Institute for Multiscale Simulation

Friedrich-Alexander-Universität
Erlangen-Nürnberg

2024 Annual Report

Prof. Thorsten Pöschel
Prof. Michael Engel

Institute for Multiscale Simulation
MSS

FAU Friedrich-Alexander-Universität Erlangen-Nürnberg

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

Editor: Nicolas Pechler

Titlepage: LASER Wire Deposition in micro-gravity. Image by Achim Sack, cover design by Nicolas Pechler.
Back cover: LASER Wire Deposition in micro-gravity II. Image by Achim Sack, cover design by Nicolas Pechler.

Institute for Multiscale Simulation

Annual Report 2024

Preface

This annual report describes the scientific, teaching, and social activities at the Institute for Multiscale Simulation of Particulate Systems at Friedrich-Alexander-Universität Erlangen-Nürnberg in 2024.

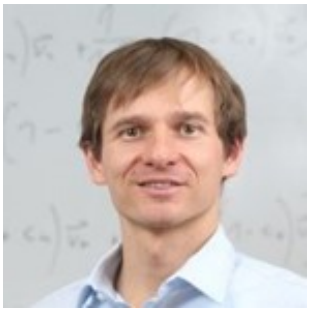
Erlangen, December 2024
Thorsten Pöschel, Michael Engel

1. Staff Members

Professors

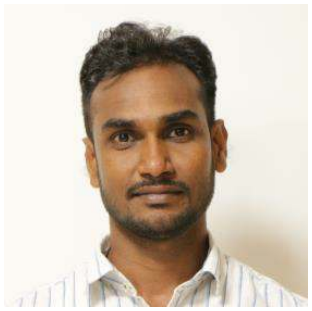
Prof. Dr.
Thorsten Pöschel

Prof. Dr.
Michael Engel



Priv.-Doz. Dr.
Patric Müller

Visiting Researchers

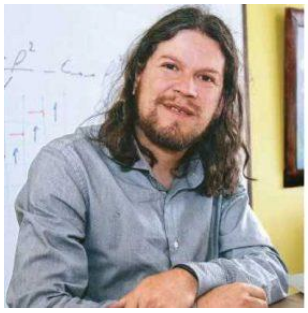


Prof. Dr.
Praveen Kumar Bommineni

Prof. Dr.
Leopoldo Gómez

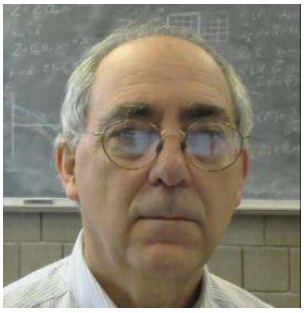
Dr.
Marek Mihalkovic

Prof. Dr.
Tomoko Mizuguchi



Prof. Dr.
José-Daniel Muñoz

Prof. Dr.
Sakurako Tanida



Prof. Dr.
Mike Widom

Habilitation Candidates

Dr.
Carlos L. Bassani

Dr.
Alberto Leonardi

Dr.
Sudeshna Roy

Postdoctoral Researchers

Dr.
Olfa Lopez-D'Angelo

Dr.
Holger Götz

Dr.
Achim Sack

PhD Students

Meysam Bagheri
M. Sc.

Felix Buchele
M. Eng.

Utku Canbolat
M. Sc.

Geovane de Jesus Rodrigues
M. Sc.

Jyoti
M. Sc.

Wing To Ku
M. Sc.

Valentina Marzulli
M. Sc.

Harsha Namdeo
M. Sc.

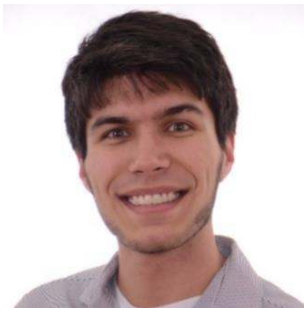
Navid Panchi
M. Sc.

Nicolas Pechler
M. Sc.

Huzaif Rahim
M. Sc.

Dr.
Nydia Varela Rosales

Hakan Şanal
M. Sc.



Angel Santarossa
Lic. (M.Sc.)

Zhiyu Song
M. Sc.

Federico Tomazic
M. Sc.

Kaijie Zhao
M. Sc.

Master and Bachelor Students

Daniel Adam
B.Sc.
Bachelor student

Nadja Al Akkam
M.Sc.
Master student

Yi-Ting Chiang
B.Sc.
Master student

Suleyman Gafarli
M.Sc.
Master student

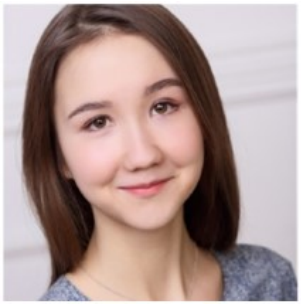
Chia-Jui Hsieh
B.Sc.
Master student

Harsha Namdeo
M.Sc.
Master student

Julian Pollet
B.Sc.
Master student

Prashanth Prakash Kamath
B.Sc.
Master student

Laura Steub
B.Sc.
Master student

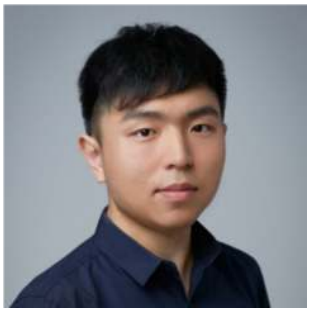


Kamilla Zaripova
M. Sc.
Master student

Technical and Administrative Staff

Ulrike Hansl
Team Assistant

Walter Pucheanu
Master Technician & Head of the Mechanics Workshop



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

Student Assistants

Nadja Al Akkam
M.Sc.

Felix Böhmer

Luca Hagen

Frederik Keil

Paavai Rajasekar Kavitha

Isabella Schneider
B.Sc.

Priyanka Singh

Hisham Zidan

2. Teaching Activities

image: fau.de

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

Wissenschaftlich Rechnen für Ingenieure (CIV1-V)
Lecture Prof. Thorsten Pöschel
Exercise Felix Buchele

Scientific Computing in Engineering (CIV2-V)
Lecture Prof. Thorsten Pöschel
Exercise Felix Buchele

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 Dr. Patric Müller
Exercise Dr. Patric Müller
Lab session Dr. Patric Müller
Walter Pucheanu
Felix Buchele
Nicolas Pechler

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

Partikelbasierte Strömungsmechanik (PSTM)
Lecture Dr. Patric Müller
Exercise Dr. Patric Müller

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

Granular Matter and Applications
Lecture Dr. Sudeshna Roy

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

Data Science for Engineers (DSE-L)
Lecture Prof. 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) 2024
Supervisor Geovane de Jesus Rodrigues
Huzaif Rahim

CEP Advanced Seminar 2024
Lecture Prof. Robin Klupp Taylor
Supervisor Meysam Bagheri
Carlos L. Bassani
Utku Canbolat
Nicolas Pechler
Huzaif Rahim

Projektkurs Chemische und Biologische Prozeßtechnik (CBPT) 2024
Supervisor Geovane de Jesus Rodrigues
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)

12.01.2024	Meysam Bagheri	*Cascading cracks in drying suspensions*
26.01.2024	Angel Santarossa	*Granular jamming gripper with integrated suction*
02.02.2024	Federico Tomazic	*Layer formation during crystallization of supraparticles in spherical confinement.*
09.02.2024	Patric Müller	*Automated tomographic assessment of structural defects of freeze-dried pharmaceuticals*
16.02.2024	Carlos L. Bassani	*Mesomorphology of clathrate hydrates from molecular ordering: I. Particle-based and continuum models of molecular attachment*
23.02.2024	Carlos L. Bassani	*Mesomorphology of clathrate hydrates from molecular ordering: II. Phase field models for the emergence and evolution of porous patterns*
08.03.2024	Achim Sack	*LADA - LASER wire welding in weightlessness*
15.03.2024	Felix Buchele	*Simulating catalytic reactions across scales*
12.04.2024	Kaijie Zhao	*Decoration of clathrate lattices with trigonal bipyramids*
19.04.2024	Suleyman Gafarli	*Development of a kinetic model for the Methanol-to-Olefins synthesis over an industrial catalyst*
26.04.2024	Marek Mihalkovic	*Composite alloys inspired by hard sphere mixtures and pair potentials*
03.05.2024	Navid Panchi	*Accurate, efficient and scalable implementation of Debye scattering equation solution*
10.05.2024	Felix Buchele	*Stochastic diffusion model for heterogeneous catalysis*
17.05.2024	Wing To Ku	*Mid-fidelity fluid structural simulation in rotorcraft aerodynamics*
24.05.2024	Harsha Namdeo	*Reconstruction of pair potential using nanoparticle configurational data*
31.05.2024	Olfa D'Angelo	*Open questions and perspectives on granular media*
07.06.2024	Jyoti	*Branched flow of light in disordered photonic lattice*
14.06.2024	Hakan Şanal	*Finiteness Conditions in rings and modules with respect to isomorphism classes*
19.07.2024	Sakurako Tanida	*Elevator traffic jam: Why do they arrive together?*
26.07.2024	Zhiyu Song	*Effective interaction between ligand-coated nanoparticles*
02.08.2024	Huzaif Rahim	*Influence of friction and initial packing on the steady state structure in sheared granular media*
09.08.2024	Holger Götz	*Effective acceleration field of a cushioned wall*

23.08.2024	Geovane de Jesus Rodrigues	*Performing experiments under low/hypergravity*
30.08.2024	Meysam Bagheri	*Emergence of crack patterns in drying suspensions*
13.09.2024	Kamilla Zaripova	*Symmetry breaking of nanocrystal shapes via formation of surface defects with kinetic Monte Carlo*
04.10.2024	Felix Buchele	*An image-based approach to characterize porous media*

3. MSS Seminar

174. **Dr. Sudeshna Roy**
Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Exploring diverse applications of granular materials flow
February 21, 2024

175. **Dr. Othmane Aouane**
Forschungszentrum Jülich GmbH, Helmholtz-Institute Erlangen-Nürnberg, Germany
Rheology of elastic capsules in a confined shear flow
March 20, 2024

176. **Prof. Mike Widom**
Carnegie Mellon University, USA
Information-theoretic approaches to calculating thermodynamic entropy
April 17, 2024

177. **Dr. Marek Mihalkovic**
Institute of Physics, Slovak Academy of Sciences, Slovakia
Composite alloys inspired by hard sphere mixtures and pair potentials.
April 26, 2024

178. **Dr. Holger Götz**
Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Jamming and convection in granulates
May 22, 2024

179. **Prof. Anki Reddy Katha**
Indian Institute of Technology Tirupati, India
Dynamics of intruders in a granular medium
May 29, 2024

180. **Dr. Greg Huber[1] and Walter Trump[2]**
[1]Chan Zuckerberg Biohub, San Francisco, California, USA
[2]Gymnasium Stein, Germany
Riddles of the sphinx tilings
June 12, 2024

181. **Dr. Nydia Roxana Varela-Rosales**
Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Computational design and thermodynamic stability of aperiodic crystals and their approximants
June 15, 2024

182. **Prof. Praveen Bommineni**
National Institute of Technology Warangal, India
Entropy traps in spherical confinement
July 10, 2024

183. **Prof. Klaus Kroy**
Universität Leipzig, Germany
Mesoscopic signatures of colloidal heating, motility, and retarded and non-reciprocal interactions
July 17, 2024

184. **Prof. Vivek Buwa**
Indian Institute of Technology Delhi, India
Multiscale modelling & simulations of multiphase flows: Applications to packed bed reactors
September 10, 2024

185. **Rajesh Pavan Pothukuchi**
Indian Institute of Science, Bangalore, India
Mechanistic details of the organizer-assisted nucleation of gold nanoparticles (AuNPs) by the Turkevich method
September 18, 2024

186. **Prof. Tobias Kraus**
Leibniz Institute for New Materials and Saarland University, Germany
Self-assembled sensor materials
September 20, 2024

187. **Prof. Felix H. Schacher**
Friedrich Schiller University Jena, Germany
Inside block copolymer micelles - A journey of crosslinking strategies along interfacial boundaries
November 6, 2024

188. **Prof. Sakurako Tanida**
Department of Aeronautics and Astronautics, School of Engineering, University of Tokyo, Japan
How zoned buses achieve synchronization
November 27, 2024

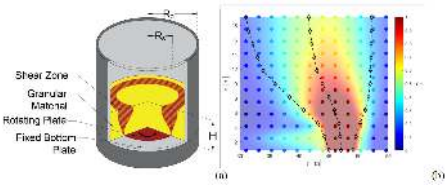
174th MSS Seminar
Wednesday, February 21, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Exploring diverse applications of granular materials flow

Dr. Sudeshna Roy

Institute for Multiscale Simulation, University of Erlangen-Nuremberg

Granular materials are integral components in additive manufacturing, geotechnical engineering, and various industrial processes. This presentation explores three interconnected applications of granular materials flow. Firstly, we explore powder spreading in additive manufacturing, investigating how particle shapes, elastic modulus, and process parameters influence temperature distribution within the powder bed. Extending this analysis to bi-disperse shape mixtures uncovers complexities in particle interactions, where the effects on flow behavior remain elusive. Subsequently, we explore the micro-macro correlations of granular mixtures and elucidate the role of particle friction and stiffness on macro properties using local critical state data within the shear band. Finally, we analyze secondary flows, informed by local shear band data, to provide insights into particle motion and flow dynamics. Our comprehensive investigation, integrating theoretical, and computational approaches, contributes to a deeper understanding of granular materials flow and its impact on industrial processes.



(a) Split-bottom shear cell geometry and (b) shear zone in split-bottom shear cell.

175th MSS Seminar
Wednesday, March 20, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Rheology of elastic capsules in a confined shear flow

Dr. Othmane Aouane

Forschungszentrum Jülich GmbH, Helmholtz-Institute Erlangen-Nürnberg, Germany

In the last two decades, the lattice Boltzmann method (LBM) has emerged as an attractive choice for modelling complex fluid phenomena, including multiphase/multicomponent flows, particle suspensions, and turbulence. Compared to conventional Navier-Stokes solvers, this method enables simple implementation of complex boundary conditions and is well-suited for highly scalable parallel computing. This presentation will primarily focus on the rheology of a suspension of elastic capsules. A capsule is a liquid droplet core encapsulated by an elastic polymeric membrane with a diameter spanning a few nanometers to a few millimetres. The fluid motion is solved using the lattice Boltzmann method, and the particles are described by a combined finite element/immersed boundary method. We have studied the rheology of strain-hardening spherical capsules, from the dilute to the concentrated regime, under a confined shear flow in three dimensions. We have considered the effect of capillary number, volume fraction, and membrane inextensibility on particle deformation, the suspension's effective viscosity, and normal stress differences. Interestingly, the suspension viscosity exhibits a universal behaviour for the parameter space defined by the capillary number and the membrane inextensibility when introducing the geometrical changes of the particle at the steady state in the definition of the volume fraction [1]. Furthermore, the same reasoning applies to other types of capsules [2].

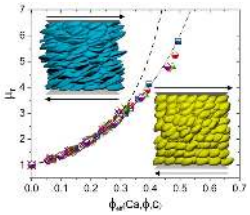


Figure: Suspension viscosity

[1] O. Aouane, A. Scagliarini and J. Harting, J. Fluid Mech 911:A11 (2021)
[2] P. Gaglietta, F. Pelusi, M. Sega, O. Aouane and J. Harting J. Fluid Mech 971:A13 (2023)

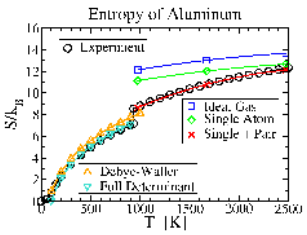
176th MSS Seminar
Wednesday, April 17, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Information-theoretic approaches to calculating thermodynamic entropy

Prof. Michael Widom

Carnegie Mellon University

The thermodynamic entropy of matter equals (in suitable units) the information required to precisely specify its state. In a fully random substitutional alloy of N chemical species, log(N) bits of information per site are required to specify the site occupations. In an ideal gas of volume V, the information required to locate each molecule grows as log(V). If the alloy is not fully random, or the gas is not ideal, then prior information contained in positional correlations becomes redundant, and the thermodynamic entropy falls below its ideal value to a quantifiable extent. We will illustrate practical applications of this principal that allow us to model the substitutional entropy of high entropy alloys; melting points of elements; phase separation and eutectics in liquid alloys; and the HCP/BCC transition of elemental titanium.



References:
A. D. Kim and M. Widom, "Interaction models and configurational entropies of binary MoTa and the MoNbTaW high entropy alloy", Phys. Rev. Mater. 7 (2022) 063803
Y. Huang and M. Widom, "Vibrational entropy of crystalline solids from covariance of atomic displacements", Entropy 24 (2022) 618
Y. Huang, M. Widom and M.C. Gao, "Ab-initio free energies of liquid metal alloys: application to the phase diagrams of Li-Na and K-Na", Phys. Rev. Materials 6 (2021) 013802

178th MSS Seminar
Wednesday, May 22, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

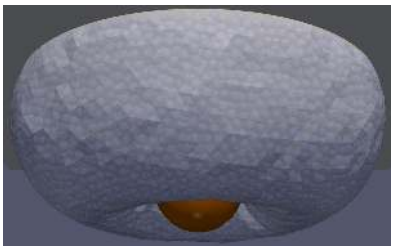
Jamming and convection in granulates

Holger Götz

Institute for Multiscale Simulation, University of Erlangen-Nuremberg

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 a 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 which makes it possible to simulate membranes together with a granulate using DEM. I use this method to characterize and improve both applications.

In addition to jamming, I deal with granulates in vibrated cylinders under zero gravity conditions. The vibrations cause convection, which despite the absence of gravity does not necessarily have an axis of symmetry perpendicular to the direction of the vibration. In my work, I show two such convection patterns and explain why they occure.



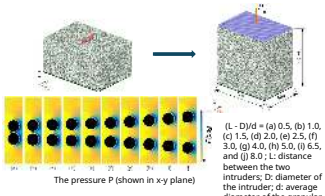
179th MSS Seminar
Wednesday, May 29, 15:30,
Room 00.156,
Cauerstraße 3, Erlangen.

Dynamics of intruders in a granular medium

Prof. Anki Reddy Katha

Chemical Engineering, Indian Institute of Technology Tirupati

The talk will present the origin of the long-ranged forces between two large intruders in a granular medium in the evolution and the subsequent buckling of force chains, which may be an essential step in understanding the segregation and Brazil nut effect in granular media. In addition, the Magnus effect and wiggling dynamics in a granular medium will be discussed.



The pressure P (shown in x-y plane)

(L - D)/d = (a) 0.5, (b) 1.0, (c) 1.5, (d) 2.0, (e) 2.5, (f) 3.0, (g) 4.0, (h) 5.0, (i) 6.5, and (j) 8.0 ; L: distance between the two intruders; D: diameter of the intruder; d: average diameter of the granular bed particles.

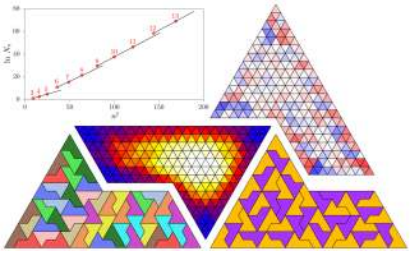
180th MSS Seminar
Wednesday, June 12, 15:30,
Room 00.156,
Cauerstraße 3, Erlangen.

Riddles of the sphinx tilings

Greg Huber[1] and Walter Trump[2]

[1]Chan Zuckerberg Biohub, San Francisco, California, USA
[2]Department of Physics, Gymnasium Stein, Stein, Germany (retired)

The sphinx tile is a simple, non-symmetrical shape which comes in left and right enantiomers and is proposed as a building block to explore chiral interactions in crowded spaces. The basic theory of sphinx tilings is lacking, so we have developed a succession of exact methods to find these tilings within finite frames. For large frames, the numbers of configurations become so large that statistical mechanics obtains and Monte Carlo methods are required. Our explorations raise a number of new mysteries which will be discussed.



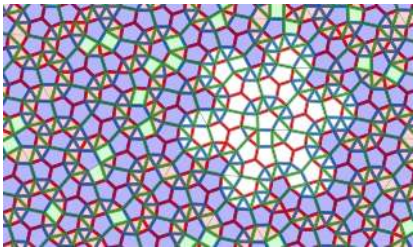
181st MSS Seminar
Tuesday, June 18, 14:00,
Room 00.156,
Cauerstraße 3, Erlangen.

Computational design and thermodynamic stability of aperiodic crystals and their approximants

Nydia Roxana Varela-Rosales

Institute for Multiscale Simulation, University of Erlangen-Nürnberg

This work seeks to further advance the exploration of aperiodic crystals from a theoretical standpoint. We will introduce simulation models for 2D and 3D quasicrystals and their approximants and present systematic studies showing their thermodynamic stability.



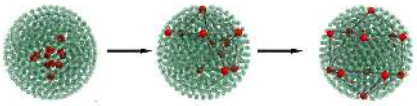
182nd MSS Seminar
Wednesday, July 10, 15:30,
Room 00.156,
Cauerstraße 3, Erlangen.

Entropy traps in spherical confinement

Dr. Praveen Bommineni

Department of Chemical Engineering, National Institute of Technology Warangal

In this presentation, we show evolution of large particles in a pool of small particles in a spherical confinement and subsequently the role of confinement in selectively trapping large particles into minimum free energy positions on the confinement surface. Potential mean force (PMF) based free energy calculations indicate that these minimum free energy positions correspond to icosahedra vertices.



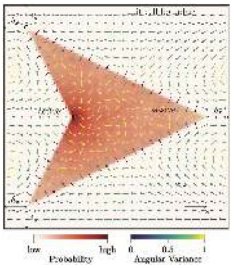
Evolution of large particles (red) in small particles (green) in the spherical confinement with time.

183rd MSS Seminar
Wednesday, July 17, 15:30 hrs,
Room 00.156,
Cauerstraße 3, Erlangen.

Mesoscopic signatures of colloidal heating, motility, and retarded and non-reciprocal interactions

Prof. Klaus Kroy
Institut für Theoretische Physik (ITP), Leipzig University

On a mesoscale, suspensions of colloidal particles that are locally out of equilibrium can to some extent be described like isothermal suspensions with effective parameters. Such parameters can often be calculated for sufficiently symmetric setups, but the convenient mappings may ultimately break down. I will discuss informative mesoscale signatures of local nonequilibria for a range of minimal models, involving local heating, self-propulsion, and time-delayed and non-reciprocal interactions of colloidal particles. The emergent phenomenologies comprise hot Brownian motion, active heat engines, static and dynamic polarization-density patterns, ensuing autonomous ratcheting, and time-reversal symmetry breaking fluctuations at phase transitions.

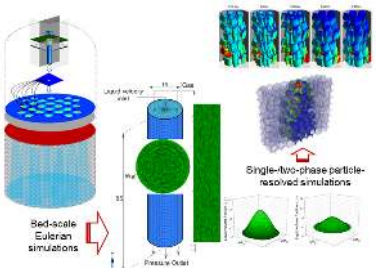


184th MSS Seminar
Tuesday 10th September, 2024, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

Multiscale Modelling & Simulations of Multiphase Flows: Applications to Packed Bed Reactors

Vivek V. Buwa
Schlumberger Chair Professor
Department of Chemical Engineering, Indian Institute of Technology Delhi, New Delhi, India

Several industrial processes involve a wide variety of multiphase flow processes. Prof. Buwa will present his group's work on multi-scale modelling of packed bed reactors. We will present the development of Eulerian multifluid model to simulate reactor(bed)-scale liquid distribution and the challenges associated with the closure models. He will show how particle-resolved simulations can be used to understand the heat-/mass-transfer limitations for solid-catalysed reactions. He will share his recent work on simulations of particle-scale two-phase flow.

