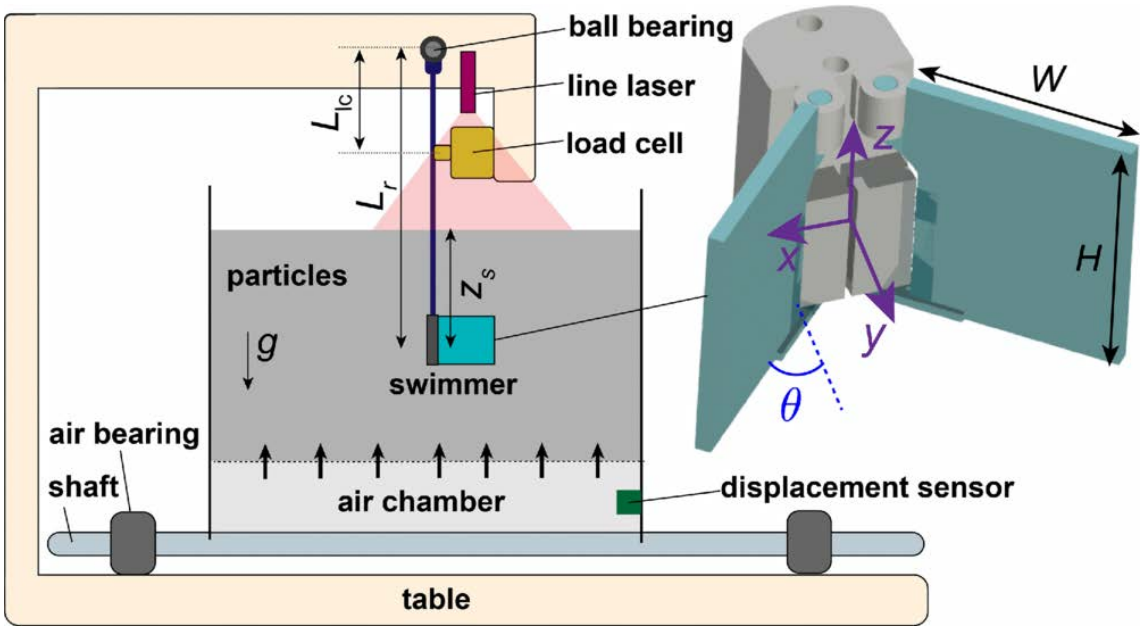
(a) Schematic illustration of the rigid intruder penetrating a granular bed, with particles colored by their initial height. (b) Depth-dependent penetration force for intrusions with different translational velocities (solid lines) and rotational angular velocities (dashed lines).

T. Wen, S. Roy, T. Pöschel, G. Xu, X. Zeng, Froude scaling of rotating intrusion drag in microgravity regolith. *Physical Review E* **(in press)** (2025).

Locomotion of a scallop-inspired swimmer in granular matter

Hongyi Xiao, Harol Torres, Achim Sack, Thorsten Pöschel

Abstract:
Understanding swimming in soft yielding media is challenging due to their complex deformation response to the swimmer's motion. We experimentally show that a scallop-inspired swimmer with reciprocally flapping wings generates locomotion in granular matter. This disagrees with the scallop theorem prohibiting reciprocal swimming in a liquid when its inertia is negligible. We use x-ray tomography and laser profilometry to show that the propulsion is created by the combined effects of jamming and convection of particles near the wings, which break the symmetry in packing density, surface deformation, and kinematics of the granular medium between an opening and a closing stroke.



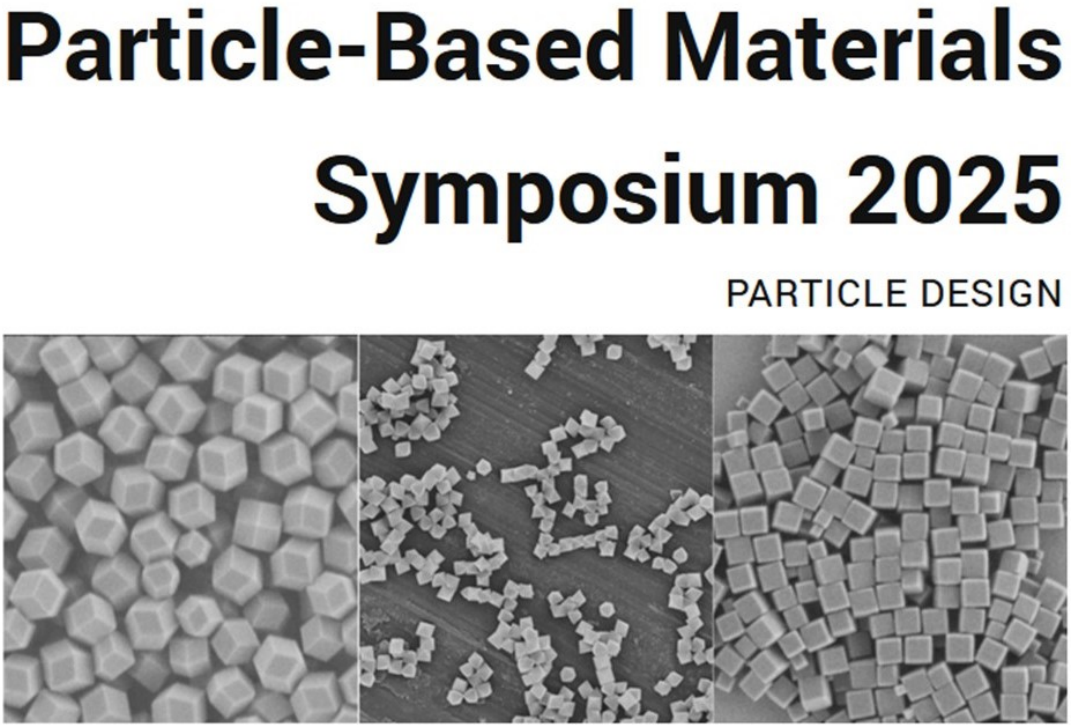
Experimental setup to study reciprocal swimming in a basin filled with granular material. A load cell records the force acting on the swimmer and a displacement sensor records the translation of the reservoir. Laser profilometry reveals the shape of the free surface.

H. Xiao, H. Torres, A. Sack, T. Pöschel, Locomotion of a scallop-inspired swimmer in granular matter. *Physical Review Applied* **24**, 034049, DOI: 10.1103/52rv-8mpz (2025).