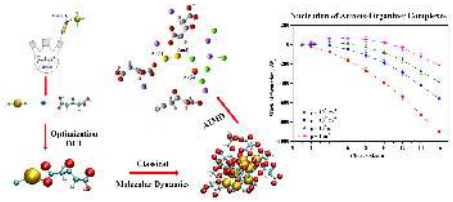


185th MSS Seminar
Wednesday 18th September, 2024, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

Mechanistic details of the organizer-assisted nucleation of gold nanoparticles (AuNPs) by the Turkevich method

Rajesh Pavan Pothukuchi
Department of Chemical Engineering, Indian Institute of Science, Bangalore, India

Turkevich's method for synthesizing citrate-stabilized highly stable gold nanoparticles (AuNPs) is most popular. Previous studies showed the need to incorporate the role of di-carboxy acetone (DCA) as organizer for Au+ ions in explaining the kinetics of AuNP formation. In this work, we identified the probable structure of complex formed between DCA and $AuCl_2^-$. This complex is highly insoluble in water and immediately nucleates to form cluster, using AIMD we showed the disproportionation of Au+ to metallic Au.

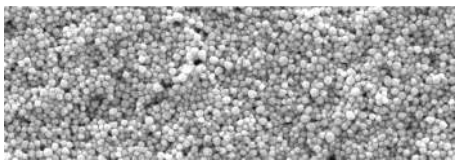


186th MSS Seminar
Friday 20th September, 2024, 12:15
Room 00.156,
Cauerstraße 3, Erlangen

Self-assembled Sensor Materials

Tobias Kraus
INM – Leibniz Institute for New Materials and Saarland University

We assemble molecules and particles into "sensor materials" that change optical or electronic properties and report relevant environmental parameters. They require electronically coupled particles and molecules in self-assembled superlattices — their design will be discussed in detail. Sensor materials do not require power sources and can be produced at low cost. I will discuss aspects of selectivity, recycling, and biodegradation for sensor materials that can remain in the environment, for example for precision agriculture.



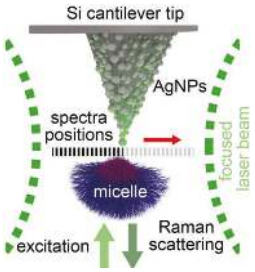
187th MSS Seminar
Wednesday 6th November, 2024, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

Inside Block Copolymer Micelles – A Journey of Crosslinking Strategies along Interfacial Boundaries

Prof. Felix H. Schacher

Institute of Organic Chemistry and Macromolecular Chemistry,
Friedrich Schiller University Jena, D-07743 Jena, Germany

We established tip-enhanced raman spectroscopy and force-distance AFM techniques to probe polymer nanoparticles and polyether-based block copolymer micelles with regards to (nanoscopic) mechanical properties and the presence of covalent crosslinks. In the latter case, we employed Diels-Alder chemistry for crosslinking of poly(furfuryl glycidyl ether) (PFGE) segments using different bismaleimides (BMI) and showed that the spectroscopic BMI signature is preferentially found in the micelle cores. With that, we have methods at hand that can be used beyond nano-local monitoring of crosslinking efficiency, but might become powerful tools to evaluate the positioning of payloads in general within block copolymer micelles.



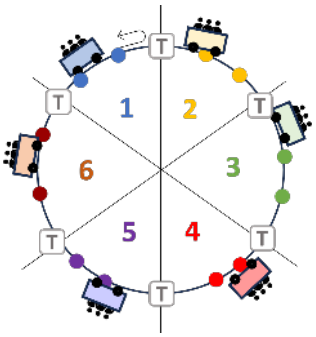
188th MSS Seminar
Wednesday 27th November, 2024, 15:30
Room 00.156,
Cauerstraße 3, Erlangen

How zoned buses achieve synchronization

Sakurako Tanida

Department of Aeronautics and Astronautics, School of Engineering, University of Tokyo

As transportation systems grow increasingly interconnected, understanding the principles of their synchronization is essential for efficient route design. In this study, we investigate synchronization dynamics in transportation systems structured into zones, where routes are only partially or indirectly connected, using discrete model simulations. Our results show that synchronization is strongly affected by the number of zones within the system. Using a mathematical model with self-consistent equations, we demonstrate how the zone structure of a transportation system influences synchronization patterns.



4. Conference Presentations

Talks

Achim Sack	*Elektrische Impedanztomographie* 4th ROBIN Project Meeting Leipzig | Germany, 18 – 19.12.2023
Thorsten Pöschel	*Granular Convection in Micro-Gravity* IUTAM Symposium on Rapid Granular Flows and Turbulent Particle Suspensions, organized by the Indian Institute of Technology Bombay | India, 21 – 25.01.2024
Thorsten Pöschel	*Structure and History of Granular Sediments* AOT-TP-Seminar Erlangen | Germany, 6.02.2024
Amir Nazemi	*Understanding the Propulsion of a scallop-like swimmer in Granular Media* 2024 APS March Meeting Minneapolis | USA, 04 – 08.03.2024
Felix Buchele	*A novel, first-principles-based, mesoscopic surface reaction model for particle-based flow simulations* DECHEMA Fachgruppensitzung MPH/AT/CFD Bremen | Germany, 20. – 21. 03.2024
Michael Engel	*Modeling Mesomorphological Structure Formation in Drying Droplets* Spray Drying Symposium Würzburg | Germany, 8 – 9.04.2024
Olfa D'Angelo	*Soft Robotics* Workshop on Discrete Simulation and Continuum Modeling of Granular Matter Puglia | Italy, 05 – 11.05.2024
Holger Götz	*Granular jamming in membranes* Inaugural Conference of the Open Network on Discrete Element Method (DEM) Simulations, Aalto University Espoo | Finland, 14 – 16.05.2024

Carlos L. Bassani — *Emergence of Mesomorphology from Molecular Ordering: Faceted Nanocrystals and Porous Clathrate Hydrates*
ATOMS Seminar Series, 16.05.2024
Webinar available online:
`https://www.youtube.com/watch?v=B0BdLDudIQo`

Michael Engel — *Simulating Hierarchical Structure Formation in Drying Droplets*
Platform for Advanced Scientific Computing (PASC24)
Zürich | Switzerland, 3 – 5.06.2024.

Thorsten Pöschel — *Entwicklung und Einsatz robuster elektrischer Mess- und Bildgebungsverfahren zur hochaufgelösten Erfassung von thermohydraulischen Parametern in Großversuchsanlagen der nuklearen Sicherheitsforschung - Implementierung und Experimente - ROBINIE*
Treffen der GRS (Gesellschaft für Reaktorsicherheit)
Köln | Germany, 04.06.2024

Thorsten Pöschel — *EIT imaging for the high-resolution imaging of fluid flow for nuclear safety research*
Tagung der Gesellschaft für Anlagen- und Reaktorsicherheit
Köln | Germany, 05.06.2024

Carlos L. Bassani — *Experiments and Modeling of Gas Hydrate Wall Deposition Mechanisms in Multiphase Sheared Systems*
ECGH 2024 - European Conference on Gas Hydrates
Trieste | Italy, 11 – 14.06.2024

Carlos L. Bassani — *Mesomorphology of Clathrate Hydrates from Molecular Ordering*
ECGH 2024 - European Conference on Gas Hydrates
Trieste | Italy, 11 – 14.06.2024

Patric Müller — *Laser melting processes of metals in reduced gravity*
4th Symposium on Materials and Additive Manufacturing
Bremen | Germany, 12 – 14.06.2024

Carlos L. Bassani — *Coordination Number-Biased Energy describes Nanocrystals with Kinetic Wulff Shapes*
Gordon Research Conference - Noble Metal Nanoparticles: Research and Development of Novel Materials for Catalysis, Energy Conversion and Sensing
South Hadley | USA, 16 – 21.06.2024

Thorsten Pöschel — *Fractal Structure of Nano-Powders*
Universität Liège – Fakultätsseminar
Liège | Belgium, 01.07.2024.

Thorsten Pöschel — *Passing through time and space scales*
ON-DEM Meeting, Vilnius Tech
Vilnius | Lithuania, 31.7.-2.8.2024

Michael Engel — *Structural Complexity in Colloidal Self-Assembly*
Special Lecture for NITech Frontier Research Institutes, Nagoya Institute of Technology
Nagoya | Japan, 07.08.2024.

Carlos L. Bassani	*Predicting nanocrystal growth into different shapes via kinetic Monte Carlo simulation* ECGH 2024 - 38th Conference of the European Colloid & Interface Society Copenhagen | Denmark, 1 – 6.09.2024
Michael Engel	*Structural Complexity in Colloidal Self-Assembly* Ph.D. Workshop Leibniz Institute of Polymer Research Schmiedeberg | Germany, 12.09.2024.
Carlos L. Bassani	*Predicting nanocrystal growth into different shapes via kinetic Monte Carlo simulation* PBM 2024 - Particle-Based Materials Symposium 2024 Bremen | Germany, 23 – 24.09.2024
Michael Engel	*Stable Quasicrystal from Tetrahedron Nanocrystals* PBM 2024 - Particle-Based Materials Symposium 2024 Bremen | Germany, 23 – 24.09.2024.
Praveen Bommineni Michael Engel	*Binary Crystals Formation from Molecular Simulations of Hard Disk Mixtures* 52nd Biennial Assembly of the German Colloid Society Dresden | Germany, 30.09 – 02.10. 2024.
Michael Engel	*Modeling and Observation of Structure Formation in Drying Droplets* AIChE Annual Meeting San Diego | USA, 27 – 31.10.2024.
Michael Engel	*Stable Quasicrystal from Tetrahedron Nanocrystals* AIChE Annual Meeting San Diego | USA, 27 – 31.10.2024.
Nicolas Pechler	*Elektrische Impedanztomographie* 5th ROBIN Project Meeting Zurich | Switzerland, 05 – 06.11.2024
Thorsten Pöschel	*Scientific Presentation* FRASCAL-Seminar Erlangen | Germany, 08.11.2024
Carlos L. Bassani	*Kinetically Trapped Nanocrystals with Symmetry-Preserving Shapes* Webinar Series GEOMPACK - Geometry & Packing in Material Structure & Biology 20.11.2024
Thorsten Pöschel	*Comparison and benchmarking of bulk properties of a capillary bridge model* Traffic and Granular Flow 24 Lyon | France, 02.12.2024
Sudeshna Roy	*Shear flow of wet granular matter: Influence of the capillary bridge model using MercuryDPM* Traffic and Granular Flow 24 Lyon | France, 02.12.2024
Thorsten Pöschel	*Symmetry and asymmetry in granular convection* 7th Southern Workshop on Granular Materials Puerto Varas | Chile, 05.12.2024

Thorsten Pöschel	*Smoothed Particle Hydrodynamics Simulation for Wire-Based LASER Metal Deposition in Additive Manufacturing* CompFlu-2024, IIT Hyderabad Hyderabad | India, 15 – 19.12. 2024

Posters

Nicolas Pechler	*Electrical Impedance Tomography for Void Fraction Analysis in Two-Phase Flow* KERNTECHNIK 2024 Leipzig | Germany, 11. – 13.06.2024
Carlos L. Bassani	*Coordination Number-Biased Energy describes Nanocrystals with Kinetic Wulff Shapes* Gordon Research Seminar - Noble Metal Nanoparticles: Harnessing the Potential of Noble Metal Nanostructures for Diverse Applications: An Intersection of Physics, Chemistry and Biology South Hadley | USA, 15 – 16.06.2024
Carlos L. Bassani	*Coordination Number-Biased Energy describes Nanocrystals with Kinetic Wulff Shapes* Gordon Research Conference - Noble Metal Nanoparticles: Research and Development of Novel Materials for Catalysis, Energy Conversion and Sensing South Hadley | USA, 16 – 21.06.2024
Olfa D'Angelo	*Structural features of jammed-granulate metamaterials* Gordon Research Seminar - Granular Matter (GRS) South Hadley | USA, 22 – 23.06.2024
Holger Götz	*Granular Convection in Zero-Gravity* Granular Matter Conference GRC, Stonehill College Easton | USA, 23 – 28.06.2024
Hongyi Xiao	*Locomotion of a scallop-like swimmer in granular media* 8th International Soft Matter Conference Raleigh | USA, 29.07 – 02.08. 2024
Navid Panchi	*AES-Debye: Accurate and Efficient Implementation of Debye Scattering Equation* European Powder Diffraction Conference (EPDIC - 18) Padova | Italy, 27.08 – 01.09.2024
Harsha Namdeo	*Modeling Colloidal Interactions and Assemblies for Optimal Functional Materials* Collaborative Research Centre 1411 (CRC 1411) Waischenfeld | Germany, 25 – 26.11. 2024

Electrical Impedance Tomography for Void Fraction Analysis in Two-Phase Flow

Nicolas Pechler, Achim Sack, Thorsten Pöschel
Friedrich-Alexander-Universität , Institute for Multiscale Simulation, Erlangen, Germany
Nicolas.Pechler@fau.de

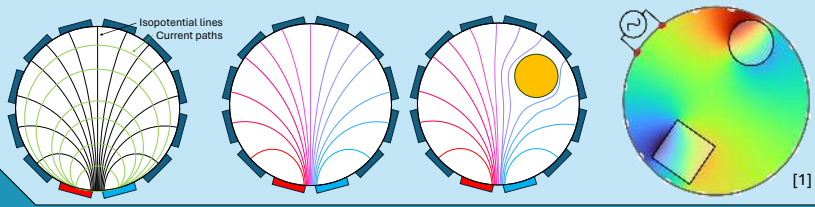
Aim

- Non-invasive imaging of void fraction and cross-section under harsh conditions
- Suitable for real-time monitoring of two-phase flow in power plant cooling circuits

ROBIN AP 2.1
gefördert durch das BMBF
FKZ: 02NUK068A

Electrical Impedance Tomography

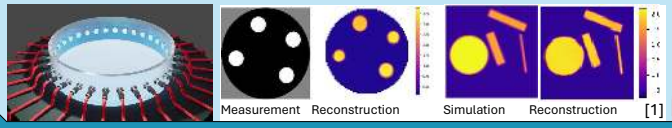
- Determination of the impedance distribution inside the volume by surface measurement
- 64 electrodes: 2 electrodes for current injection, 64 electrodes for potential measurement
- Current injection leads to a potential distribution measured by the electrodes
- Placing an object changes the potential distribution according to its conductivity
- The excitation patterns (current injection pairs) are permutated and measurement is repeated
- Real-time monitoring by frequency multiplexing over 64 signal channels simultaneously
- Each electrode has its own excitation frequency; its impact on the system is measured on all electrodes



[1]

2D Reconstruction & AI Training

- Reconstruction necessary for cross-section imaging (ill-posed problem)
- Traditional reconstruction algorithms are too slow for real-time monitoring
- We've shown in the past that AI is a feasible approach for 2D reconstruction [1]



[1]

3D Data Generation Setup

- AI training on the 3D problem needs a huge dataset
- Measurement data is generated by automated displacer placement
- Pipe section model: ⌀ = 125 mm, l = 1200 mm
- Staggered electrodes on three rings (16-32-16)
- Co-axial electrodes for simultaneous excitation and measurement
- 64 Channel 1 Msps sampling for frequencies up to 500 kHz

References:
[1] Ayman A Ameen, Achim Sack and Thorsten Pöschel (2024), *TSS-ConvNet for electrical impedance tomography image reconstruction*. Physiological Measurement, Volume 45, Number 4

GEFÖRDERT VOM
Bundesministerium für Bildung und Forschung
FAU Friedrich-Alexander-Universität Erlangen-Nürnberg
KERNTECHNIK

Coordination Number-Biased Energy describes Nanocrystals with Kinetic Wulff Shapes

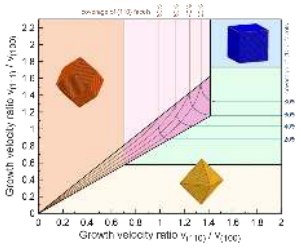
Carlos L. Bassani, Michael Engel

Institute for Multiscale Simulation (MSS), Department of Chemical and Bioengineering (CBI), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany

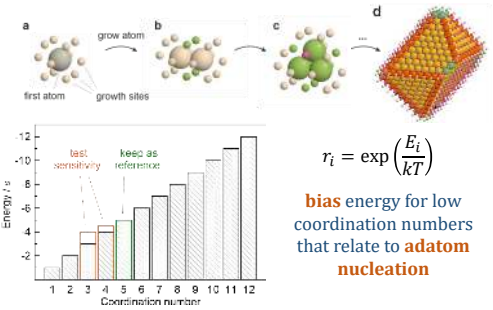
Motivation

- **Why do different nanocrystal shapes form?**
- How to predict the emergence of nanocrystals with **10 to 100 nm** keeping **atomic resolution**?
- Crystallographic directions with **slower growth velocity** limit nanocrystal growth

Geometric Construction



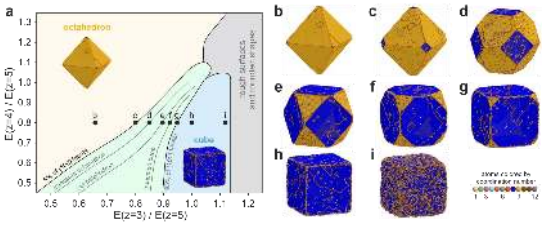
Rejection Free Kinetic Monte Carlo



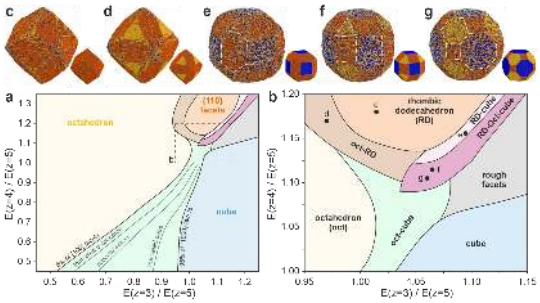
$$r_i = \exp\left(\frac{E_i}{kT}\right)$$

bias energy for low coordination numbers that relate to **adatom nucleation**

Shape Diagrams

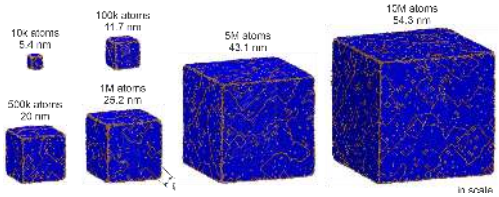


simulation conditions: nanocrystal of 1 million atoms, perfect fcc structure, bond energy = 1, kT = 0.2, only growth events

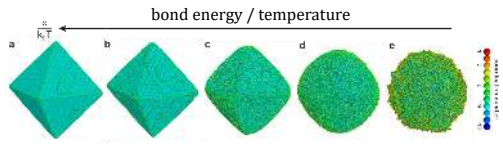


simulation conditions: same, but 60% growth events, 40% dissolution events

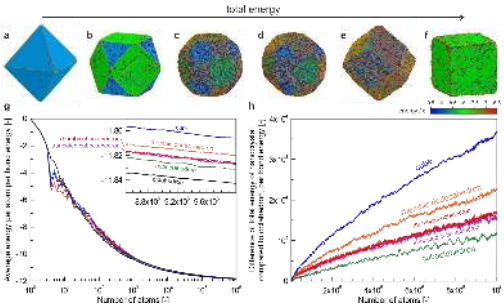
Realistic Nanocrystal Size



Roughening and Rounding



Kinetically Trapped Nanocrystals



Discussion

For high ratio between bond energy and temperature, growth follows a layer-by-layer mode (atoms grow only to most energetically favorable sites), forming nanocrystals with smooth facets. **Adatom nucleation** limits growth velocity. When biasing the energy related to adatom nucleation (herein, coordination numbers 3, 4, and 5 for fcc), the **ratio of growth velocity between crystallographic directions** (100), (110), and (111) changes and the nanocrystals assume shapes of all the family of truncations between cube, octahedron, and rhombic dodecahedron. Each shape presents a different total energy. They are kinetically trapped in local energy minima, known as **kinetic Wulff shapes**.

contact: carlos.bassani@fau.de, michael.engel@fau.de

Manuscript in preparation: C.L. Bassani, M. Engel. Coordination Number-Biased Energy describes Nanocrystals with Kinetic Wulff Shapes. To be submitted to ACS Nano, 2024.
Relevant literature: [1] T.-H. Yang, Y. Shi, A. Janssen, Y. Xia. Surface Capping Agents and Their Roles in Shape-Controlled Synthesis of Colloidal Metal Nanocrystals. Angew. Chem. Int. Ed. 2020, 59, 15378. **[2]** M. Grzelczak, J. Pérez-Juste, P. Mulvaney, L. M. Liz-Marzán. Shape Control in Gold Nanoparticle Synthesis, in: Colloidal Synthesis of Plasmonic Nanometals, Jenny Stanford Publishing, 2020. **[3]** Y. Kang, J. Beom Pyo, X. Ye, R.E. Diaz, T.R. Gordon, E.A. Stach, C.B. Murray. Shape-Controlled Synthesis of Pt Nanocrystals: The Role of Metal Carbonyls. ACS Nano 2013, 7, 645–653. **[4]** M.R. Hauwiller, L.B. Frechette, M.R. Jones, J.C. Ondry, G.M. Rotskoff, P. Geissler, A.P. Alivisatos. Unraveling Kinetically-Driven Mechanisms of Gold Nanocrystal Shape Transformations Using Graphene Liquid Cell Electron Microscopy. Nano Lett. 2018, 18, 9, 5731–5737

Friedrich-Alexander-Universität
Department Chemie- und Bioingenieurwesen
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ENGINEERING OF ADVANCED MATERIALS
FAU COMPETENCE CENTER
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Jammed-granulate metamaterials for soft robotics

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

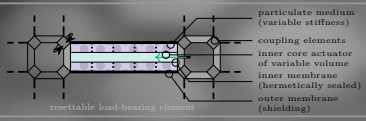
Institute for Multiscale Simulation, Universität Erlangen-Nürnberg, Cauerstraße 3, 91058 Erlangen, Germany

INTRODUCTION

soft robotics — robots composed of compliant materials

jamming-based actuators — large stiffness range, minimal volume variation

metamaterials — materials with engineered properties, drawn from that of *constituents & structural features*



METHODS

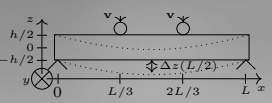
SIMULATION SETUP

DEM simulation, details [PRR **6**, 013061 (2024)]: contact model [PRE **53**, 5382 (1996)], no cohesion, $d = 3.5\,\mathrm{mm} \pm 20\%$, $\sim 11\,000$ particles

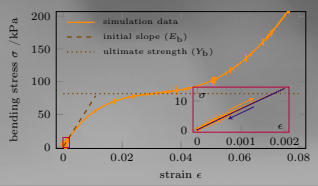
beam geometry: $L = 40\,\mathrm{cm}$, cross section $4\,\mathrm{cm} \times 8\,\mathrm{cm}$

quasi-static deformation ($v = 0.2\,\mathrm{mm\,s^{-1}}$), controlled by deformation

Euler-Bernoulli beam theory: $\sigma = F\frac{L}{bd^2}$, $\epsilon = \Delta z \frac{108h}{21L^2}$



METHODS



PROTOCOLS

PROTOCOL A: packing density ϕ_{bend} function of friction μ_p

$\mu \equiv \mu_{\mathrm{init}} = \mu_p$

seeding → growth until $\phi \geq \phi_{\mathrm{init}}$ → confining pressure → bending starts $\phi_{\mathrm{bend}}(\mu_p)$