12. Service for the Scientific Community

PBM 2025
Symposium
Co-organized by Prof. Michael Engel

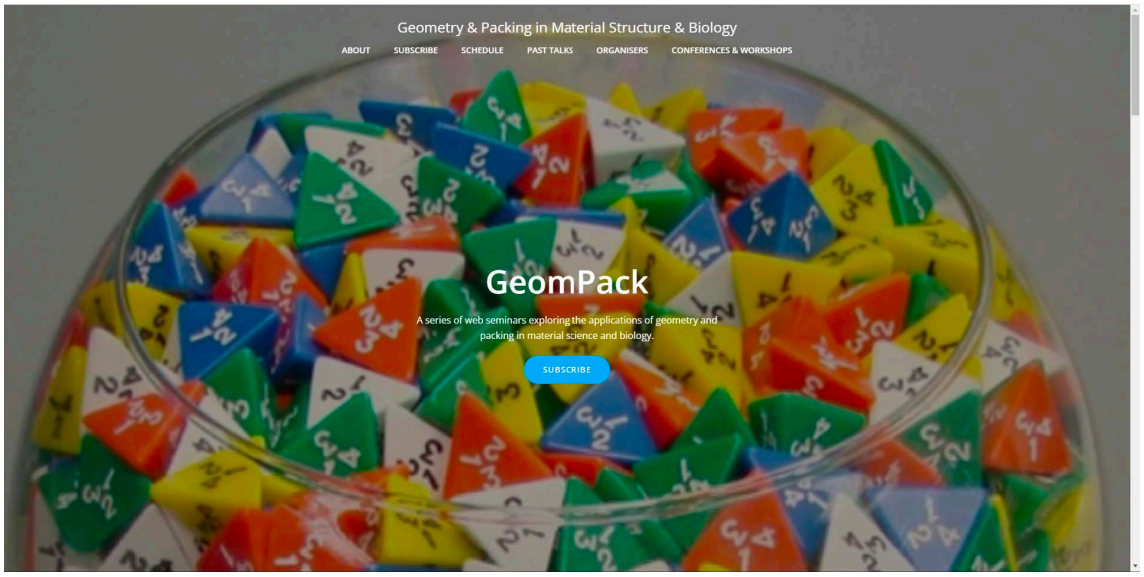
Prof. Michael Engel co-organized PBM 2025 together with Prof. Karl Mandel and Prof. Nicolas Vogel: Particle-Based Materials Symposium 2025 was a symposium to bring together scientists and engineers that aim to use particles for the creation of functionality in materials, from the sysnthesis to the integration into thin films, bulk matrices, fibers or other geometries. The symposium om 2025 focused on partcle design, with sessions covering synthesis and formulations, simulations and models, functional properties, as well analysis and characterization. It took place in Erlangen in October 2025.



Geompack
Webinar
Co-organized by Prof. Michael Engel

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.
`https://geompack.com/`
In 2025, two webinars took place:

- **11th June 2025**: *"Geometry, pattern, and mechanics of notochords "* by Sharon Lubkin.
- **25th June 2025**: *"Arts-and-crafts inspired self-assembly: folding, cutting, and coloring triangulated sheets to make tubules and toroids"* by Thomas Videbaek.



Particles 2025
Invited Session
Co-organized by Priv.-Doz. Sudeshna Roy

In the period October 20 - 22, 2025, S. Roy (Friedrich Alexander University Erlangen, Germany), H. Xiao (University of Michigan, United States), and D. Nasato (Technical University of Munich TUM, Germany) coordinate an invited session at PARTICLES 2025 in Barcelona, Spain. Additive manufacturing has revolutionized manufacturing processes and opened new possibilities for design, customization, and production across various industries. Aerospace companies, such as GE Aviation, use it to create lightweight components like turbine blades and fuel nozzles, improving fuel efficiency. In medical engineering, it enables the fabrication of tailored implants and customized prosthetics, enhancing patient outcomes. The automotive industry leverages it for rapid prototyping, tooling, and component production, as demonstrated by Bugatti's brake calipers. Although additive manufacturing has the potential for the realization of intricate designs previously impossible to execute, the manufacture efficiency (e.g., printing speed and labor cost) and quality (e.g., strength, toughness, and surface texture) are still far from ideal. Quantitative optimization of the manufacturing processes requires a deeper level of understanding and modeling for the interplay of process design and material properties.
This dedicated invited session on additive manufacturing will provide valuable insights and perspectives on this rapidly evolving field. It will serve as a prominent platform for researchers to explore the diverse and intricate intersections between particle technology and additive manufacturing. By highlighting the latest developments, challenges, and opportunities of particle-based simulations in additive manufacturing, our session aims to foster a deeper understanding of this emerging technology within the field of granular systems. The session will cover a range of topics important to additive manufacturing, including but not limited to:

- Powder spreading and material structure
- Particle sintering and phase change dynamics
- Enhanced computational approaches for particle simulations
- Powder rheology, and flow behavior
- Experimental calibration and validation of particle-based simulations
- Post processing, industrial implementation, and case studies