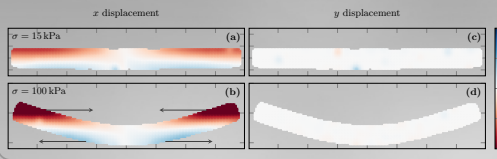
PROTOCOL B: fixed density ϕ_{bend} at bending onset $\forall \mu_p$

$\mu \equiv \mu_{\mathrm{init}}$ $\mu = \mu_p$

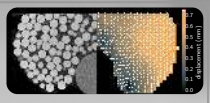
seeding → growth until $\phi \geq \phi_{\mathrm{init}}$ → confining pressure → bending starts $\phi_{\mathrm{bend}}(\mu_{\mathrm{init}})$

step I — step II — step III — step IV

NEUTRAL PLANE LOCATION



neutral plane: no stress, no deformation surface (midplane)



TEMPORAL EVOLUTION

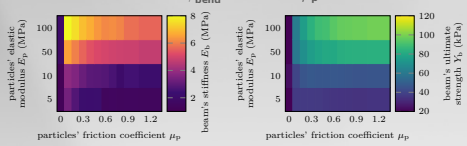
- *early* (before Y_b): initially, neutral plane & geometrical midplane coincide
- *throughout bending*: plane **shifts upwards**
- *later stage* (past Y_b): extremities bend inwards, shift exacerbated

SPATIAL LOCATION

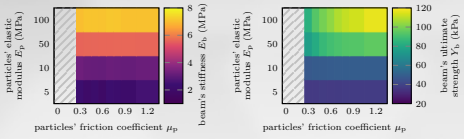
- *above:* compression, particles' motion towards beam's center
- *below:* tension, particles' motion away from beam's center
- *extremities:* largest displacement at extremities (*cf.* granular gripper X-ray CT: more geometric freedom and direct contact with membrane → preferential retraction in surface)

MICRO TO MACRO

PROTOCOL A: ϕ_{bend} function of μ_p



PROTOCOL B: $\forall \mu_p$, same ϕ_{bend}

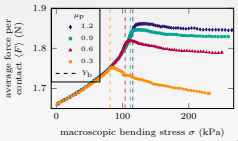


BEAM'S ELASTIC MODULUS

- **depends on preparation through packing density ϕ**
- at fixed ϕ, independent of particles' friction μ_p
- generally increases with particles' stiffness, E_p
- proportionality relation: beams' elastic modulus $E_b \sim E_m\,\Delta p\,E_p$, membrane stiffness, E_m, confining pressure, Δp, particles' stiffness E_p [Granul. Matter **25**, 58 (2023)]

BEAM'S ULTIMATE STRENGTH

- increases with E_p, μ_p and ϕ: at fixed E_p, $Y_b(\mu_p) = (Y_b^0 - Y_b^\infty)e^{-\alpha\mu_p} + Y_b^\infty$
- **corresponds to force network collapse:**



STRUCTURAL FEATURES

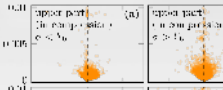
DEFORMATION MECHANISMS

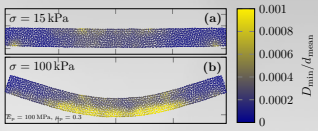
- *affine:* large-scale, homogeneous, coordinated motion; $D_{\min} \to 0$
- *localized:* one particle breaks neighbors-formed cage; $D_{\min} > 0$

quantified by $D_{\min}$ [PRE **57**, 7192 (1998)]: mean-square deviation from affine of particle i to neighbors j, within $\Delta t = t' - t = 2.5\,\mathrm{s}$:

$$D^2(i,t,t') = \frac{1}{N}\sum_j \left[\mathbf{r}_j(t') - \mathbf{r}_i(t') - (\mathbb{1}+\epsilon)(\mathbf{r}_j(t) - \mathbf{r}_i(t))\right]^2,$$

for affine deformation ϵ so that $D_{\min} = \min_\epsilon |D|$

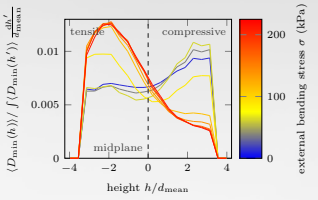




- jammed phase **deforms in affine motion**: no shear band, initially no delimitation at neutral plane

LOCAL DENSITY VARIATIONS

SPATIAL DISTRIBUTION OF LOCAL DEFORMATION

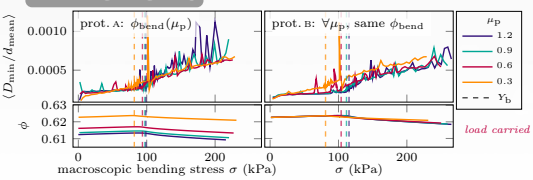


- **deviation from affine is correlated with change in local packing fraction** (v-shape of all graphs)
- past Y_b: part in tension (bottom) allows expansion, hence more individual particle motion

plot of normalized $D_{\min}$ as a function of beam's height:

- initially: $D_{\min}$ larger in top part (compressive)
- then becomes much larger in bottom part (tensile), as particles have enough space to move
- transition happens around Y_b

BENDING REGIMES



before Y_b:

- system densifies on average
- deforms in fully affine manner
- top part compressed, while pressure gradually relieved in bottom (without motion): $D_{\min}$ close to 0

after Y_b:

- as neutral plane rises, part in tension increases
- ϕ on average decreases, effectively leaving more space for particles' motion: $D_{\min}$ increases

load carried by: granular packing (top) in compression — external membrane (bottom) in tension

effect of particles' properties:

- μ_p: influence through initial packing density but not deformation mechanism
- μ_p: shifts Y_b for hard particles; no influence on Y_b for soft particles
- soft particles (not shown): higher packing density at same confining pressure, hampers non-affine deformation

CONCLUSION

preparation protocol:

- select E_p for desired compliance
- maximize packing density, e.g. preconstrain beam in pre-Y_b regime

reinitialization of beam:

- *in-situ* sensing for optimizing reinitialization frequency: find Y_b, when granulates stop carrying load (compression), possibly through extension of bottom membrane

H. Götz, T. Pöschel, O. D'Angelo, Phys. Rev. Research **6**, 013061(2024)
O. D'Angelo, A. Sack, T. Pöschel, German Patent App. DE 10 2023 130 608.1 (2023)
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Institute for Multiscale Simulation

ENGINEERING OF ADVANCED MATERIALS

Friedrich-Alexander-Universität Technische Fakultät

Granular Convection in Zero-Gravity

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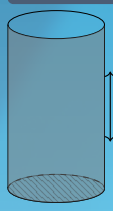
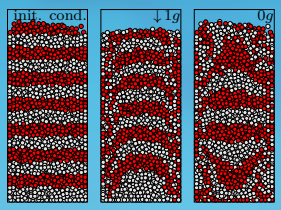
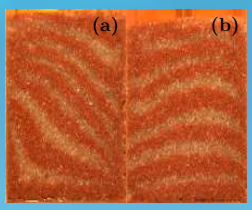
Introduction



system setup
- cylinder filled with particles
- vertical vibrations of the form $z(t) = A\sin(2\pi ft + \phi)$

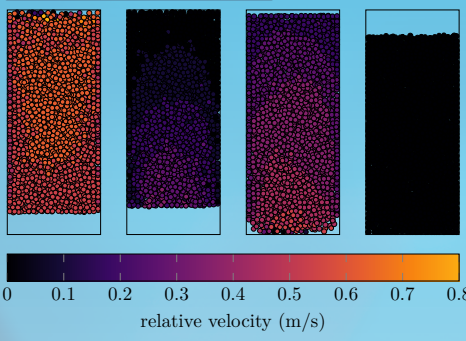


expected result
- **gravity** particles travel upwards in the center and downwards at the sides
- **zero gravity** particles movement is point symmetric to the center of mass



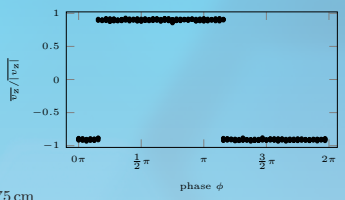
experimental results in 0g
- **(a)** particle layers are tilted. Only one convection cell appears
- **(b)** gravity pattern is recovered

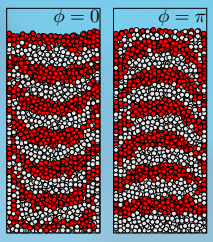
Broken up/down symmetry



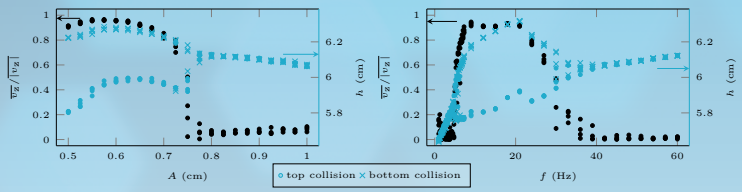
The conditions of the collisions with the top and bottom wall differ:
- **before the collision with the top wall**: the granulate is dense
- **after the collision with the top wall**: a velocity gradient is visible; the granulate can expand
- **before the collision with the bottom wall**: the granulate is less dense
- **after the collision with the bottom wall**: no visible velocity gradient; the granulate remains dense

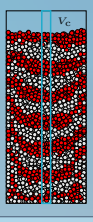
Direction is determined by initial condition, e.g., phase





When does the convection become symmetric?
- broken symmetry for $A \lesssim 0.75\,\mathrm{cm}$; repaired symmetry for $A \gtrsim 0.75\,\mathrm{cm}$
- broken symmetry for $5\,\mathrm{Hz} \lesssim f \lesssim 35\,\mathrm{Hz}$; repaired symmetry for $f \lesssim 5\,\mathrm{Hz}$, $f \gtrsim 35\,\mathrm{Hz}$





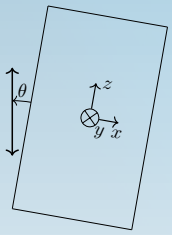
Determine symmetry:

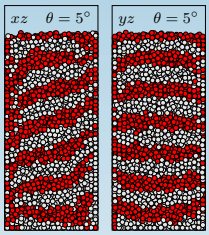
$$\overline{v_z} = \frac{1}{\rho_c}\sum_{i=1}^{N}\frac{m_i v_{z,i} V_{i\cap c}}{V_i V_c}$$

$$\overline{|v_z|} = \frac{1}{\rho_c}\sum_{i=1}^{N}\frac{m_i |v_{z,i}| V_{i\cap c}}{V_i V_c}$$

$$\rho_c = \sum_{i=1}^{N}\frac{m_i V_{i\cap c}}{V_i V_c}$$

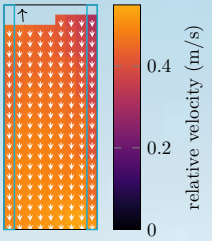
Convection in tilted cylinder



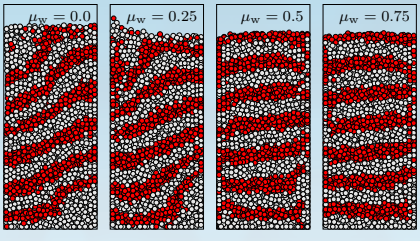


changed system setup
- vibration direction tilted against x and z
- in the xz-plane, only one convection cell appears
- in the yz-plane, the convection is unchanged

- **before the collision with the bottom wall:** particles on the left ($x < 0$) move downwards faster than particles on the right ($x > 0$)



- **effect is purely geometrical:** without friction, the convection pattern persists



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Locomotion of a scallop-like swimmer in granular media

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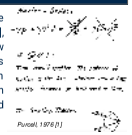
Motivation

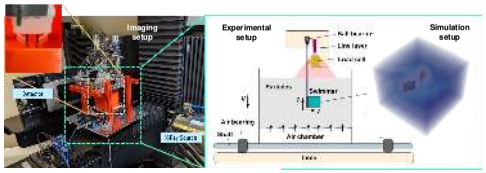
We aim to understand how simple swimming motion can generate locomotion in granular media. As stated by the scallop theorem [1], reciprocal motion cannot generate locomotion in Newtonian fluids at low Reynolds numbers. However, this is possible in complex fluids such as viscoelastic liquids [2, 3]. Granular matter is a soft and yielding medium that demonstrates both liquid-like and solid-like behaviors that can depend on pressure, rate, and history. This makes understanding and designing locomotion mechanisms challenging.



When an intruder penetrates granular matter, a stagnant zone forms near the leading face of the body, in which particles are jammed [4]. Microscopically, force chains form, percolate, and break near the moving intruder. This gives the medium an elastoplastic response and its implications in locomotion is yet to be fully understood. While it has been observed that a single reciprocally rotating rod can generate locomotion [5], particle-level information and mechanisms of locomotion have not been investigated. Thus, we further examine reciprocal locomotion in granular media using a scallop-like swimmer with two flapping-wings.

DEM simulations and experiments with X-ray imaging

- A 3D-printed scallop-like swimmer was buried into 1 mm polydisperse polystyrene particles.
- An air chamber was used to fluidize particles to reset their initial packing configuration.
- Air bearings were used to support the container so that it only feels force from the swimmer.
- X-ray computed tomography (CT) was used for analyzing the motion of the particles.

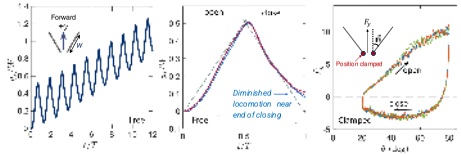


- **Discrete Element Method** (DEM) were used to simulate the particles and a pair of counter-rotating wings, based on an open-source package MercuryDPM.
- Hertz-Mindlin model was used for simulating the interaction of ~510,000 spherical particles with mean diameter of 1 mm in an 80 mm wide container, which matches the experiment.
- The displacement of the scallop was updated using a velocity Verlet algorithm.

Locomotion in frictional granular matter

- With reciprocal opening and closing strokes, the swimmer can consistently propel itself in the $+y$ direction over time.

Experimental results:

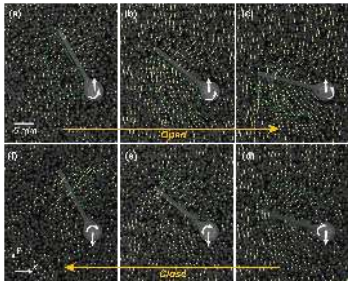


Swimmer displacement, y_s, over time, t, normalized by the period T | **Displacement in individual cycles** | **Propulsion force, F_y, in individual cycles with a clamped swimmer**

- We clamped the swimmer's position and monitor the propulsion force generation, which also shows a net force over a cycle that is in the $+y$ direction.
- The observation is insensitive to angle combination, rotation speed, and wing size varied at the quasi-static limit.

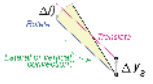
In-plane particle displacement field from X-ray CT

- To visualize particle motion in 3D, a quasi-statical experiment was performed under X-ray. A cycle was divided to several rotation steps and a full CT scan was taken for each step. In-plane displacement field measured from X-ray tomograms over a cycle shows the presence of stagnant zones in which particle displacements are aligned and follow the wing motion.
- The formation of a stagnant zones can be seen in front of the leading edges and are marked by the green boxes. The yellow arrows indicate the displacements of particles that can be tracked between two consecutive frames.



In-plane displacement field measured from X-ray tomograms taken during quasistatic swimming

View swimming as an action of the swimmer exchanging position with particles in front:

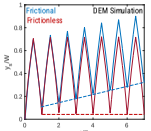


Opening: in-plane lateral particle displacement is seen, as an effective way to transport particles backward.

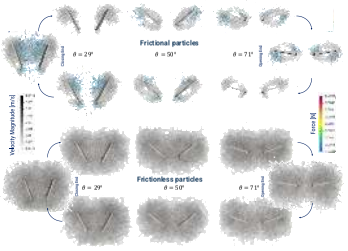
Closing: out-of-plane vertical particle rearrangements occur, as particle displacement vector is perpendicular to the wing, and many particles cannot be tracked due to vertical movement. This can be inefficient swimming.

Role of jamming and friction in forward swimming

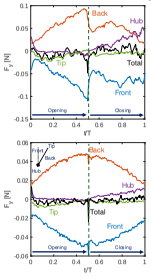
- By eliminating friction in simulation, the forward locomotion of the swimmer vanishes.
- Frictional case: force chains form only in front of the leading edges, breaking the symmetry. Strain localization occurs as the swimmer only perturb a small neighborhood of particles.
- Frictionless case: no significant force chains observed. The particle velocity field is symmetric between opening and closing, and more particles are perturbed.



Velocity and contact force visualization from DEM simulation



Force on each side of the wing



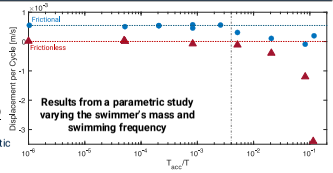
- We obtained the force applied to each surface of the wings in particle simulation. Near the end of closing, we observed significant contribution from of the hub. In separate measurements, we also see a significant contribution of tangential forces in the frictional case.

Role of inertia in backward swimming

- To investigate the role of the swimmer's inertia, we examine the ratio of time required for the swimmer to accelerate, T_{acc}, to the cycle period, T:

$$\frac{T_{acc}}{T} = \frac{(W/T)/(PW^2/M)}{T}$$

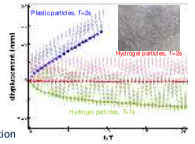
where P is the hydrostatic pressure.

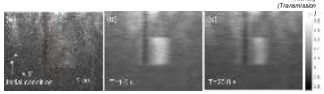


- In the frictional cases, a plateau exists at lower values of T_{acc}/T, showing a quasi-static regime. A decreasing trend was observed at higher values of T_{acc}/T, showing a transition to a dynamic regime which shows little locomotion . The two regimes separated by the vertical line.
- In the frictionless cases, the same plateau exists in the quasi-static regime but with no locomotion. At higher values of the time scale ratio, the decreasing trend is steeper than the frictional case, showing significant backward locomotion.

Locomotion in frictionless granular hydrogels

- We tested the same scallop swimmer in granular hydrogels also with 1 mm mean diameter.
- Hydrogel particles are frictionless, soft, and cohesive, giving an overall viscoelastic mechanical response with a characteristic relaxation time around 1 s.
- At low swimming frequency, the swimmer show no locomotion.
- At higher frequency comparable to the material relaxation time, the swimmer show backward locomotion locomotion.





Time-averaged X-ray radiograms (side view):

- At higher frequencies, the medium cannot relax fast enough and significant void regions exist behind trailing edges.
- At very high frequency, no locomotion was observed.

Summary

- Reciprocal motion of a scallop-like swimmer generates locomotion in both frictional granular particles and hydrogel particles, with different directions and frequency dependence.
- The swimmer's wing rotation creates stagnant zones in front of leading edges that breaks symmetry in both opening and closing strokes.
- Friction is important for the forward locomotion of the swimmer.
- The swimmer's inertia is important for the backward locomotion.

References

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[4] Kang, Wenting, et al. "Archimedes' law explains penetration of solids into granular media." *Nature Communications* 9.1 (2018): 1101.

[5] Texier, Baptiste Darbois, et al. "Propulsion by reciprocal motion into granular media." *Physical Review Fluids* 6.3 (2021): 034604.

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Understanding the Propulsion of a Scallop-like Swimmer in Granular Media

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Introduction

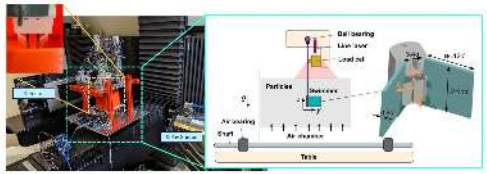
Understanding locomotion through reciprocal motion in complex media is challenging. While scallop theorem claims that any reciprocal motion, whether slow or fast, does not generate locomotion in Newtonian fluids in low Reynolds numbers, this theorem does not apply in complex media, such as viscoelastic fluids [1, 2].

Granular material is a complex medium that poses liquid-like and solid-like mechanical behaviors simultaneously, which has made understanding phenomena in locomotion challenging. When a solid body penetrates into a granular medium, a stagnant zone forms around the leading face of the body, in which particles are jammed [3]. As a consequence, the medium forms force chains that show a network of particles reacting to one another in their principal axis directions, which is the direction of most compressive principal stress [4].

For locomotion in granular media, it has been observed that a single reciprocally rotating rod can generate locomotion [5]; however, particle-level information and mechanisms of locomotion has not been investigated. Also, the system was not conserved in terms of total external torque applied to the rod. Therefore, we examined the locomotion in granular media by designing a scallop like swimmer with two flapping-wings.

DEM Simulations and Experiments with X-ray Imaging

- A 3D-printed scallop-like swimmer is buried into polydisperse polystyrene particles.
- An air chamber was used to fluidize particles and reset their initial configuration.
- Air bearings were used to support the container so that it only feels force from the swimmer.
- We performed X-ray computer tomography (CT scans to analyze the motion of the particles.



- Numerical simulations were conducted using discrete element method (DEM) to simulate the interaction between particles.
- Hertz-Mindlin model was used for interaction of ~510,000 particles with diameter of 1.0 mm which matches the experiment.

Summary

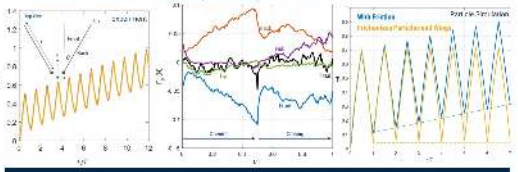
- Reciprocal motion can generate propulsion in frictional granular media.
- Swimmer's motion forms stagnant zones in front of leading edge that breaks symmetry in both opening and closing strokes.
- Particles in stagnant zones are in jammed state, as force chains observed.
- As friction influences the state of the particles, we can claim that friction is one of the primary effective parameters in locomotion of the swimmer.

References

[1] Qiu, Tian, et al. "Swimming by reciprocal motion at low Reynolds number." Nature communications 5.1 (2014): 5119.
[2] Normand, Thibaud, and Eric Lauga. "Flapping motion and force generation in a viscoelastic fluid." Physical Review E 78.6 (2008): 061907.
[3] Kang, Wenting, et al. "Archimedes' law explains penetration of solids into granular media." Nature Communications 9.1 (2018): 1101.
[4] Peters, J. F., et al. "Characterization of force chains in granular material." Physical Review E 72.4 (2005): 041307.
[5] Texier, Baptiste Darbois, et al. "Propulsion by reciprocal motion into granular media." Physical Review Fluids 6.3 (2021): 034504.

Position and Force Response

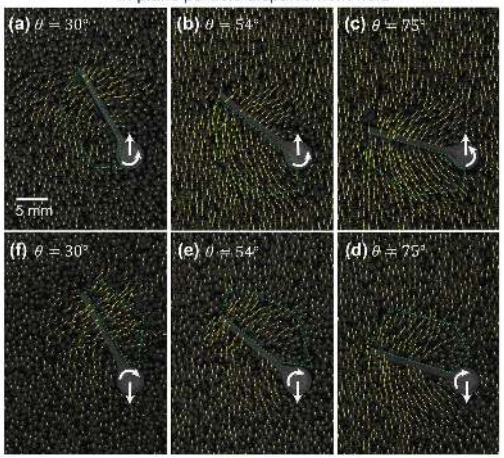
- We performed experiments and corresponding simulations and recorded the position of the swimmer over time while reciprocating by opening and closing the flapped-wings.
- Positive displacement in y-direction observed that confirms the locomotion generation using reciprocal motion in granular materials. Identical displacements were observed in both experiment and simulation.
- We obtained the force applied to each surface of the wings in particle simulation. We observed significant contribution of lift in total applied force over the closing stroke. However, total force tends to fluctuate around zero force.
- The comparison of the swimmer's position in frictionless case with base frictional case shows that locomotion of the swimmer vanishes by eliminating the friction.



Stagnant Zone and X-ray Tomograms

- The experiment was performed quasi-statically, meaning that a cycle was divided to several steps and a full CT scan was taken for each step.
- In-plane displacement field measured from X-ray tomograms over a cycle shows the presence of stagnant zones in which particle displacements are aligned and follow the wing motion.
- The formation of a stagnant zones can be seen in front of the leading edges and are marked by the green boxes.
- The white arrows indicate the wing rotation direction and the swimming direction, while the yellow arrows indicate the displacements of particles that can be tracked between two consecutive frames.

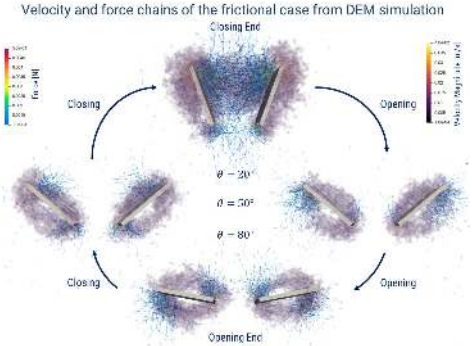
In-plane particle dispalcement field



Force Chains in Stagnant Zones

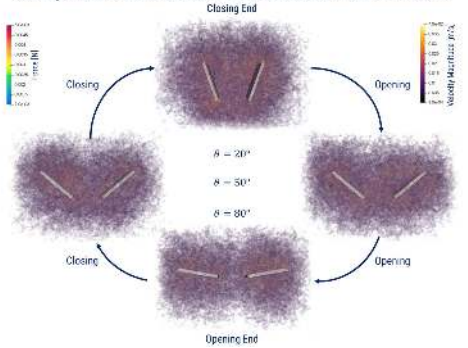
- The formation of force chains in the jammed stagnant zones is visualized in DEM simulation results below.
- The force chains are formed in front of the leading edge in both opening and closing strokes, whereas no force chains formed in front of trailing edge. This causes the symmetry breakage.
- The network intensifies as the wings angle decreases in closing stroke. However, contribution of tangential forces due to friction in the y component increases compared to normal forces, which agrees with decrease in the magnitude of the y component of force for front and back sides in closing stroke.

Velocity and force chains of the frictional case from DEM simulation



- As friction is one of the major factors of jamming and in order to ensure the jammed particles in the stagnant zones are the reason of interaction forces magnification in corresponding zones that breaks the symmetry and leads to locomotion, another particle simulation were performed, in which all particles and wings are frictionless.
- As seen in figure below, no force chains were formed in the frictionless case that can lead us to conclude that particles are not jammed to form any force chains in front of leading edges to break the symmetry.

Velocity and force chains of the frictionless case from DEM simulation



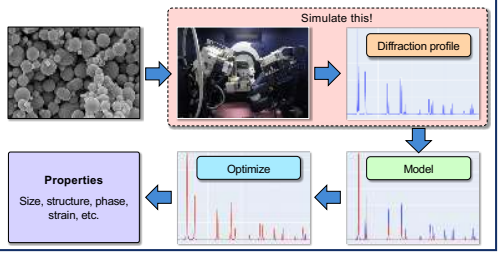
AES-Debye: Accurate, Efficient and Scalable Implementation of Debye Scattering Equation

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

[1]Institute for Multiscale simulation, IZNF, Friedrich-Alexander-Universität Erlangen-Nürnberg (Germany)
[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)

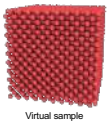
Motivation

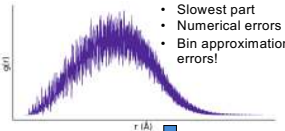
- Debye scattering equation is crucial for total scattering analysis
- Enables calculation of powder diffraction patterns for virtual samples
- Requires extensive computational resources



Debye Scattering Equation (DSE)

Calculate pair distribution function (PDF)


Virtual sample



- Slowest part
- Numerical errors
- Bin approximation errors!

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

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

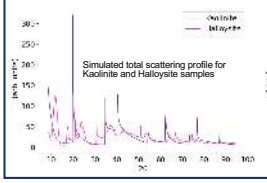
[1] A. Leonardi, D.L. Bish, J Appl Crystallogr 49 (2016) 1593–1608.

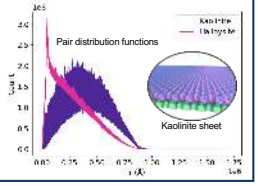
Application 1: Halloysites

- 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)


Halloysite spiral structure model created using a Kaolinite sheet

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

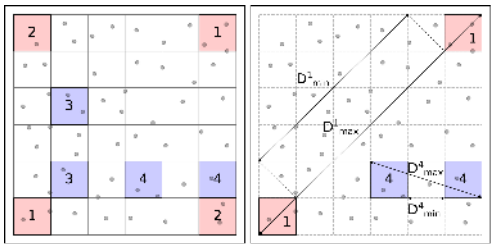




Other features

- 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

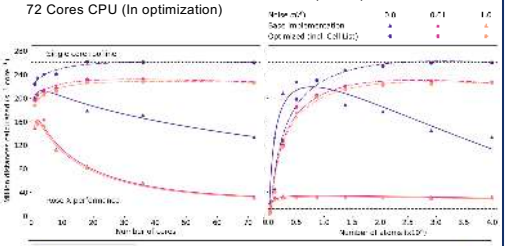
Domain Decomposition

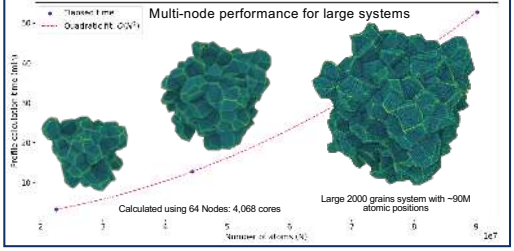


- Divide the box into equal cells
- Distribute atoms into different cells
- Create pairs of equidistant cells
- Equidistant pairs access same part of the PDF data structure memory
- Efficient cache utilization on CPU

Performance

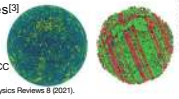
- Rose-X suffers from memory bandwidth limitation
- ~ 2x faster on Nvidia a100 GPU vs 72 Cores CPU (In optimization)
- Cells based approach helpful for realistic systems
- ~ 20x speed-up vs Rose-X

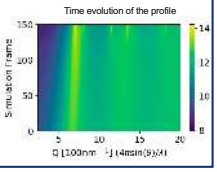




Application 2: Colloids

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


Left: Supra-particle colored with co-ordination number
Right: Crystallized FCC inside



[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.

D04

FP2

Modeling Colloidal Interactions and Assemblies for Optimal Functional Materials

Harsha Namdeo, Jyoti, Federico Tomazic, Kamilla Zaripova, Carlos Lange Bassani, Michael Engel

Institute of Multiscale Simulation (MSS), FAU

DESIGN OF PARTICULATE PRODUCTS CRC 1411

Mission of the project

Background and scope

- Nanoparticles synthesized within the CRC under varied experimental conditions exhibit different properties
- Perform **coarse-grained** simulations of these nanoparticle systems to describe the **assemblies** [1-5], **interactions** [6], **trajectories** [7] and **functional properties**
- Disordered systems can produce **angle independent structural colors**
- **Twinning** during nanocrystal growth leads to different nanocrystal shapes
- Characterize and quantify structural defects to decide what **optimum disorder** leads to the **target properties**
- Investigate the effect of **crystallographic defects** on **growth and shape** of nanocrystals.

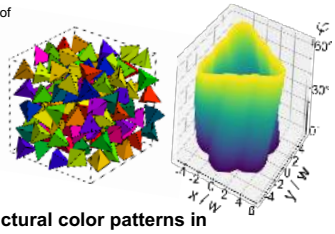
Key research questions

- **WP1** How do **complex 3D nanoparticles** interact? How to efficiently simulate this complex **anisotropic** interaction?
- **WP2** How disorder affects the angle dependence of structural color? Can this **disorder** be characterized in terms of **controllable parameters** for **dynamic systems**?
- **WP3** How does drying of droplet proceed? Are there any **characteristic structural defects** that occur? How can we target a desired **local or global order** by tuning particle properties and assembly conditions?
- **WP4** What processes drive the formation of distinct nanocrystals shapes? How do **kinetic factors** compare to **thermodynamic factors** in determining the final shape of a nanocrystal?

Results and ongoing work

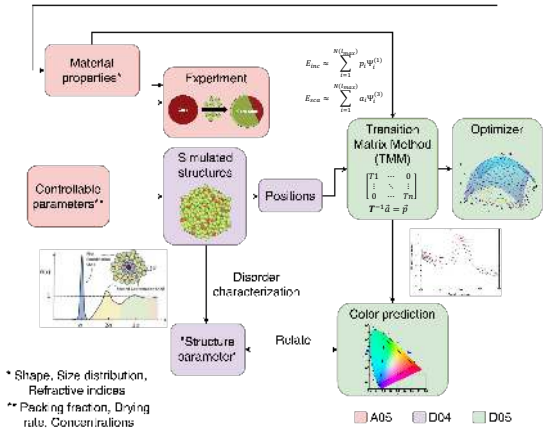
WP1 Implementation of complex particle model in three dimensions

- Investigation of the interactions of 3D complex particles [6]
- Implementation completed and interaction energies and forces calculated using **3D Derjaguin approximation**
- Calculated energies and forces tabulated and MD simulations performed using **in-house extension of HOOMD-Blue**



WP2 Prediction of structural color patterns in disordered systems

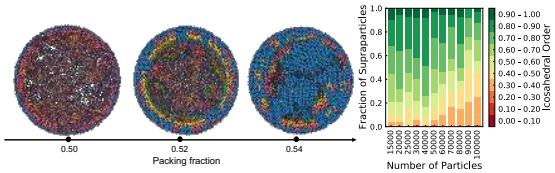
- Current objective is to study mono- and bi-disperse simulated systems
- Extension to **disordered bi-disperse core shell** and **inverse photonic** systems
- Color prediction for these structures performed using the **transition matrix method (TMM)** (D05)



- **Structure parameter** to relate between the computed colors (D05) and simulated structure (D04), which models the experiments (A05) and its controllable parameters
- Quantification of the **degree of disorder** to achieve optimal colors

WP3 Resolving kinetic effects during assembly and drying

- Drying of a colloidal cluster for mono and polydisperse sphere mixtures [7]
- Formation of "onion layers" investigated using MC, EDMD and EDMC (own code)
- Applied **novel point group symmetry parameters** to characterize the clusters

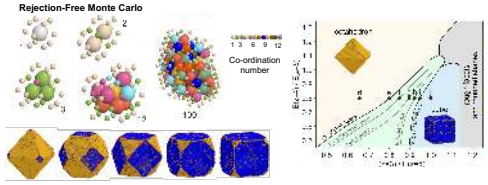


WP4 Kinetic Monte Carlo of nanocrystal growth and transformation

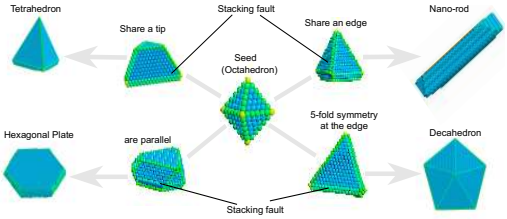
- We study the growth mechanism of nanocrystals of different shape using **Lennard-Jones** potentials at realistic system scales
- Probability of a particle growing at a growth site depends on the **Boltzmann factor**

$$p = \exp\left(\frac{-E_i}{kT}\right)$$

- System is kinetically trapped in local energy minima, resulting in the formation of diverse shapes during growth [2]



- Presence of defects creates symmetry-broken shapes



[1] Tomazic, F., Muttathukattil, A., Nabiyan, A., Schacher, F., & Engel, M. In The Journal of Physical Chemistry B (Vol. 128, Issue 45, pp. 11258–11266). American Chemical Society (ACS) **(2024)**
[2] Bassani, C. L., & Engel, M. *Preprint available on arXiv* **(2024)**
[3] Bassani, C. L., et. al. In ACS Nano (Vol. 18, Issue 23, pp. 14791–14840). American Chemical Society (ACS) **(2024)**
[4] Bommineni, P. K., Wang, J., Vogel, N., Engel, M., *submitted to Physical Review Letters* **(2024)**
[5] Wang, J., Martín-González, J., Römling, L., Englisch, S., Mbah, C. F., Bommineni, P. K., Spiecker, E., Engel, M., Vogel, N. *submitted to ACS Nano* **(2024)**
[6] Tomazic, F., Panchi, N., Engel, M. *In preparation*
[7] Tomazic, F., Martín-González, J., Varela-Rosales, N. R., Panchi, N., Vogel, N., Engel, M. *In preparation*

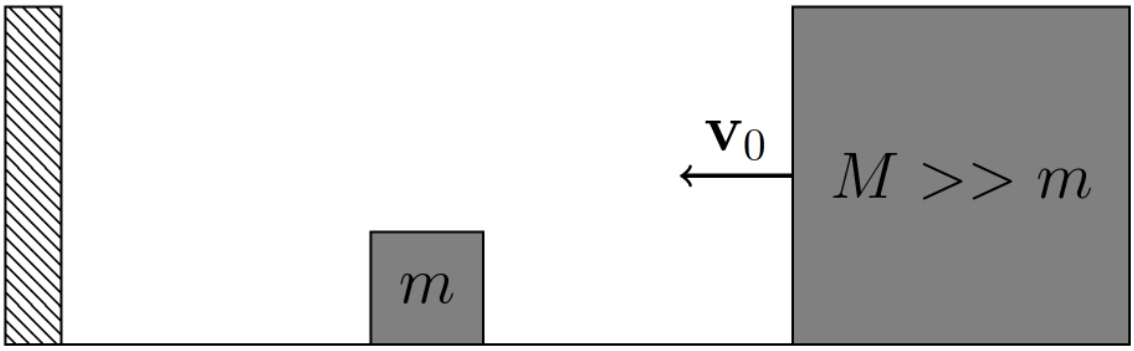
FAU Friedrich-Alexander-Universität Erlangen-Nürnberg

Funded by: DFG

5. Selected Postdoc Projects

Dr. Holger Götz
Acceleration field of an elastically cushioned wall.

We consider a heavy particle moving towards a wall, with a light particle placed in between the wall and the heavy particle. Because of the light particle, the heavy particle will never reach the wall. Instead of an instantaneous momentum inversion due to a collision with the wall, it is accelerated through many collisions with the light particle, which travels back and forth between the heavy particle and the wall. Hence, the heavy particle appears to move through an acceleration field created by the interplay between the light particle and the wall. Assuming elastic collisions, we geometrically derive an analytical and exact expression of the apparent acceleration field.

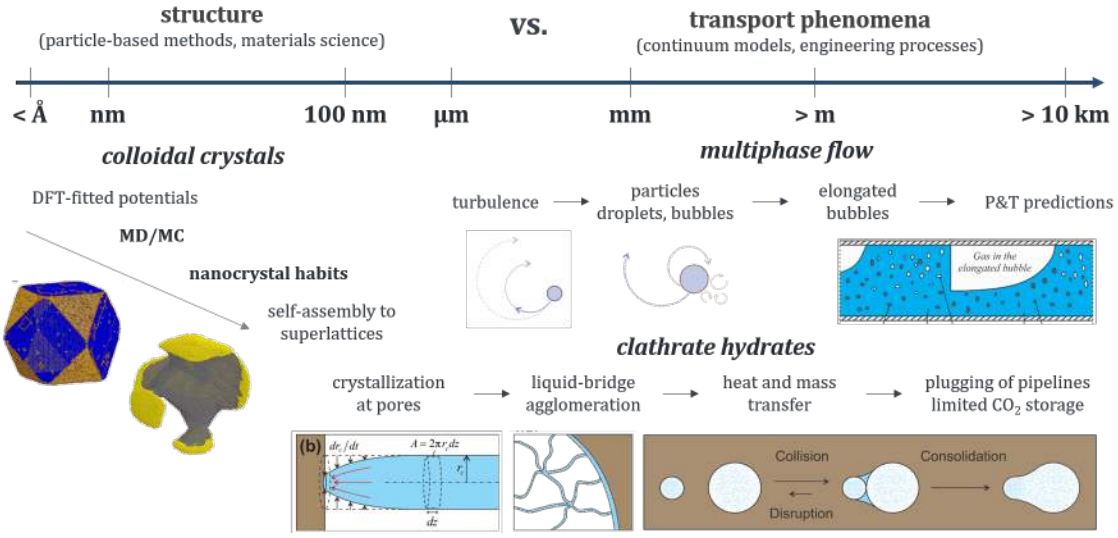


The considered system: A heavy particle with mass M moves towards a light particle with mass m and a wall.

Dr. Carlos L. Bassani

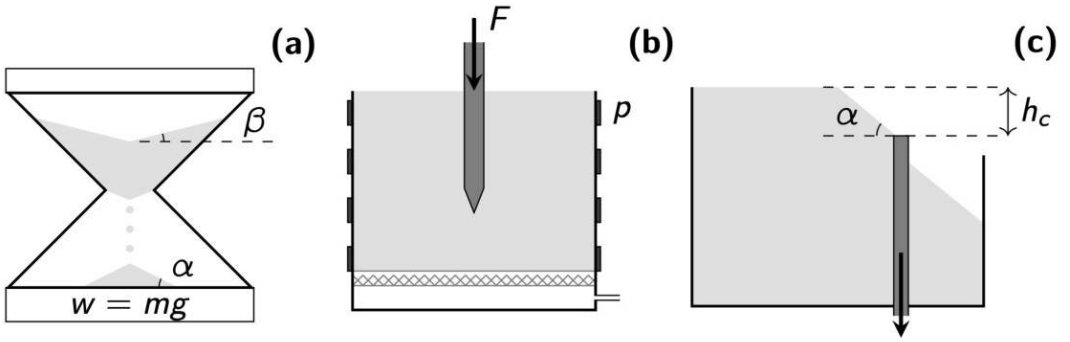
Multiscale modeling of crystals from fundamental science to engineering applications.

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 in transferring mass (diffusion/convection), momentum (pressure), and energy (temperature) to keep the crystallization process dynamically happening, described by continuum approaches (phase field models, finite volume method). The coupling of structure formation and transport phenomena is therefore key to predicting heterogeneous driving forces over the crystalline surface that lead to different growth pathways, ultimately affecting the outcome of the engineering process. Systems of interest comprise (a) emergent technologies such as the synthesis of nanoparticles of defined shape and their assembly into superstructure (colloidal crystals) as possible new materials for society use, and (b) urgent matters in the reduction of emissions by understanding multiple-component clathrate crystals as potential carbon storage materials, and their agglomeration/deposition in the possibility of reducing environmental impacts in hydrocarbon production.



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

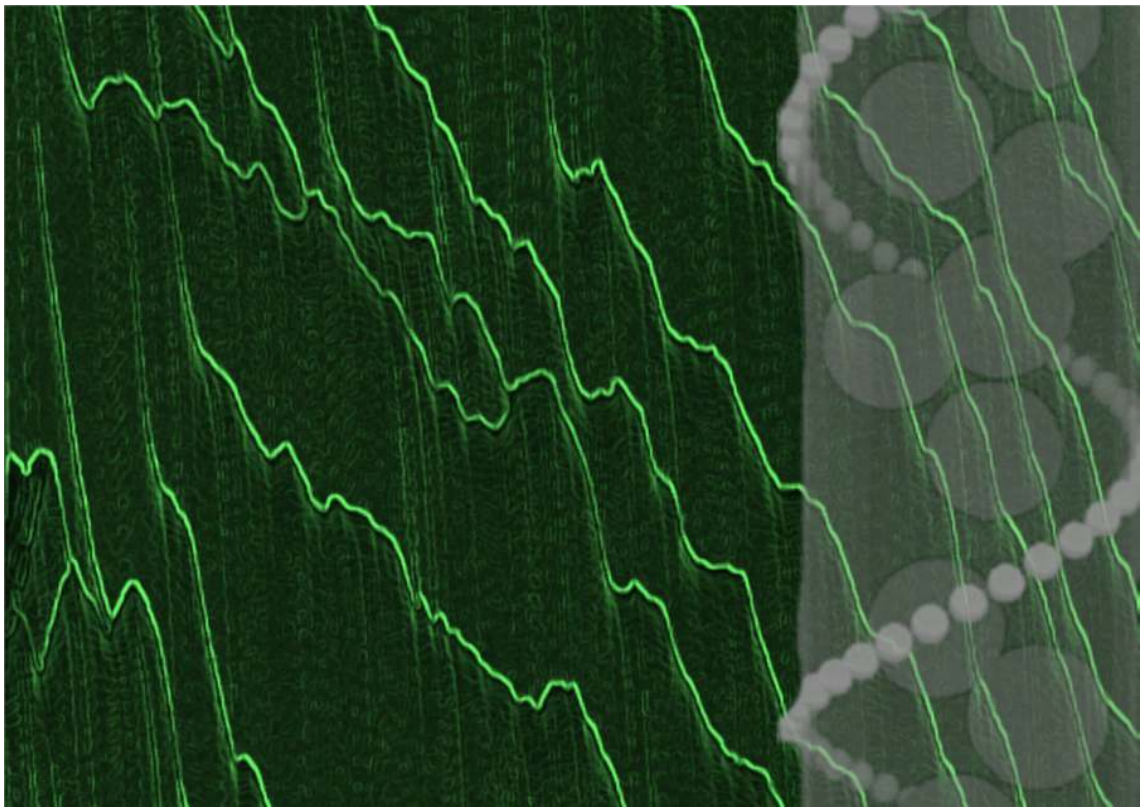
The success or failure of future space exploration missions will depend on humans' ability to understand and overcome the challenges posed by the Lunar environment – among which, dealing with the overwhelming presence of regolith. With sunlight, regolith is the main in-situ resource available on the Moon; all ISRU (in-situ resource utilization) processes rely on its acquisition, isolation and preparation. The complexity of Lunar regolith rheology is threefold: the granular material itself exhibits unique physical properties (sharp and abrasive particles with a large amount of fines); the low level of gravity modifies interactions among particles, making cohesive forces predominant; the singular Lunar environment (featuring low gravity but also high vacuum and electrostatic charges from solar winds) has a complex influence on regolith behavior. On ground, existing granular models rely on thousands of years of empirical knowledge. We lack such experience on the Moon. Gravity – more precisely Earth's gravity – is included in current rheological models, although often implicitly. For example, confining pressure and packing fraction indirectly depend on gravitational environment and will redefine soil properties; low gravity also triggers the predominance of cohesive forces, altering granular flowability. In this project, we will understand the rheology of Lunar regolith on the Moon, and translate it into models of regolith flow-behavior. Our models will inform the development of ISRU processes, and provide a benchmark for a future Lunar regolith rheological simulant. First, we will make explicit the effect of three factors on regolith rheology: physical properties of regolith, low gravity, and Lunar environment, notably through electrostatic charging. The combined influence of those factors will be studied through three experiments: an hour-glass experiment, a penetration experiment, and a collapsing wall experiment. Adapted from already existing hardware, they were selected because despite their relative simplicity of implementation, those three experiments combined provide a holistic view of granular behavior. They also directly relate to ISRU processes, past and future: from the tranche collapse and penetration data from Apollo missions, to robotic and human interactions with Lunar soil during the Artemis mission, to provide fuel for Lunar Gateway, and towards the democratization of Lunar activities, notably with NASA's commercial lunar payload services (CLPS). By combining efforts and results from those experiments, we will propose a universal description of granular rheology adapted to low gravity environments, enabling humans to explore sand-covered space bodies: our Moon, asteroids, Mars, and beyond.