Injavis – INteractive JAva VISualization

`https://engellab.de/injavis`

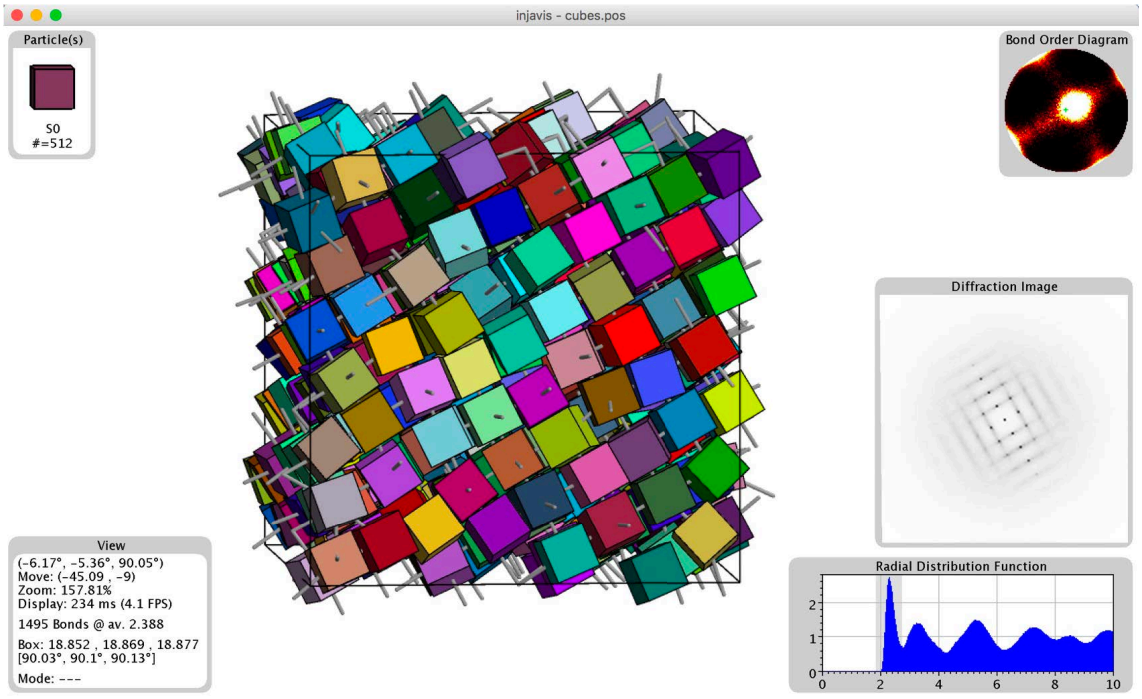
The software package Injavis (acronym for INteractive JAva VISualization) displays, analyzes, and manipulates particle simulation data. An emphasis lies on geometry and structural analysis as well as interactivity. The main input and output file format is .pos, which is a format developed specifically 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.



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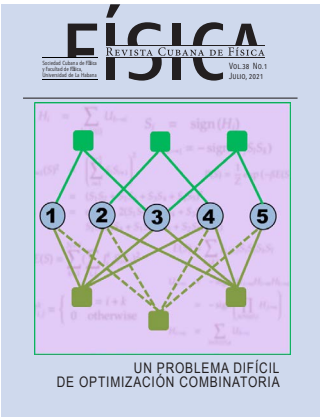

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(founding member)

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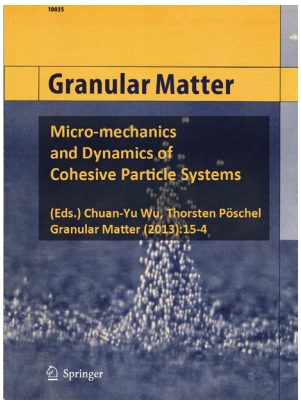
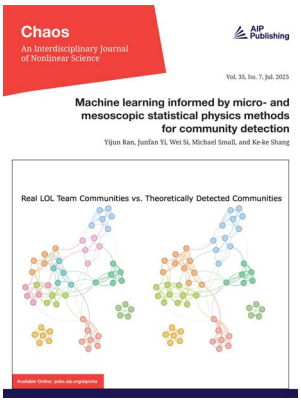
www.springer.com/journal/10035