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

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.

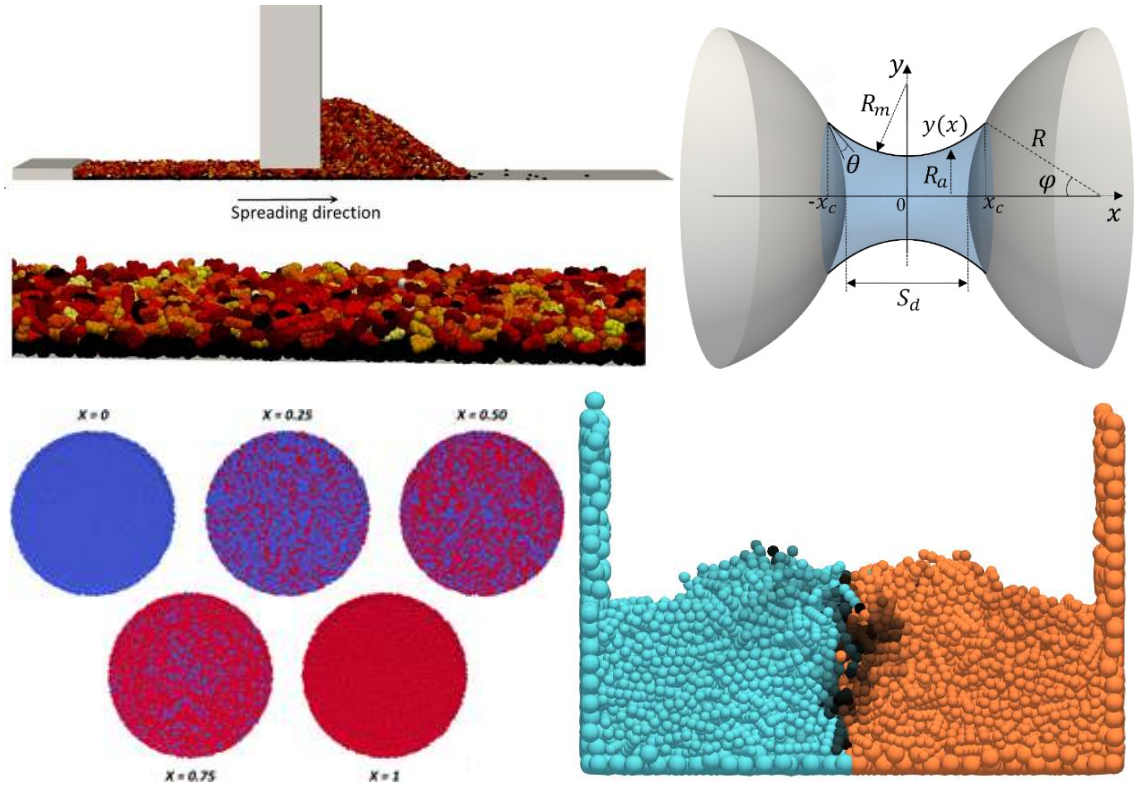


Density waves in gravity driven granular pipe flow.

Dr. Sudeshna Roy

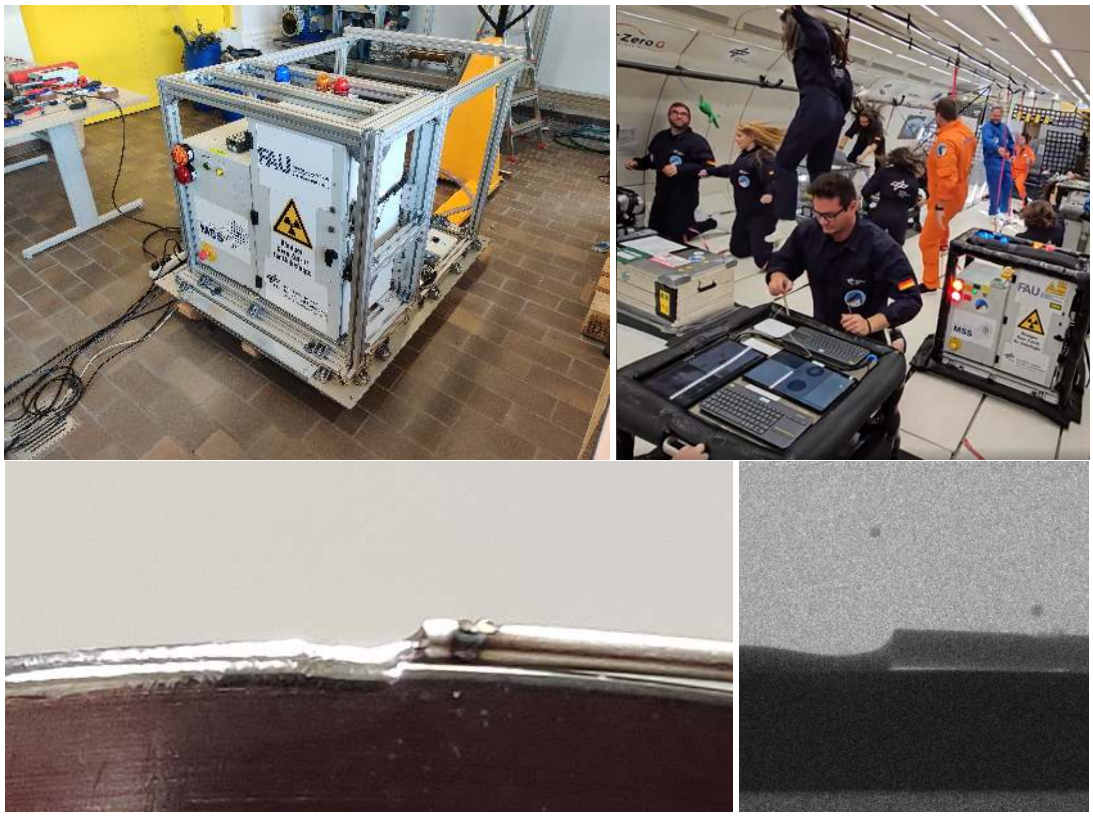
Habilitation: Multiscale Simulation of Granular Flows: Insights into Additive Manufacturing, Rheology, and Capillary Force

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.



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

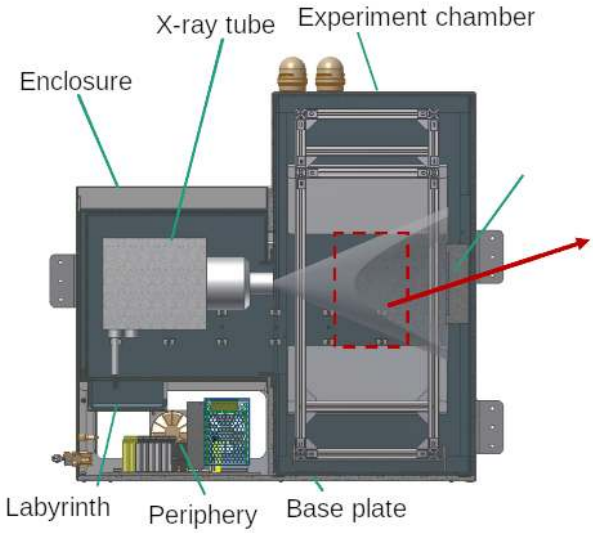
In laser wire welding, a metal wire is melted using a laser and applied to a metallic base, similar to how a 3D printer extrudes plastics. Our project explores how this process could be adapted for space missions in zero gravity, enabling the production of necessary components on-site, such as on space 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.

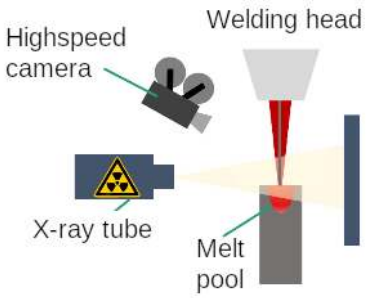


Dr. Achim Sack

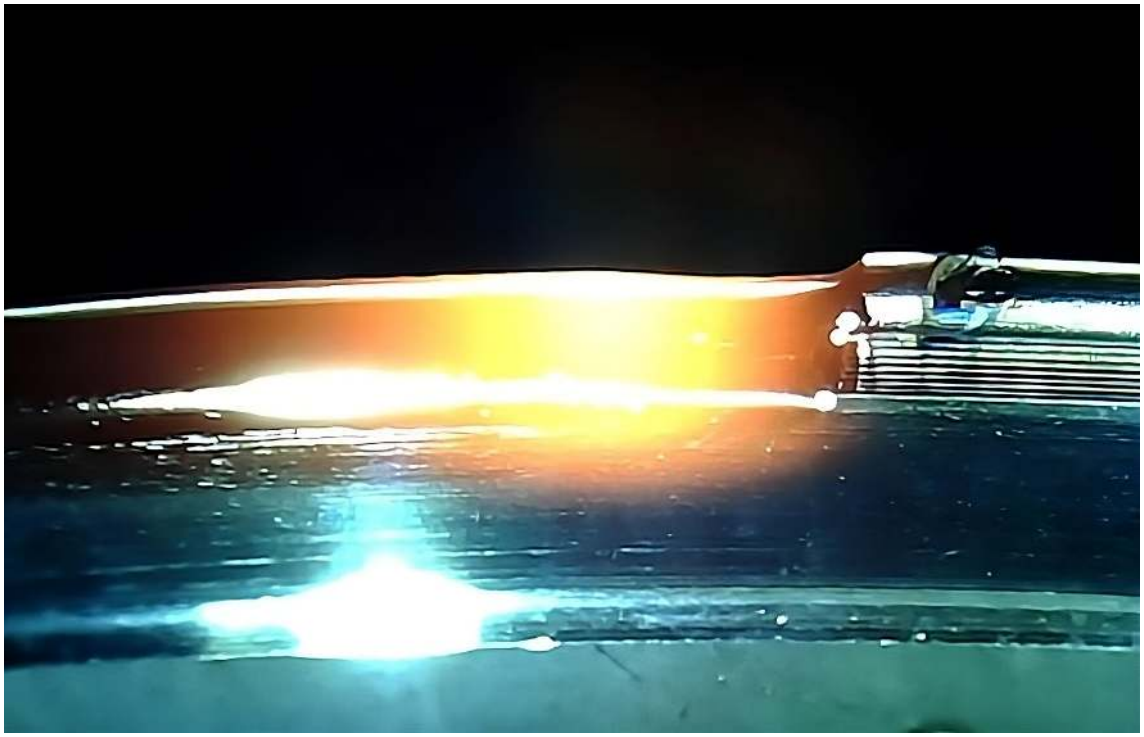
Tracer-based radiography of the melt pool dynamics during laser wire welding in weightlessness (ETI)

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.





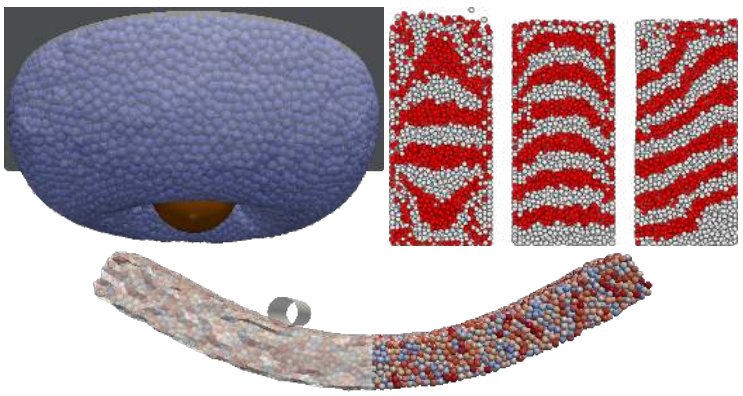
- Material: Ti-6Al-4V
- Wire diameter: 0.4 - 1 mm
  Laser: 500W, 1070nm, single mode
- Highspeed camera (40.000 fps)
- X-ray source: Hamamatsu L9181-02
  (120W, 130kV)
- Detector: Hamamatsu C12849
  (2048 x 2048 px, 25655 fps)



6. Dissertations and Habilitations

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.

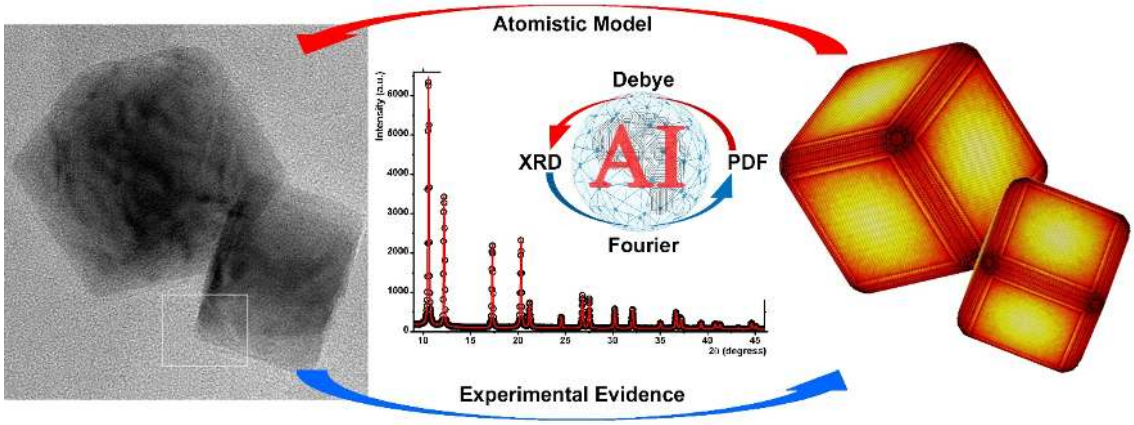


Exemplary representations of the three investigated systems: the granular gripper (top left), patterns of granular convection (top right), and a beam-shaped granular metamaterial (bottom).

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.

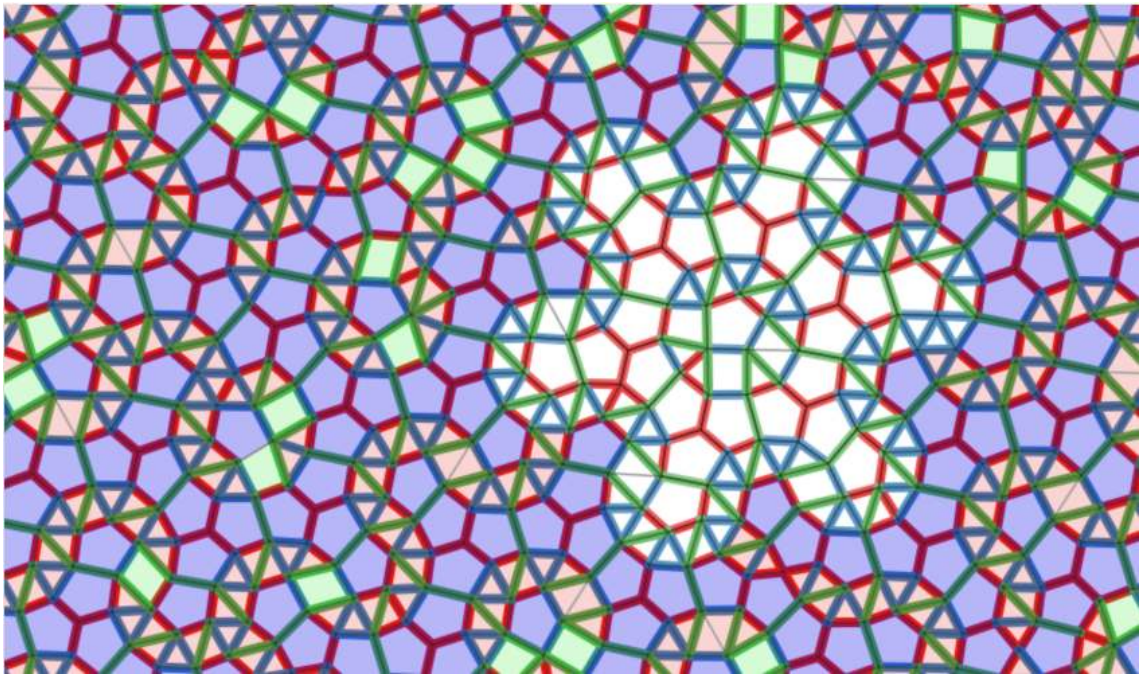


Nydia Roxana Varela-Rosales

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.

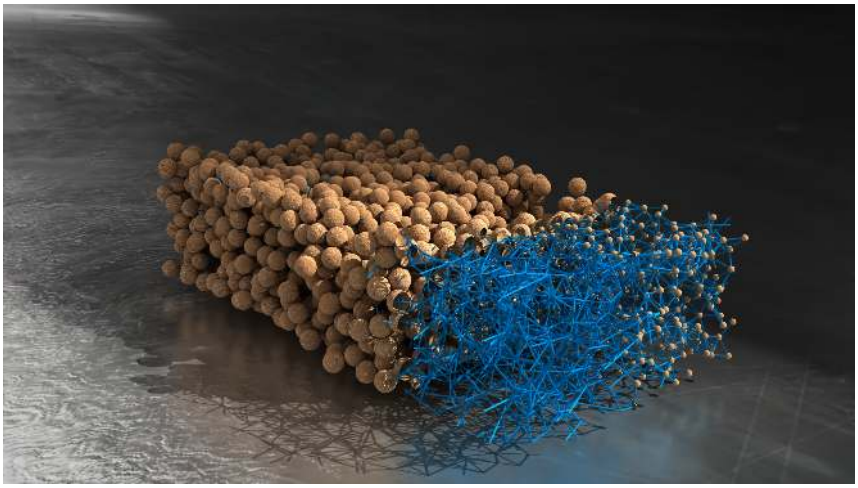


Tiles of a six-fold aperiodic crystal, with bond connections colored based on distances to nearest neighbors.

7. Ongoing PhD Projects

Meysam Bagheri
Physics of Drying Suspensions

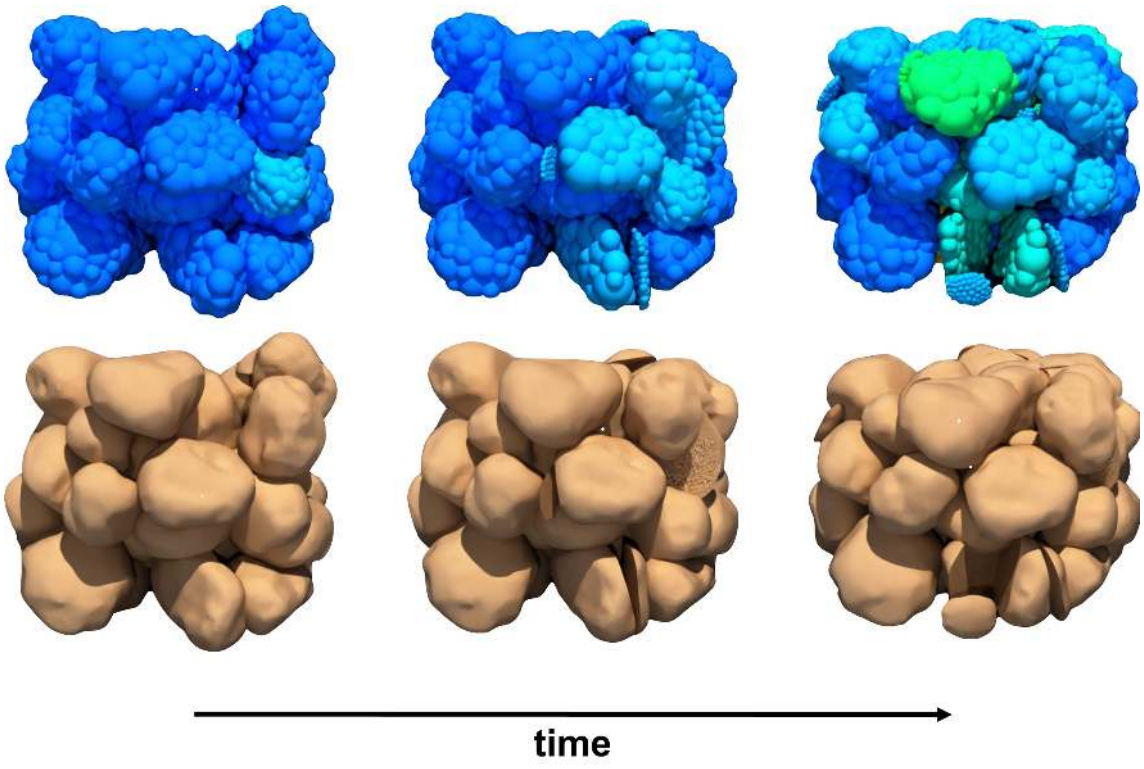
Drying suspensions display a fascinating network of cracks during the drying process. The cracks result from a number of complex interactions: the particles are concentrated into a close-packed array due to the evaporation of the fluid. Further drying results in a network of particles that are interconnected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



Utku Canbolat

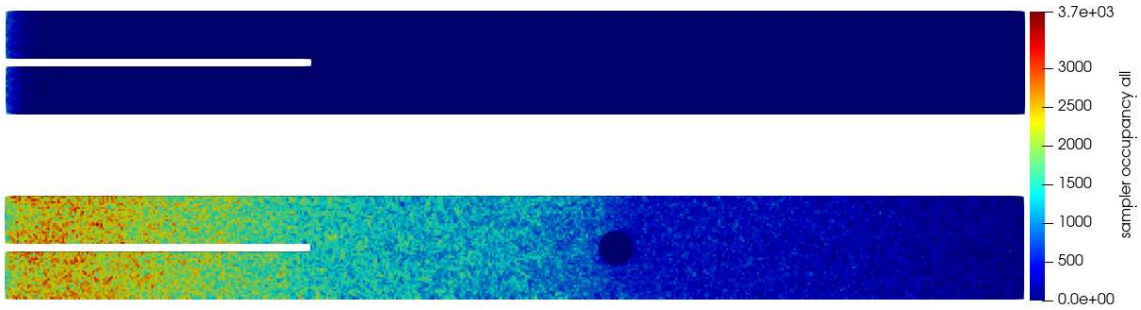
Modelling Fragmentation in Large Scale DEM Simulations

Comminution refers to the reduction of solid materials from a larger to a smaller average particle size through processes such as crushing, grinding, cutting, and vibrating. It is a critical phenomenon, particularly in fields like mining, geotechnical engineering, and process engineering. However, comminution processes are known for their high energy demands; for instance, studies show that approximately 36
The Discrete Element Method (DEM) is widely regarded as a powerful tool for simulating comminution processes. In DEM, simulation models for fragmentation generally fall into two categories: particle-replacement methods and bond-breaking methods. However, these approaches face significant challenges, including violations of volume conservation, material properties that depend on scale, and high computational costs. To address these issues, we developed a novel approach named the Image-Informed Fracture Model. This model overcomes the limitations of traditional methods by achieving significantly higher accuracy in fragmentation simulations, with manageable computational costs. It enables scaling to systems containing over 10^5 complex-shaped particles.
The model leverages multisphere representations of particles alongside surface mesh data (STL files), allowing for rapid contact detection while preserving the true morphology of the system. This year, we resolved several key issues, making the model ready for use in both scientific research and industrial applications. The model is currently undergoing validation using experimental data from the literature to ensure it produces accurate physical results.



Felix Buchele
Reactive Flow in Porous Media

Catalysts are important materials in the chemical industry and may contribute to the future of our mobility by being key parts of electrolyzers and fuel cells. Understanding flow and reaction kinetics in catalysts, however, is limited to microscopic and macroscopic points of view. With tools like Density Functional Theory (DFT), Molecular Dynamics (MD), or Kinetic Monte Carlo (KMC), the properties of catalytic surfaces can be investigated on a microscale. On the other hand, there are rate-based flow solvers and semi-empirical differential equations describing the properties of catalytic systems on a macroscopic, engineering scale. Mesoscopic tools to investigate flow within porous catalysts and chemical reactions based on first principles are virtually non-existent.
The aim of this project is therefore to develop suitable methodologies to simulate complex catalytic reactions and flow in porous catalysts. The range of adequate tools is, however, limited by the small characteristic length scales in porous catalysts. Flow in microchannels, similarly to rarefied gas flow, is governed by collisions with boundaries rather than intermolecular collisions, precluding the use of continuum methods. Thus, a particle-based Direct Simulation Monte Carlo (DSMC) code is used to simulate flow. The surface reactions are modeled following energy-barrier-based first principle equations from physical chemistry for Langmuir-Hinshelwood and Eley-Rideal kinetics, with detailed stochastic adsorption and desorption computation. The surface and its sites are modeled following lattice gas dynamics. A model for electrochemical reaction kinetics is planned for the future.



Chemical reaction on a spherical catalyst inside a microchannel. Colours indicate the number of DSMC sampler particles per cell. The plots show initialization and equilibrium of the system.

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 penetration test, typically used to probe geotechnical soil properties. In our setup for the experiment, a container is filled with granular material, and with the addition of sensors, the pressure acting on the walls and at the bottom of the container is measured. The force acting on the probe introduced into the material was also measured. Two different probes were used: a cylinder with a conical tip 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. By understanding the influence of gravity on the material flow behavior, we expect to improve existing models for regolith rheological properties description.
Additionally, we supported the team of Jonatthan Kollmer from the University of Duisburg-Essen in performing the hourglass experiment during the 43rd DLR Parabolic Flight in France. Being also part of the GRIS project, both the hourglass experiment and the penetration test are complementary in understanding the regolith flow behavior.

Jyoti

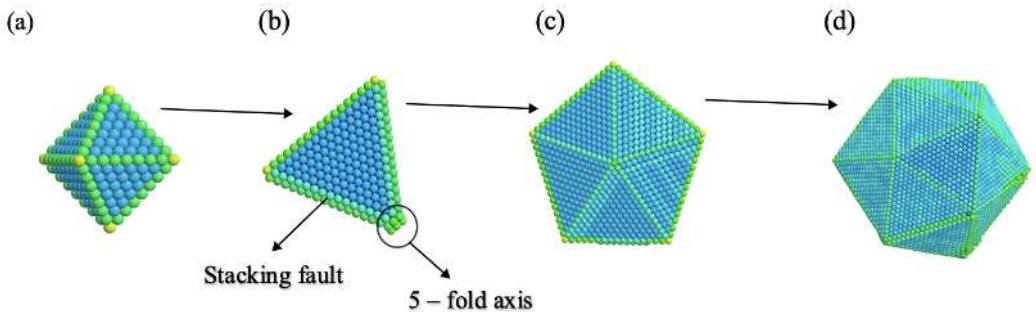
Symmetry Breaking and Growth Mechanism of Multiply Twinned Particles

The shape of nanoparticles plays a crucial in determining their physical, chemical, and biological properties, influencing their behavior in various applications. Multiply twinned nanoparticles (MTPs), in particular, exhibit fascinating properties due to their intricate morphologies and high density of twin boundaries. The shape and twinned structure of MTPs can significantly affect their stability and mechanical strength, offering insights into novel development pathways for resilient nanomaterials.

In this project, our research question is: what effect do crystallographic defects, such as dislocations and stacking faults, have on the growth and shape of nanocrystals? How do kinetic factors compare to thermodynamic factors in determining the final shape of a nanocrystal?

In the first stage, we explore the fundamental mechanism of symmetry breaking in noble metal nanocrystals by employing rejection-free kinetic Monte Carlo simulations. The interactions between particles are modeled using one of the simplest pair-potential models, the Lennard-Jones, in vacuum. To overcome the nucleation barrier, we initiate with a single crystal having face-centered cubic (fcc) symmetry (in the form of an octahedron) as a seed. To allow the formation of planar defects (stacking faults) during growth, we also consider growth sites corresponding to hexagonal cubic symmetry (hcp).

Preferential growth of particles over some facets adjacent to twin boundaries leads to symmetry breaking in the system during growth. On the formation of the first twin boundary, octahedra start deforming into tetrahedra, and when the two twin boundaries meet at an edge, a fivefold symmetry axis is established, leading to the rapid formation of multiple tetrahedra around this edge, which then evolve into decahedra and subsequently into icosahedra.



Growth Mechanism of Multiply Twinned particles. (a) Octahedron as an initial seed, which grows to (b) tetrahedra by the formation of two twin boundaries (light green), and further becomes (c) decahedra, having 5 tetrahedron units around the 5-fold axis, and finally forms (d) icosahedra.

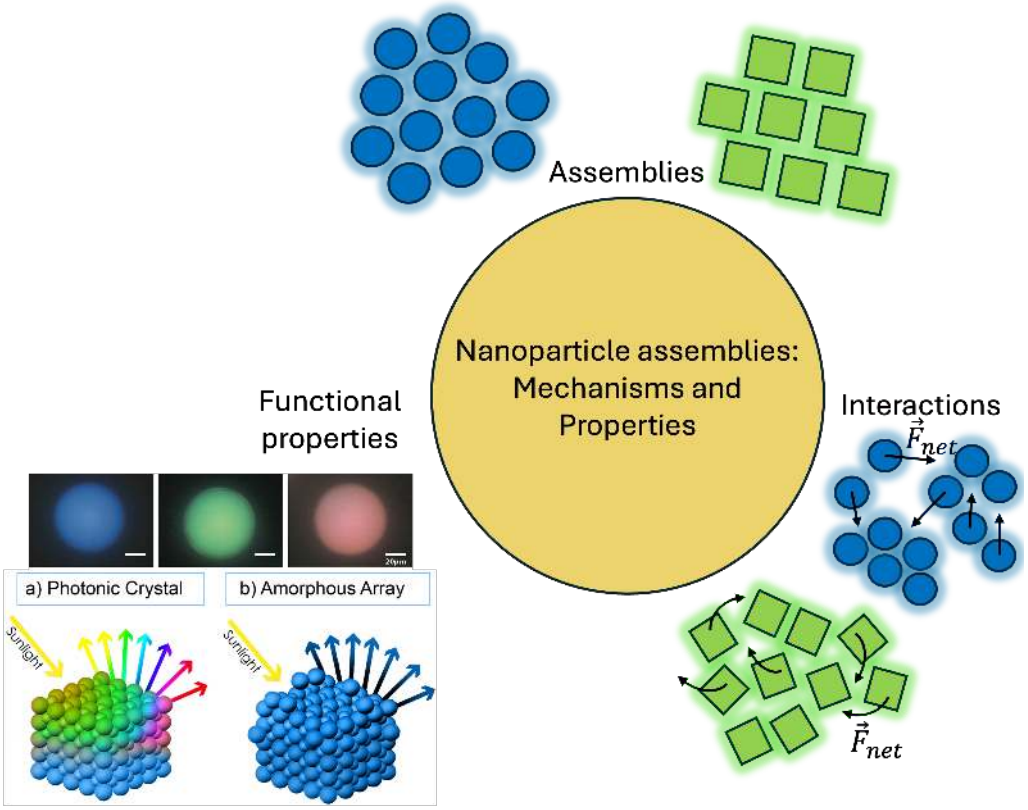
Harsha Namdeo

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 the 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.

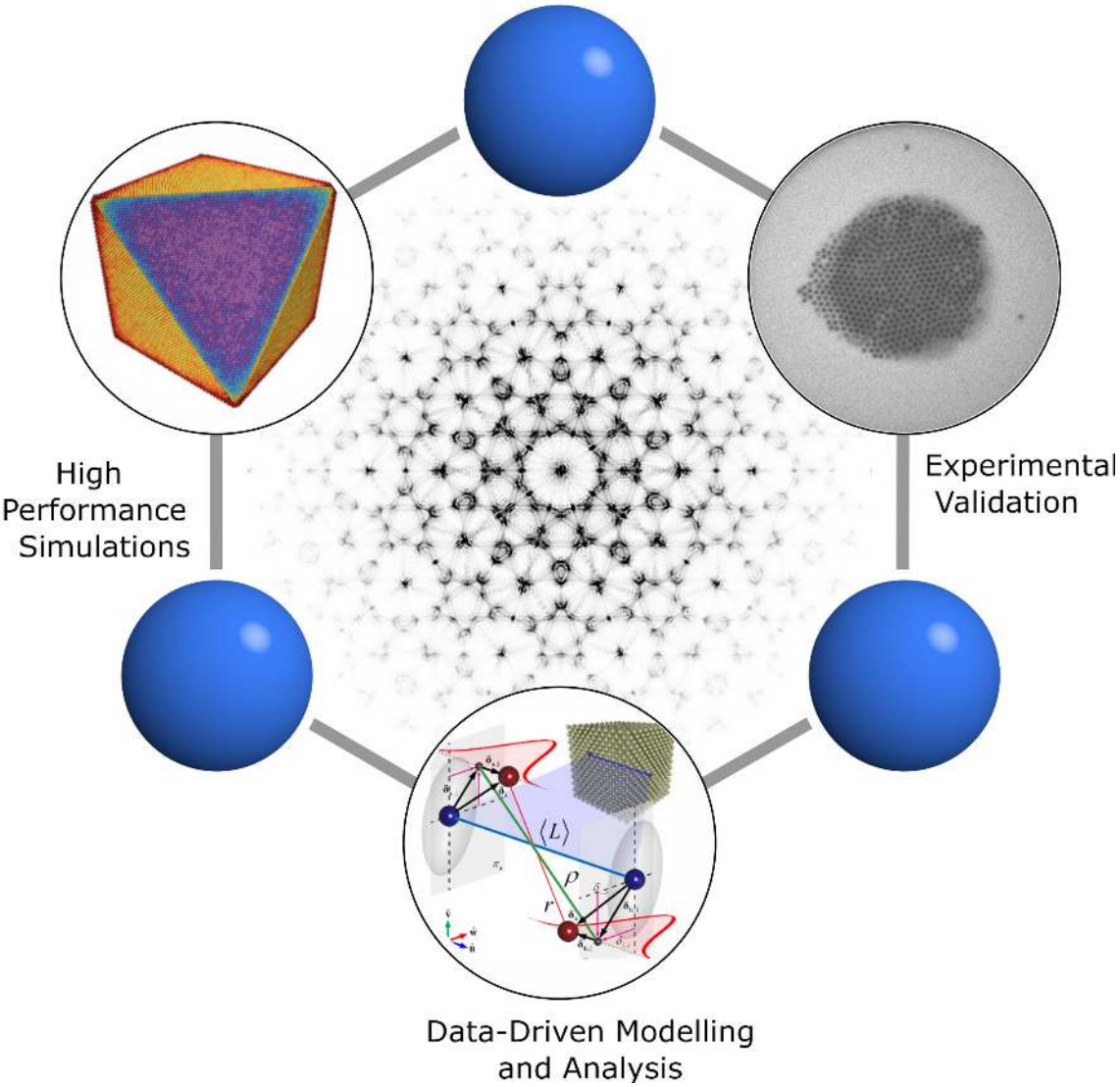


Navid Panchi

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

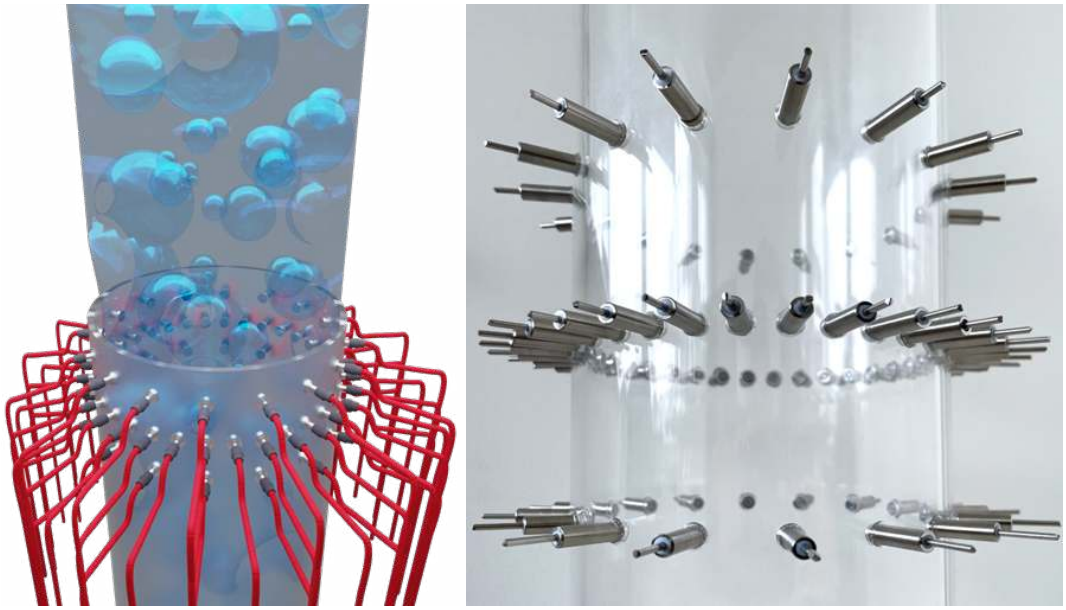
This research focuses on developing advanced data-driven, high-performance simulation methods and analysis techniques for particle-based systems. It develops algorithms for simulating diffraction patterns, examining system symmetries, and conducting symmetry analysis, with an emphasis on computational 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 large-scale experimental facilities for nuclear safety research, we are developing a sensor based on electrical impedance tomography. This sensor is intended to enable non-intrusive monitoring of two-phase flows in pipelines, allowing for the assessment of flow regimes, fluid velocity fields, and void fields.
Electrical impedance tomography (EIT) is a non-invasive imaging technique used to visualize and monitor the internal conductivity distribution of an object. This is done by 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 want to 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.



Concept image of an EIT sensor. EIT pipe model with 64 electrode sensor.

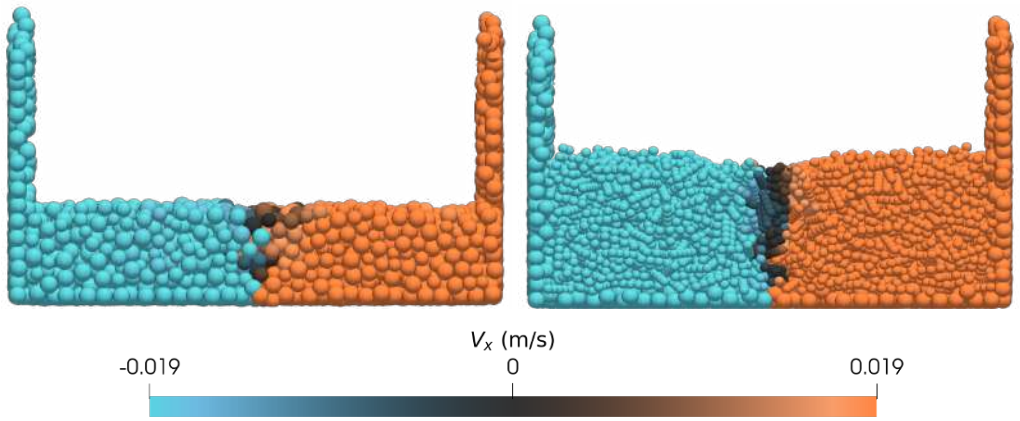
Huzaif Rahim

The Granular Weissenberg Effect

When granular materials of shape-anisotropic particles, such as elongated grains, are sheared in a split-bottom shear cell, they accumulate in the center, forming a heap. This heap corresponds to a depression observed on the shear band surface, which is absent in the flows of spherical particles. This behavior is similar to the Weissenberg effect in non-Newtonian fluids, where secondary flows lead to rod climbing or heaping effects. While granular flows differ fundamentally from fluids due to their discrete nature, they share mechanisms, such as alignment and stress distribution.

This study investigates how particles' aspect ratio (AR) affects their alignment, packing density, and stress distribution in the shear band. Using a linear split-bottom shear cell, we observed that particles align more closely with the shear direction as AR increases. This alignment increases the local packing density and influences stress distribution and bulk rheology. For spherical particles, dilation occurs due to Reynolds dilatancy. However, with higher AR, particle alignment counteracts this dilation, resulting in compaction. At AR = 5, compaction dominates, leading to dense packing and a depression on the shear band surface.

Particle alignment also reduces stress in the shear direction, making the flow smoother. The macroscopic friction coefficient, $\mu(AR)$, increases with AR, due to more particle contacts. Granular flows exhibit shear-thinning behavior across all AR values. Elongated particles, particularly with AR=5, exhibit higher viscosity than spherical particles.



DEM simulation of wooden pegs. The shear cell is filled with (left): spherical particles, showing a flat surface, and (right): elongated particles, showing a depression on the shear band surface, lacking significant depth.

Hakan Şanal

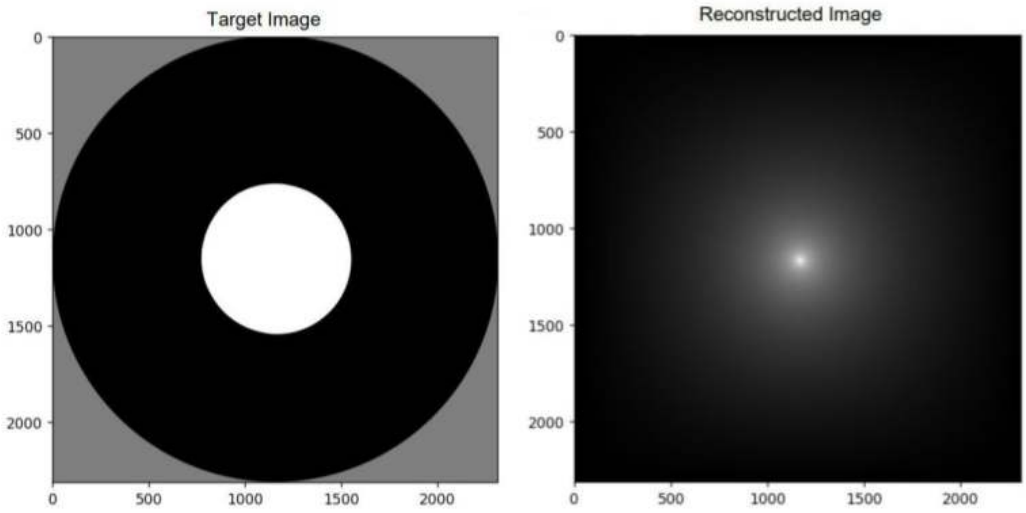
Direct Reconstruction Algorithms for Electrical Impedance Tomography (EIT)

EIT is a non-invasive imaging method used to visualize the internal conductivity distribution of an object by injecting electrical currents through electrodes and measuring the resulting voltage patterns. Applications include monitoring thermohydraulic flows in pipelines and detecting material anomalies.

Our work addresses EIT's key limitation: low spatial resolution. Traditional iterative methods often require significant computational resources, making them impractical for real-time imaging. Instead, we focus on direct methods, particularly the D-Bar Method and Calderón's Method, which have seen significant advancements. Our research emphasizes Calderón's Method and its derivatives, refining these approaches for real-world applications.

The project involves developing and validating Calderón-based reconstruction algorithms tailored to our application, with ongoing refinement to optimize performance and enhancing these algorithms for real-time operation and improved spatial resolution.

In collaboration with the experimental team, our goal is to integrate these algorithms into a real-time imaging setup for monitoring two-phase liquid-gas flows in pipelines. This will enhance power plant safety by providing high-resolution insights into flow regimes and fluid distributions.

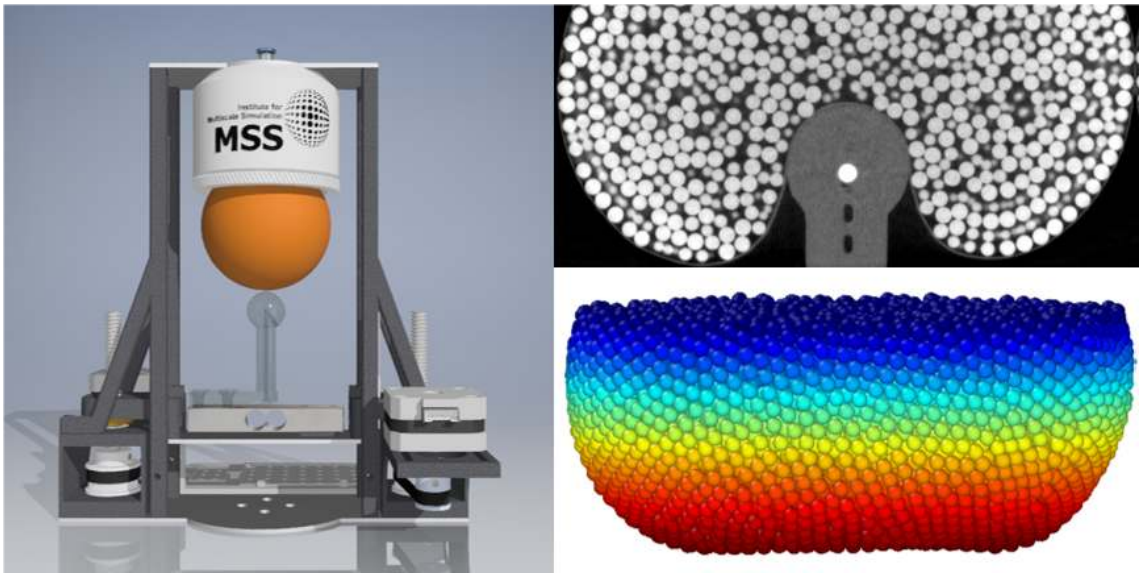


Angel Santarossa

Jamming-Based Robotic Granular Grippers: X-Ray Imaging

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

Despite its advantages, current-generation systems are far from being fully developed and optimized, by which their application to the industrial sector is still unsuccessful. In this sense, the interior dynamics of the granular material remain almost unresearched. My PhD project focused on the experimental study of granular gripping systems. The experimental branch of this work included the design and construction of granular gripper prototypes, the generation of data to calibrate simulation models, and the study of the internal granular structure of these grippers through X-ray computer tomography. The in-depth understanding of the particle-scale processes in these gripping systems was then used to enhance their grasping capacity and performance.