Prof. Thorsten Pöschel
Editor since 2006

Chaos - Special Issue
AIP Publishing
https://pubs.aip.org/aip/cha/issue/



Prof. Thorsten Pöschel, Prof. Marcus Beims,
Prof. Pedro G. Lind,
Guest Editors

13. PhD Graduations

Angel Santarossa,
Experimental research and enhancement of granular gripping systems

Faculty: Chemical Engineering / Dr. -Ing.
Date: May 09, 2025

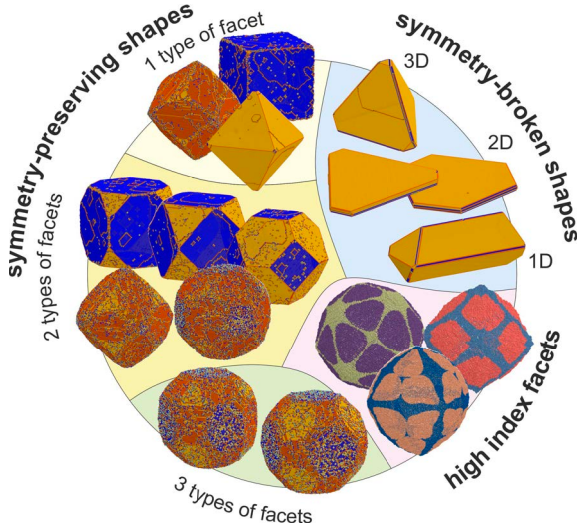
Federico Tomazic,
Particle Self-Assembly into Complex Suprastructures: The Role of Shape and Interaction

Faculty: Chemical Engineering / Dr. -Ing.
Date: June 3, 2025

14. Awards

Image of the Month: EAM Calendar January 2025

Carlos Bassani's artwork has been chosen to be featured in the 2025 EAM (Engineering of Advanced Materials) calendar. The piece was showcased as the featured image for the month of January.



Carlos picture accepted for the 2025 EAM calender

Best Poster Award at PBM2025
Jyoti Pannu's work, presented at the PBM2025 symposium, won the award for best poster. The symposium took place from 7 - 8.10.2025.

15. University Administration

Activities within the University Self-Administration

Library Commission of the University, Representative of the Faculty of Engineering	Prof. Thorsten Pöschel
Competence Unit for Scientific Computing (CSC), Founding Member, Head of Application Lab Particles	Prof. Thorsten Pöschel
Executive Board of the Interdisciplinary Centre for Nanostructured Films	Prof. Thorsten Pöschel Prof. Michael Engel
Scientific Committee of the BayWISS Joint Academic Partnership Energy (Wissenschaftlicher Ausschuss des BayWISS Verbundkollegs Energie)	Prof. Thorsten Pöschel
Habilitation Committee of the Technical Faculty (Kommission für Habilitationen und wissenschaftlichen Nachwuchs)	Prof. Thorsten Pöschel
Executive Board of the Department for Chemical and Biological Engineering	Prof. Thorsten Pöschel Priv.-Doz. Dr. Patric Müller
Recognition Committee at the Government of Swabia according to the Regulation for the Regulation of Compensation Measures in Accordance with the Bavarian Engineering Act (Anerkennungsausschuss bei der Regierung von Schwaben nach der Verordnung zur Regelung von Ausgleichsmaßnahmen nach dem Bayerischen Ingenieurgesetz) (BayIngAMV)	Prof. Thorsten Pöschel
Study Program Manager (Studiengangsverantwortlicher), Chemical Engineering — Nachhaltige Chemische Technologien (CEN)	Prof. Michael Engel
Advanced Materials and Processes (MAP), Executive Board Member and Focal Subject Head for Computational Materials Science and Process Simulation	Prof. Michael Engel