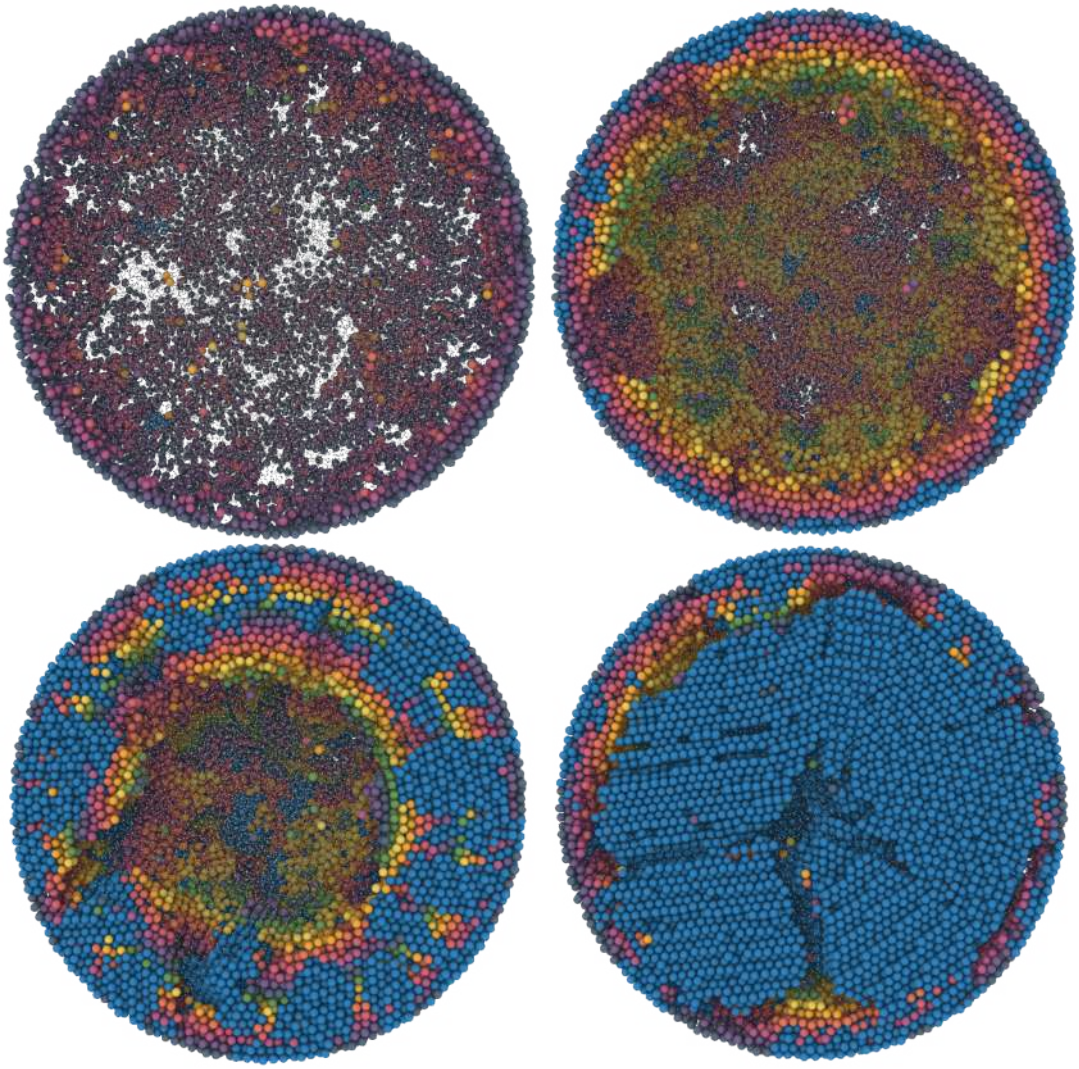


The experimental setup of the gripper (left), an X-ray image of the interior structure of a granular gripper (upper-right), and a 3D reconstructed image from X-ray tomography (bottom-right).

Federico Tomazic

Modelling Particle Aggregation and Assembly into Optimal Structures

Nanoparticles are used as building blocks to assemble robust functionalized suprastructures, with applications in nanophotonics and chromatography. We use computational techniques to relate the interactions between building blocks to the formation of a desired self-assembled suprastructure.
By modeling the crystallized polymeric ligand bundles on a nanoparticle as a sphere-rod model, we find that the dimension of the ligand bundle determines the shape of the self-assembled structures. We use event-driven simulations to reproduce the drying of a colloidal dispersion into spherical supraparticles, and we study how the ordered layers on the surface of the droplet affect the final order in the supraparticles.
Finally, to model the interaction between anisotropic nanoparticles, we develop a method to calculate the potential between two differently oriented nanoparticle faces. We apply this method to tripods, two-dimensional non-convex nanoparticles. We tabulate the potential between two tripods at different orientations. We then perform molecular dynamics simulations that recover the precomputed potential to observe how different potentials affect the self-assembly.

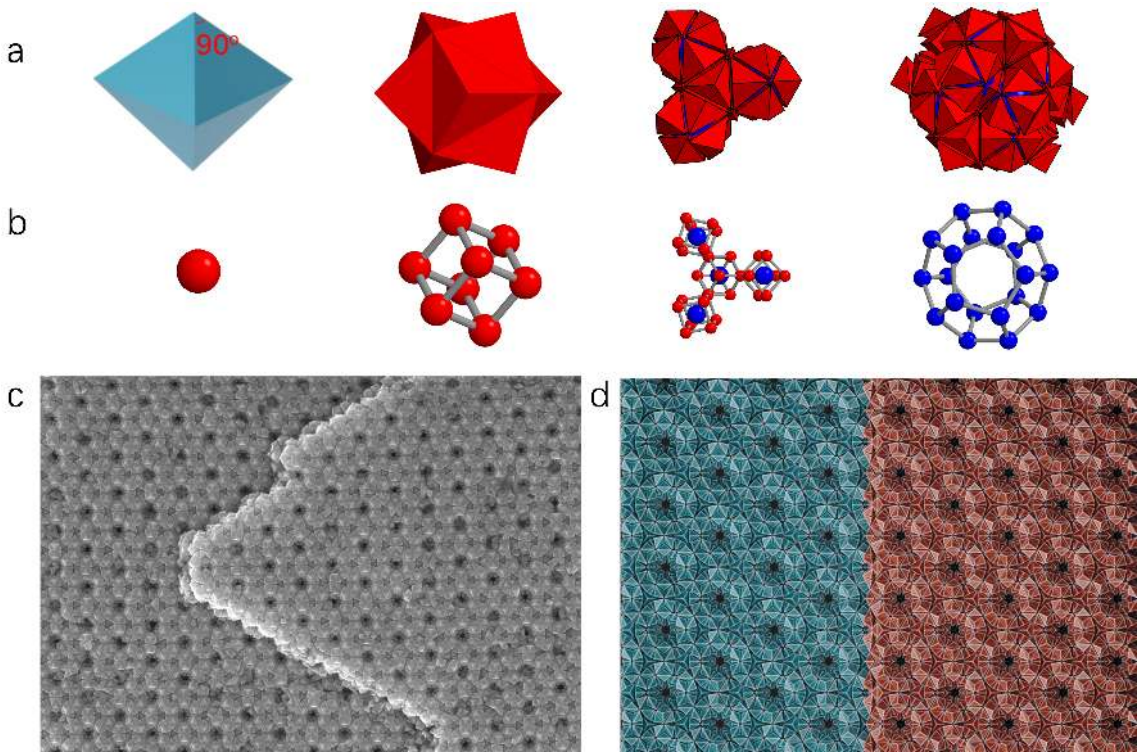


Self-assembly of nanoparticles into optimal structures. Layers formation for particles in spherical confinement such as a droplet. Different colors represent different layers, with blue indicating crystalline structures.

Kaijie Zhao

Hierarchical Structure Analysis of Self-Assembly of 100 Trigonal Bipyramids

The advancement in synthetic methods for monodisperse anisotropic particles enables the exploration of vast possible different nanocrystal structures. Our collaborators from Rice University have recently managed to synthesize new trigonal bipyramids (TBPs) with {100} facets, where the facets are at 90 degrees to each other. These building blocks self-assemble into a complex crystal structure under microscopy. We then perform a bottom-up structure analysis, which reveals that this crystal is equivalent to a Clathrate II. Eight {100} TBPs first gather face to face to form a "stellated" octahedron, and four more stellated octahedra can "grow" on the central octahedron by sharing four distant bipyramid tips. In this way, we successfully constructed the cubic unit cell with 816 {100} TBPs, which is by far the largest unit cell of a self-assembled structure from anisotropic nanoparticles.



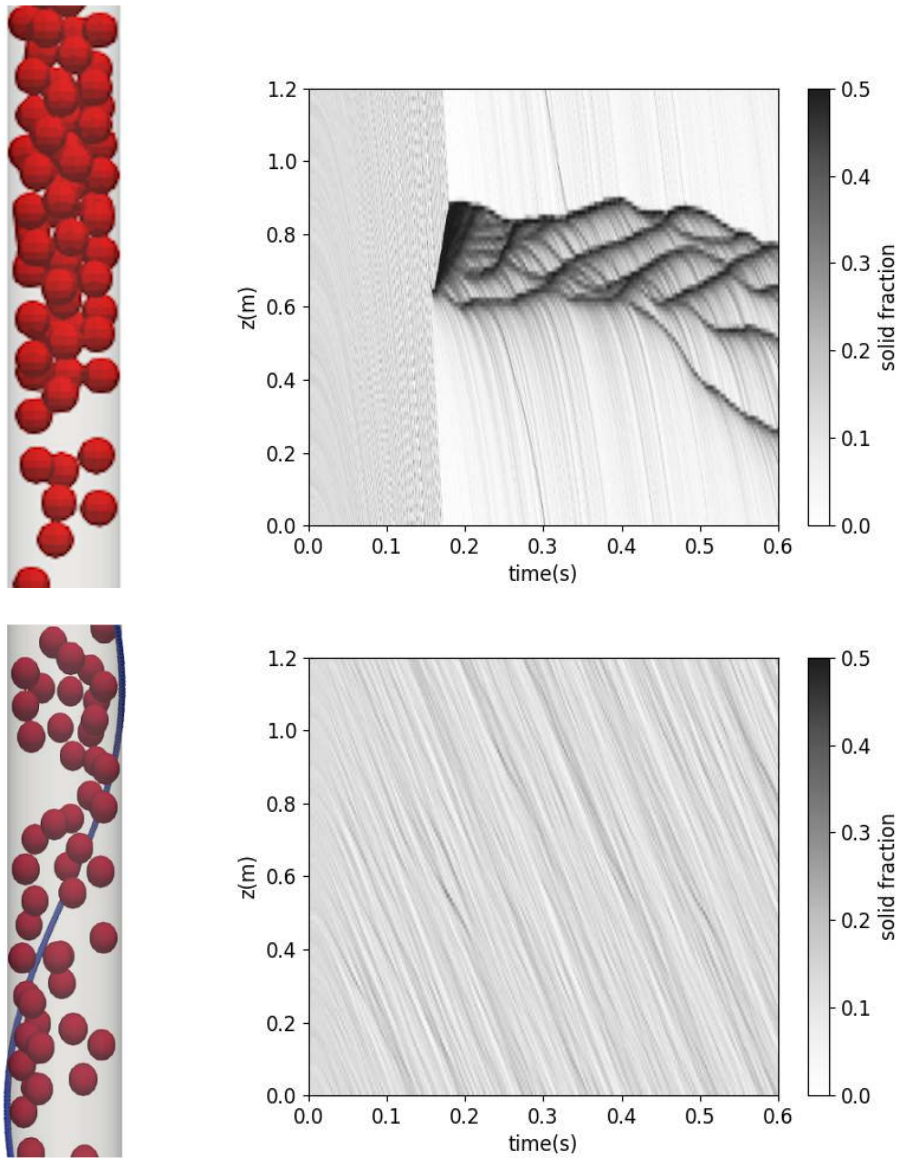
Hierarchy of the self-assembled {100} trigonal bipyramid. (a) & (b): Hierarchies of building blocks and their simplified models. From left to right: trigonal bipyramid, stellated octahedron, tetrahedral bonding, and dodecahedral cage. Red spheres are the mass center of the trigonal bipyramids and blue spheres are the mass center of the stellated octahedra, respectively. (c): SEM image of the nanocrystal. (d): Geometric construction of clathrate II.

Wing To Ku

Homogenization of Granular Pipe Flow

The transport of particulate matter through narrow pipes occurs in many industrial processes, such as in the food industry and in civil and chemical engineering. This type of transport is intrinsically unstable, with large variations in solid fraction (density waves) and even clogging potentially occurring in the pipes. These issues can lead to destructive pressure transients on the inner walls.

Although external energy inputs, such as electric fields or mechanical perturbations, can be used to mitigate the problem, this project aims to develop a passive method to homogenize the flow. Building on previous work, I have simulated granular pipe flow systems using the discrete element method (DEM). I investigated the effect of different wall structures on the efficiency and homogeneity of granular pipe flow. To better simulate real-world applications, other flow characteristics, such as polydispersity of granules, bend pipes, and interstitial fluid, have been included.



A section of granular pipe flow, showing the formation of plugs (upper left), the corresponding density waves (upper right), the introduction of a helical wall texture (lower left), and the homogenization of flow (lower right).

8. Students Projects

Master theses

Nadja Al Akkam
Rheology of Lunar Regolith and its Simulants

This thesis investigates the rheology of lunar regolith simulant, a granular material produced to mimic the sand that covers the Moon, known as regolith. Using data from NASA's Apollo missions (1963 - 1972), as most of the information on 'real' lunar regolith comes from these missions, and also conducting experiments with EAC-1A and LHS-2E simulants, including classical ring shear tests and vertical wall collapse tests, to investigate key parameters that influence the rheological material behavior and provide insight into the observed properties of lunar regolith.
The vertical wall collapse test is inspired by the Apollo trench tests and was conducted in air and vacuum (20 mbar). The experimental setup consists of a box filled with granular material; the front wall is progressively lowered, exposing the material held in place by cohesion. Repeated material failures are captured by two cameras, providing a view from above and from the front. Image analysis was used to determine the angle of repose as a function of slope height and to derive the strength parameters in the Mohr-Coulomb framework: cohesion and internal friction angle. Both strength parameters are used to describe the material and are compared with data from lunar regolith and research results on lunar regolith simulants. Overall, the results indicate a strong dependence of material behavior, defined by the cohesion and internal friction angle, on intrinsic material properties such as bulk density and moisture content, and on extrinsic factors: the environment such as gravity, atmospheric pressure, and applied pressure.

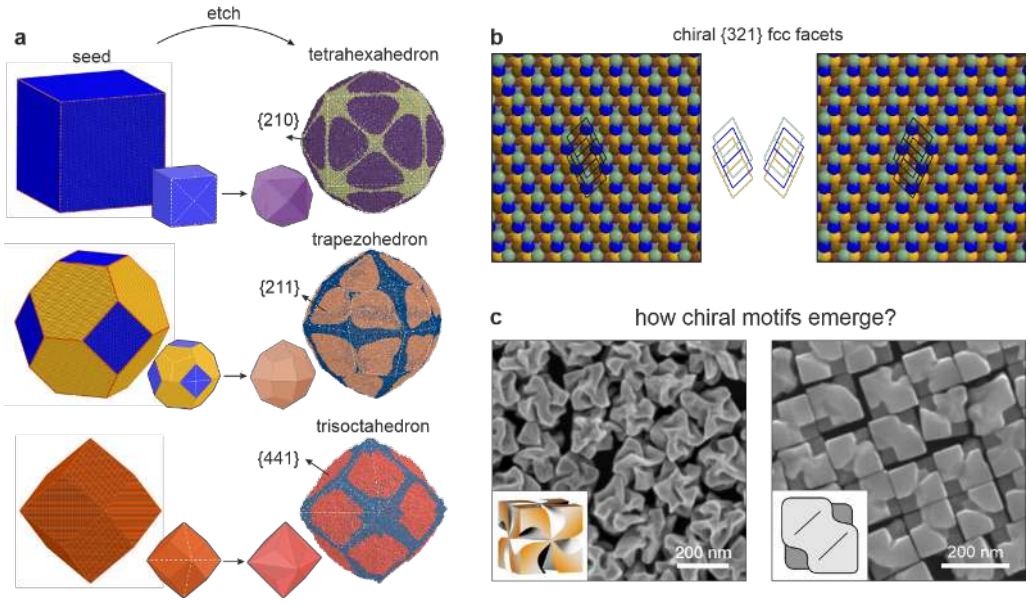
Chia-Jui Hsieh

Simulation of Nanocrystals with High Index Facets

The shape of nanocrystals is closely linked to their functional properties, and thus achieving controllable synthesis over specific facet-bound nanocrystals is essential for the performance in applications such as catalysis, plasmonics, and photonics. Nanocrystals with high index facets are composed of low-coordinated step-terrace atoms acting as active sites, resulting in enhanced catalytic activity. However, the synthesis of high index facets is challenging due to their high surface energy and tends to vanish during the end of growth stage.

Although many successful syntheses have been achieved through seed-mediated methods, the mechanisms underlying facet formation and the impact of seed morphology remain unclear. Based on rejection-free kinetic Monte Carlo, this study aims to understand the mechanisms of high index facets bounded nanocrystal formed by etching a seed.

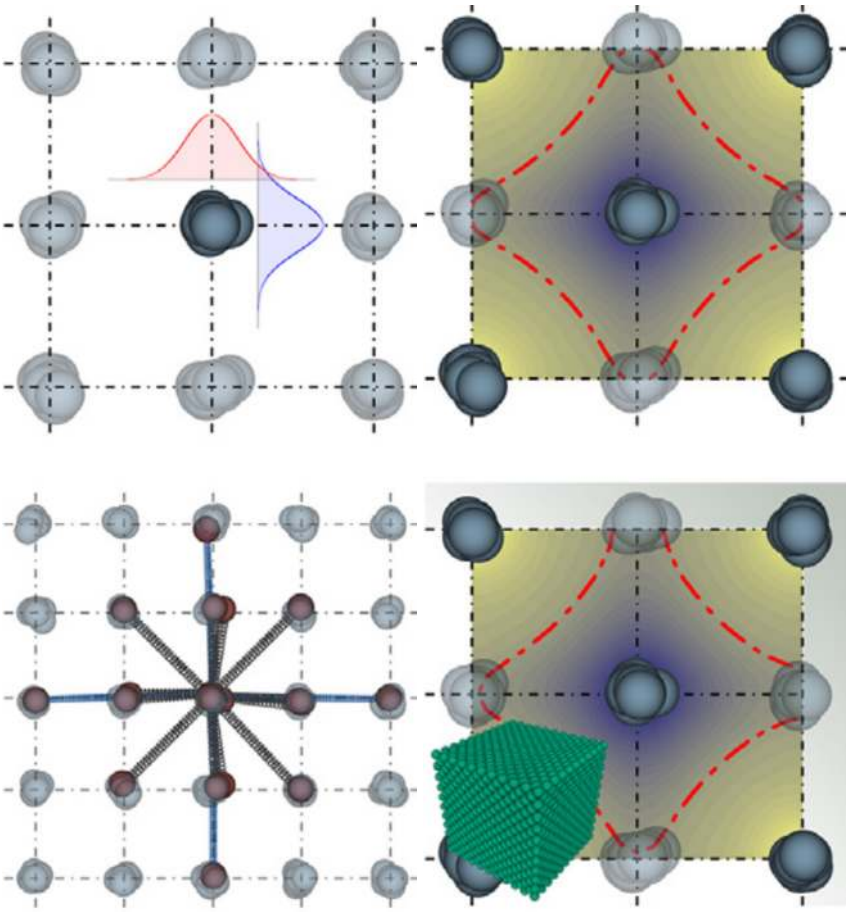
Etching simulations from an initial nanocrystal shape predicted three types of nanocrystals with high index facets, namely tetrahexahedron, trapezohedron, and trisoctahedron. Key determinants on the formation of high index facets are the initial seed shape (tested for cube, truncated octahedron, and rhombic dodecahedron seeds), the energy of surface atoms with coordination numbers 6 and 7, temperature, and the ratio of growth to etching events. We propose shape diagrams to classify the nanocrystal shapes found in the simulation. The results shed light on the evolution process of high index facets, from atomic scale mechanisms to nanoscale morphology and faceting. This understanding is essential for optimizing the design and performance of advanced nanocrystal engineering.



Yi-Ting Chiang

Automated Extraction of Disorder Model from Simulation Data for Diffraction Modeling

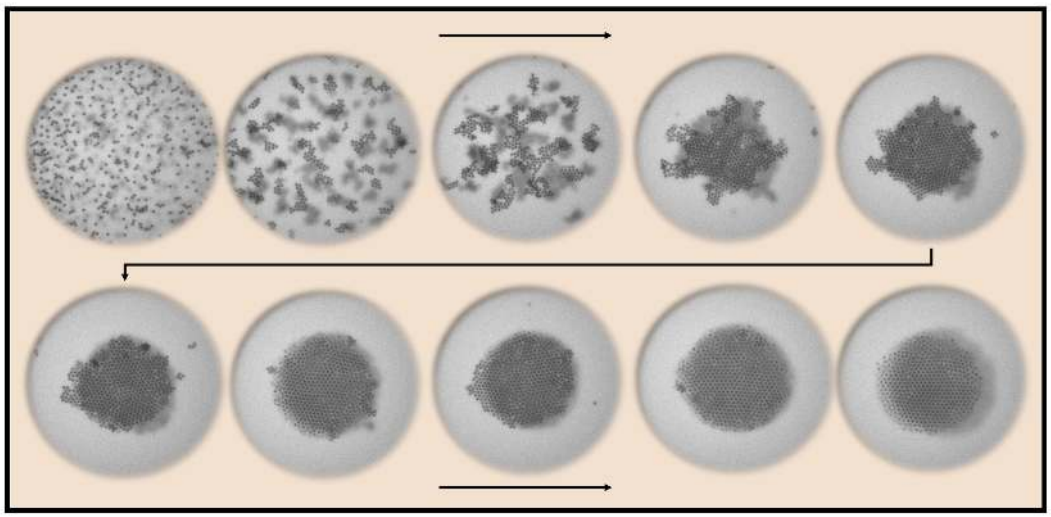
Diffraction profiles hold a wealth of information about material structures, but extracting this information requires careful modeling using mathematical functions. These models are essential for isolating or interpreting various types of disorder present in a material. One significant type of disorder stems from dislocations, which critically influence material properties. Understanding these effects is crucial for accurately predicting the behavior of materials in applications ranging from optoelectronics to battery technology. Traditionally, developing these models has been a time-intensive process, as each model must be carefully tailored to account for specific effects. To streamline this, we propose leveraging Machine Learning to automatically derive these models from simulation data, with the goal of applying them to experimental diffraction profiles. This approach could accelerate the analysis process, enabling faster insights into novel material behavior and performance.



Harsha Namdeo

Reconstruction of Pair Potential from Nanoparticle Configurational Data

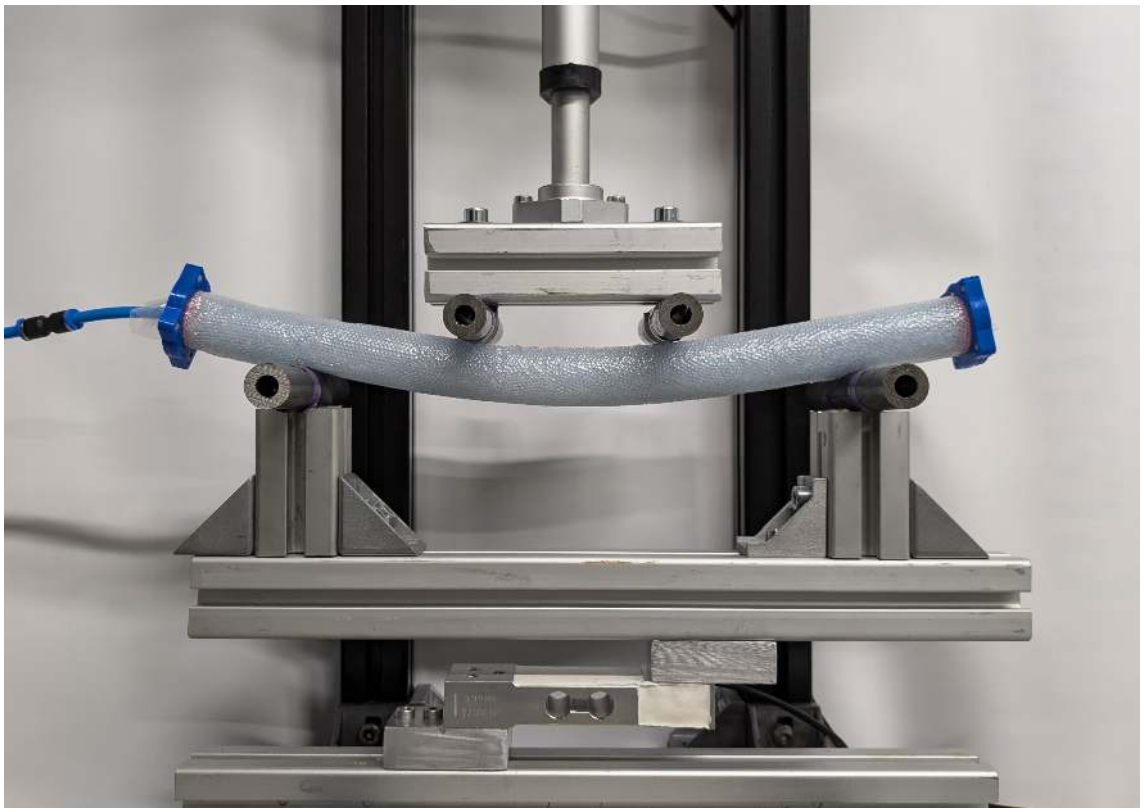
Nanoparticles and their self-assemblies have attracted significant attention in recent years due to their potential applications across various fields. In colloidal systems, these nanoparticles organize into distinct structures influenced by the forces between them. Achieving precise control over these assemblies requires a thorough understanding of these interactions. This project aims to develop a framework for reconstructing the pair potential in self-assembling colloidal systems using only configurational data from experiments. By adopting an observable-based approach, we can align our simulated configurations with those observed experimentally, evaluating different observables to understand their strengths and limitations in characterizing particle arrangements. Additionally, we employ a neural network to learn a pair potential based on the radial distribution function (RDF) as an observable. As a future extension, this approach will be adapted for anisotropic particles to uncover interaction potentials that govern their assembly into targeted structures.