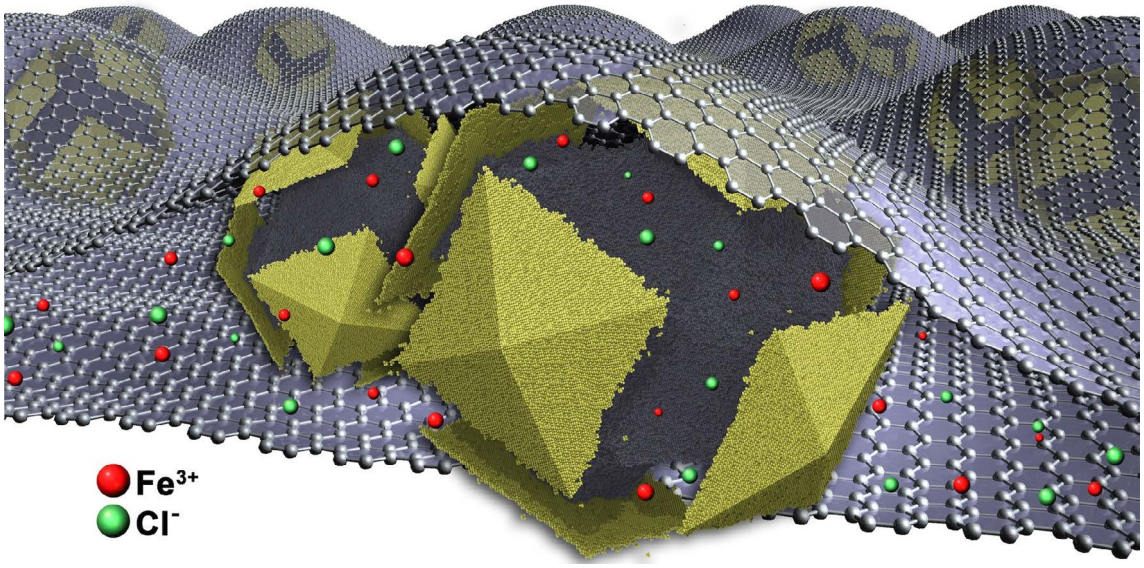
Deputy Chair, Study Commission (Studienkommission), Chemical and Biological Engineering (CBI), Chemical Engineering— Nachhaltige Chemische Technologien (CEN), Biotechnologie	Prof. Michael Engel
Study Commission (Studienkommission), Clean Energy Processes (CEP)	Prof. Michael Engel
Spokesman of the Early-Stage Researchers (habilitands) of the Department for Chemical and Biological Engineering	Priv.-Doz. Dr. Patric Müller
Admission Committee for Master's Students in Clean Energy Process in the Department for Chemical and Biological Engineering	Priv.-Doz. Dr. Sudeshna Roy
Advanced Materials and Processes (MAP), Executive Board Member	Dr. Carlos L. Bassani
PR-Team of the Department for Chemical and Biological Engineering	Stefanie Suttner
Admittance Committee for the Master Program on Advanced Materials and Processes (MAP)	Dr. Carlos L. Bassani

16. Public Attention and Public Outreach

Lange Nacht der Wissenschaften 2025

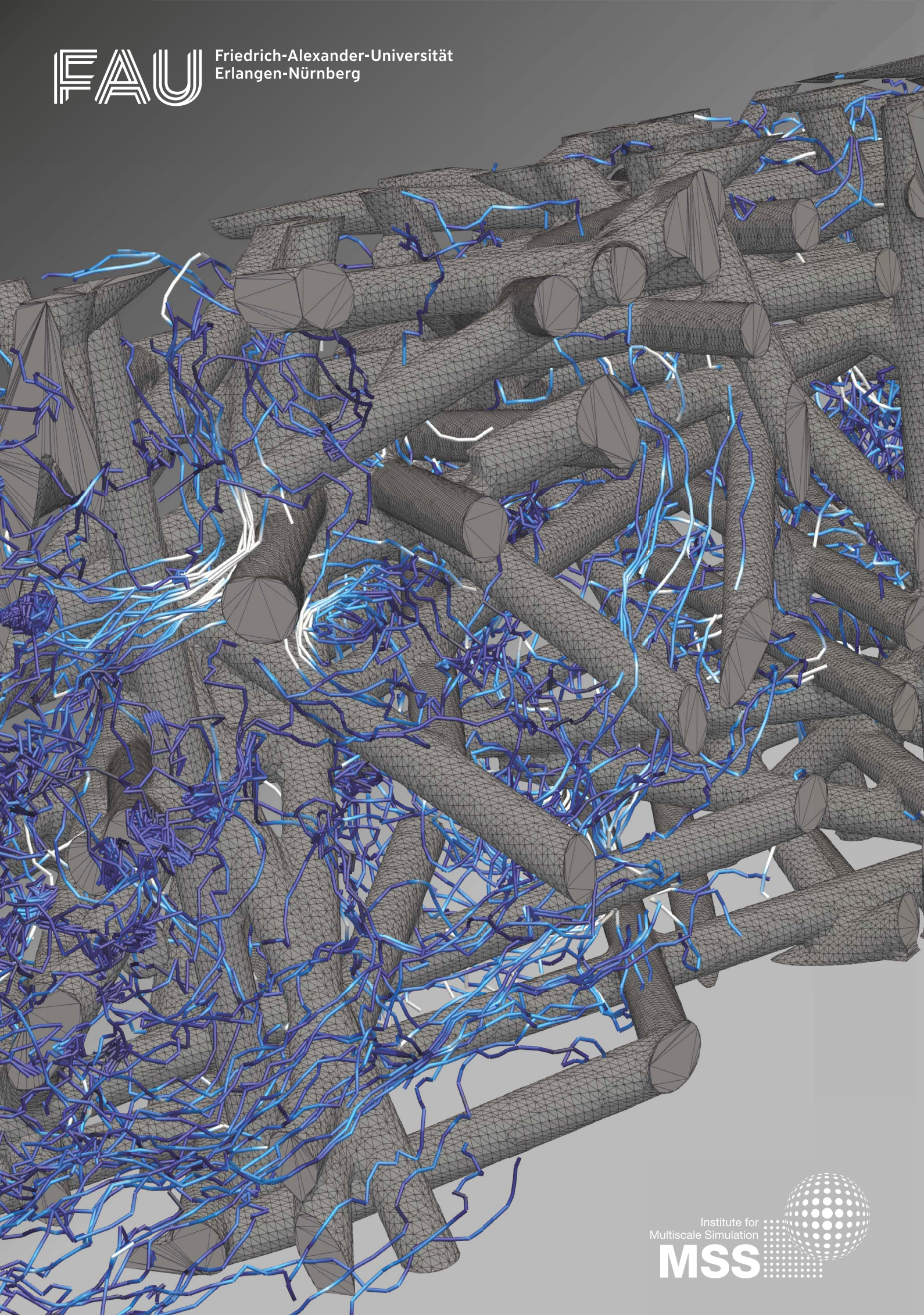
The Lange Nacht der Wissenschaft is a fantastic chance for having contact with an external audience. Last year, the MSS participated with the attractions "Interactive particle simulations", "Flow paths in disturbed granulates" and "Digital hourglass". During the exposition, visitants could have a first contact with the background of 3D printing techonolgy, as well digital image processing. The Engel Lab presented an interactive outreach activity focused on particle simulations of atoms and nanoparticles. Participants were introduced to these systems, learned how simulations are used to study their behavior, and had the opportunity to run simulations themselves using computers, tablets, and their own smartphones. We extend our gratitude to all attendees for their participation and their enthusiasm for science and technology.

Flow paths in disturbed granulates experiment in exposition for the Lange Nacht der Wissenschaften



Schematic of nanoparticles confined between two graphene sheets. The Engel Lab uses computer simulations of this setup to better understand in situ studies of nanoparticle etching.

FAU Friedrich-Alexander-Universität Erlangen-Nürnberg



Institute for Multiscale Simulation

MSS