Julian Pollet

Mechanical Properties of Granular Jammed Metamaterials

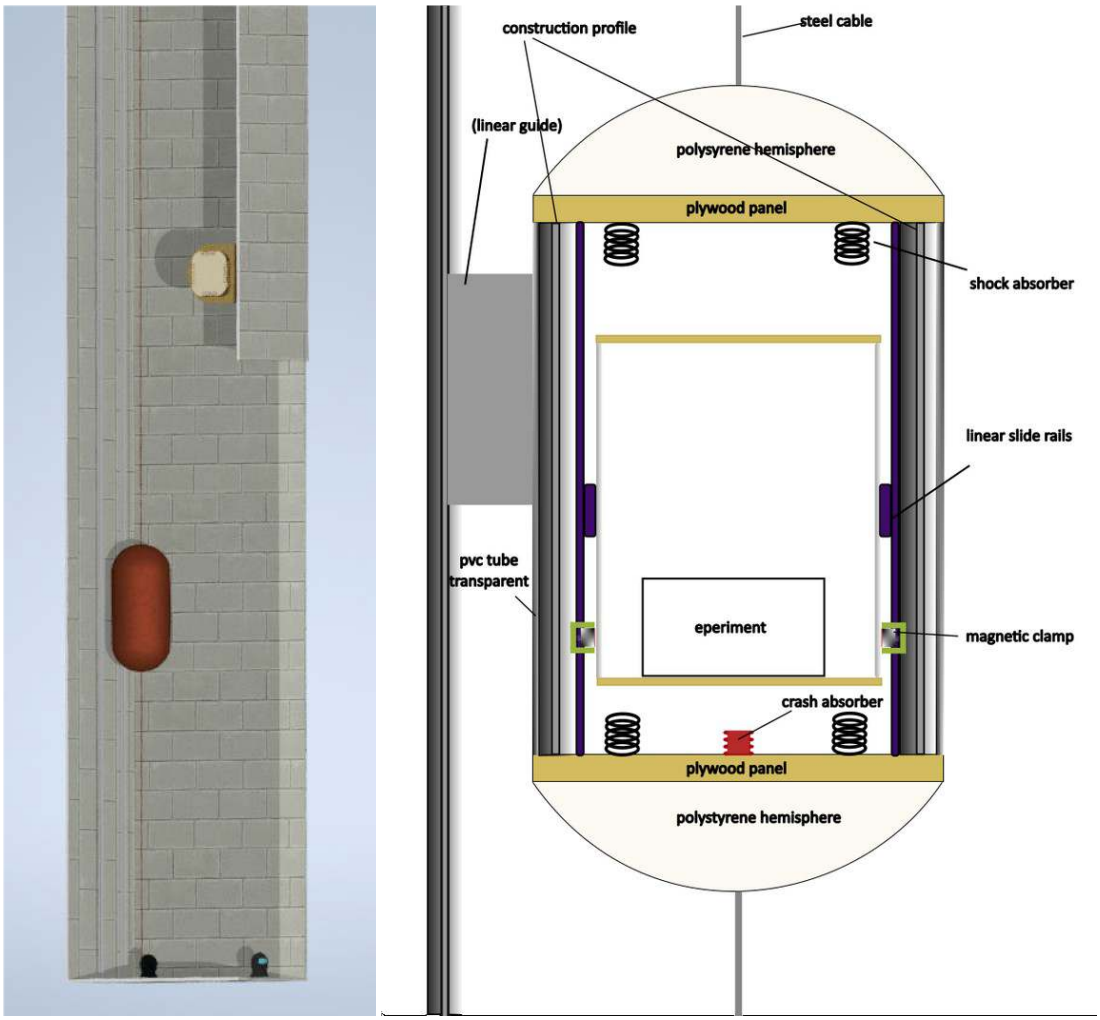
The goal of this master's thesis is to investigate the mechanical properties of granular jammed metamaterials, supervised by Dr. Olfa D'Angelo. For this, two metamaterials that share a similar design principle are compared: both utilize membranes and small round particles to achieve tunable stiffness. The first metamaterial beam features a single outer membrane encasing the particles. When a vacuum is applied, the particles jam together, causing the beam to stiffen due to the increased friction and restricted particle movement. The second beam uses a two-layer membrane system. The inner membrane is filled with air, while a second membrane filled with particles surrounds the air-filled membrane. When overpressure is applied to the inner membrane, it compresses the particles against the outer membrane, inducing a jamming effect similar to the first beam but triggered by the internal overpressure instead of a vacuum.
Different kinds of membranes and particles, varying in geometry, density, and elasticity, are tested in a 4-point bending setup to determine the metamaterial's properties. By using image analysis to measure the deflection and a load cell to record the force applied to the material, we can gain further insights into the material's behavior, such as determining its Young's modulus or deriving a stress-strain curve. Additionally, the internal behavior of the particles will be investigated using a CT scan.



Laura Steub

Gravitational Force Research Elevator – G FREE

Gravity often plays an important in the study of granular media. To conduct experiments under variable levels of gravity, this thesis will combine the design and construction of a small elevator within a maintenance shaft at the MSS laboratories. After an acceleration of 1.5m, a free fall in an up and down motion over a height of 10.5m each will provide up to 2.93s of zero gravity time. Experiments from near-zero to about 1.5g should be possible with corresponding experimental times. The experiment will be held in a guided free-flyer system, with capsule movement being controlled by a motorized winch.



Left: Planned setup of the vario-gravity lift; right: Planned setup of the capsule

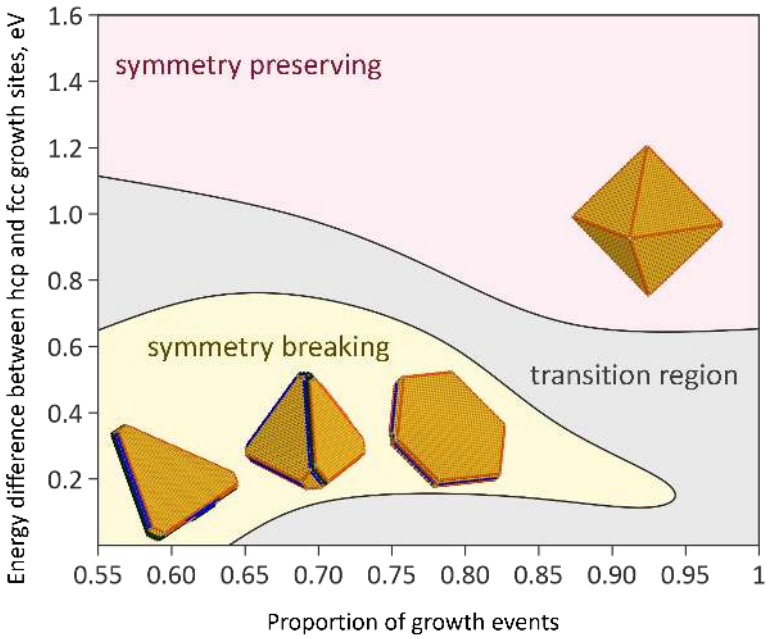
Kamilla Zaripova

Symmetry Breaking of Nanocrystal Shapes via Formation of Surface Defects with Kinetic Monte Carlo

The shape control during nanocrystal growth is essential for the development of nanomaterials with tunable functional properties including catalysis, plasmonics, and photonics. Nanocrystal shapes can be characterized as symmetry-preserving, i.e., the final shape has the same symmetry as a unit cell of a crystal lattice, and symmetry-broken, that is, the symmetry of the resulting shape differs from the one of a unit cell. The first category is well described by Wulff shape construction models. However, the mechanisms leading to symmetry breaking remain unclear.

Based on rejection-free kinetic Monte Carlo simulations, this study investigates the underlying mechanism of symmetry breaking in noble metal nanocrystals. By allowing the simulation to form planar defects (stacking faults) on {111} facets of a nanocrystal, characterized by hexagonal close-packed (hcp) stacking on a face-centered cubic (fcc) surface, three types of symmetry broken shapes are observed, namely tetrahedra, hexagonal nanoplates, and triangular nanoplates. The mechanism of symmetry breaking stems from the preferential growth of atoms on edges between a facet containing a stacking fault and a regular fcc facet. This induces facilitated growth of the adjacent facets to the facet containing the stacking fault, leading to their elimination.

To grow a tetrahedron, at least two non-parallel facets must undergo the formation of the stacking fault to eliminate 4 out of 8 octahedral facets. A nanoplate requires at least one stacking fault, and any further planar defects need orientation parallel to the first stacking fault. Shape transformations between hexagonal and triangular nanoplates are possible depending on the number and sequence of stacking faults. If the initial shape is hexagonal, then another stacking fault creates a difference in growth kinetics between two adjacent side facets of the nanoplate, transforming it into a triangular nanoplate. Alternatively, another stacking fault on a triangular nanoplate restores the growth kinetics between two adjacent side facets, creating a hexagonal shape. Because the formation of planar defects is stochastic, these symmetry-broken shapes coexist. Coexistence with symmetry-preserving shapes, which for the fcc are octahedra, is also investigated. These results bridge fundamental knowledge from atomic scales (energy) to mesoscales (growth velocities, shapes) that are of importance to the engineering of nanomaterials.



Suleyman Gafarli

Development of a Kinetic Model for the Methanol-to-Olefins Synthesis Over an Industrial Catalyst

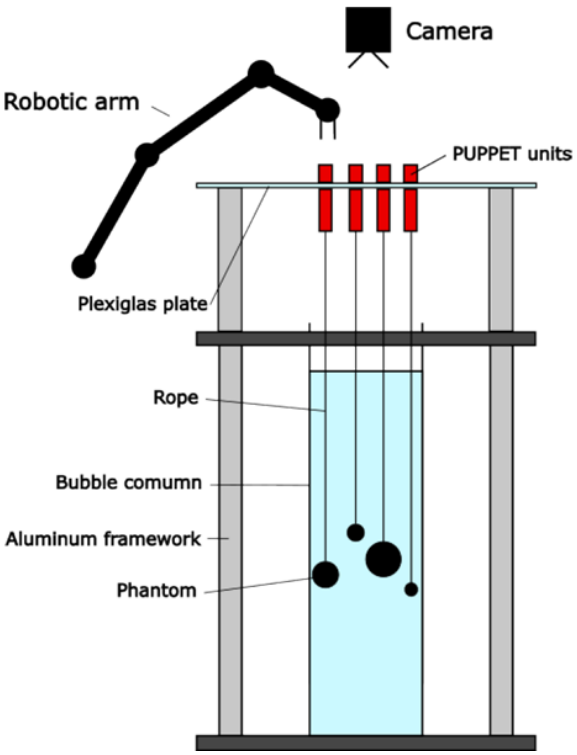
Sustainable aviation fuels (SAFs) are expected to play a crucial in the defossilisation of the aviation industry. The so-called Power-to-Liquid (PtL) technology enables promising SAF production pathways associated with lower demand for natural resources, such as arable land and water, compared to SAF produced from biological feedstocks. The methanol pathway for producing PtL fuels offers several advantages over other production routes, e.g., the possibility of achieving an increased yield of jet fuel.

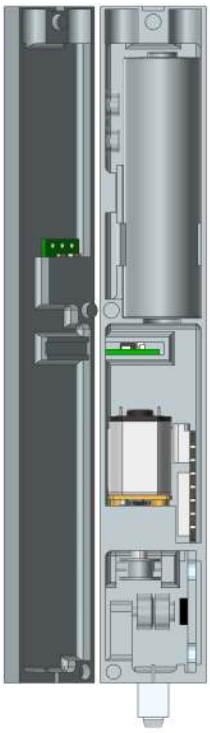
The methanol-to-olefins (MtO) process is a key step for the production of jet fuel starting from methanol. The objective of this thesis is to develop a kinetic model for the MtO synthesis over an industrial catalyst. Kinetic models available in the scientific literature were implemented into a model of a fixed-bed MtO reactor, which was validated using published data. The reactor model was further extended to be able to simulate a wide range of experimental conditions simultaneously and to flexibly predict the reactor effluent composition for the conversion of methanol with and without co-feeding olefins. Furthermore, a kinetic fitting tool was established to regress the kinetic parameters from experimental data via nonlinear optimization techniques. A comparison of experimental and calculated mass fractions indicated that most compounds were predicted within a 20% error range. However, to fully exploit the potential of the developed model, a comprehensive set of experimental data is required for further refinement.

Bachelor theses

Daniel Adam
Implementation of a 3D Phantom Generator for the Acquisition of Validation Data for EIT Image Reconstruction

Electrical impedance tomography (EIT) is an imaging technique employing electric current as the energy source to image the impedance, or resistance, of the measured volume. However, the reconstruction of the image from the measured data presents an ill-posed inverse problem and requires complex algorithms which either take a long time or create images in low resolution. Neural networks offer a promising solution by combining both speed and accuracy, provided they are sufficiently and precisely trained. While there are several ways to create this training data, a particularly low-cost and simple option is to simulate an impedance distribution with non-conducting phantoms, arranged in a known way in front of the sensor. This thesis aims to propose a concept for a 3D phantom generator that can be used to acquire validation data for EIT image reconstruction and to implement this concept for a laboratory-scale experiment.





Other projects

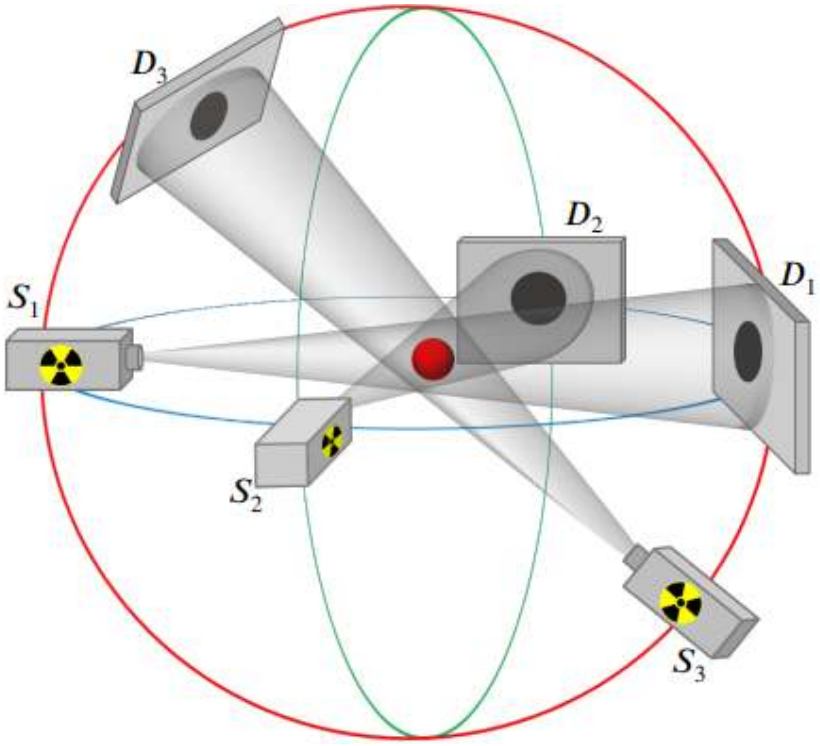
Luca Hagen

Particle Tracking Using Multi-Beam X-Ray Radiography

We developed an iterative algorithm to determine the position of tracer particles from multiple X-ray projections of granular samples, addressing limitations of traditional tomography in dynamic systems. Unlike conventional CT, which requires extensive Radon transformations and numerous projections, our geometric-algebraic approach uses fewer projections, enabling high-speed imaging with temporal resolutions of thousands of frames per second.

This method excels in high-density systems, where particle overlap causes occlusions, by iteratively reconstructing particle paths and improving accuracy. Its adaptability to different experimental setups and conditions, such as varying pressures or temperatures, makes it a versatile tool for fields like granular flow dynamics, experimental rheology, and materials science.

The project advances our understanding of particle dynamics, supporting studies on phenomena such as shear, compaction, and jamming, while paving the way for future enhancements in high-speed radiographic imaging and algorithmic efficiency.



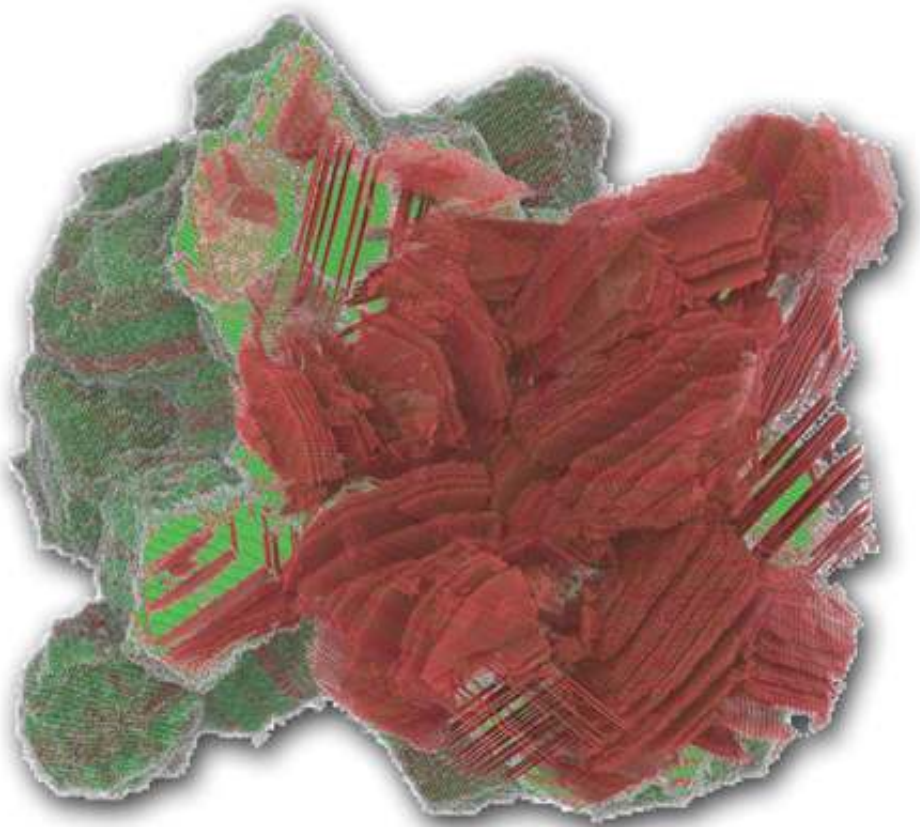
Schematic representation of a multi-beam X-ray CT system with three source-detector pairs (S1-D1, S2-D2, S3-D3) for high-speed, dynamic particle tracking in granular materials.

Navid Panchi

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

The solution of the Debye scattering equation is pivotal in the analysis of total scattering data. Although common solutions rely on brute-force or binning-based algorithms, these approaches are affected by inherent numerical approximations, which compromise accuracy. To address this issue, the Rose-X algorithm was introduced, offering a promising avenue to achieve both computational efficiency and high accuracy. Building on this foundation, we introduce an improved iteration of the original code.

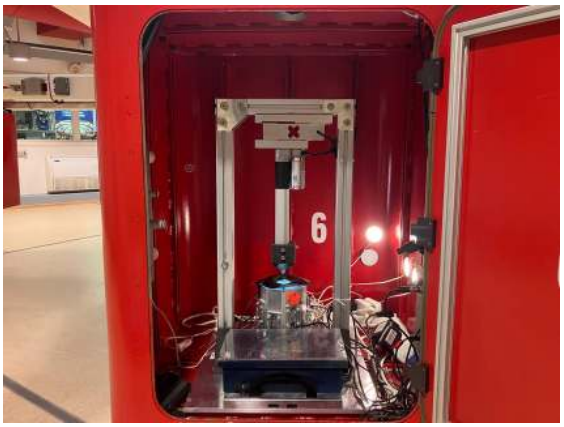
AES-Debye achieves a speedup of 20x over the Rose-X implementation through rigorous performance optimizations and strategic domain decomposition to optimize memory access operations. The code exploits a fusion of OpenMP, MPI, and CUDA programming paradigms to leverage diverse hardware configurations. We provide heuristic benchmarks to dynamically set various implementation parameters, ensuring optimal performance across diverse hardware environments. An open-source Python binding is also provided, empowering users to customize and extend the code, along with a LAMMPS plugin for ease of integration into existing workflows. Lastly, we showcase the code's accuracy and scalability by computing an accurate powder diffraction profile for a large sample with over 90 million atomic positions in a matter of minutes.



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.



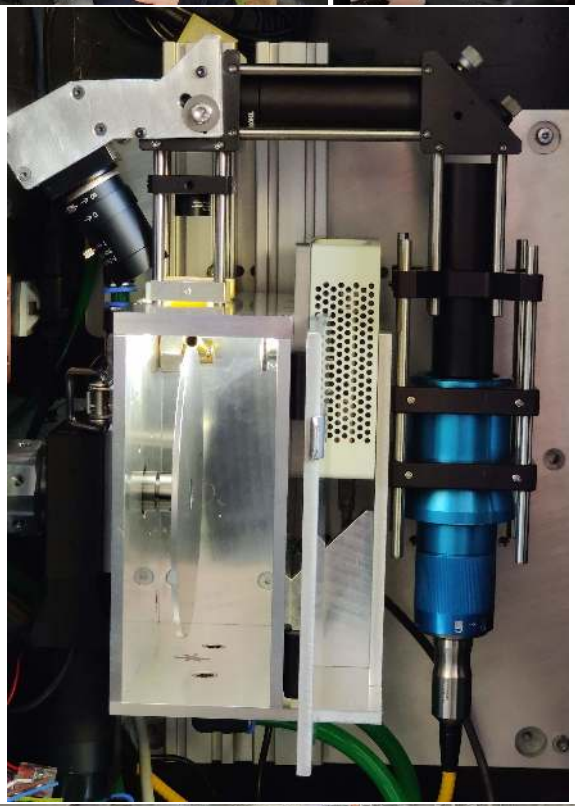
43rd DLR parabolic flight campaign

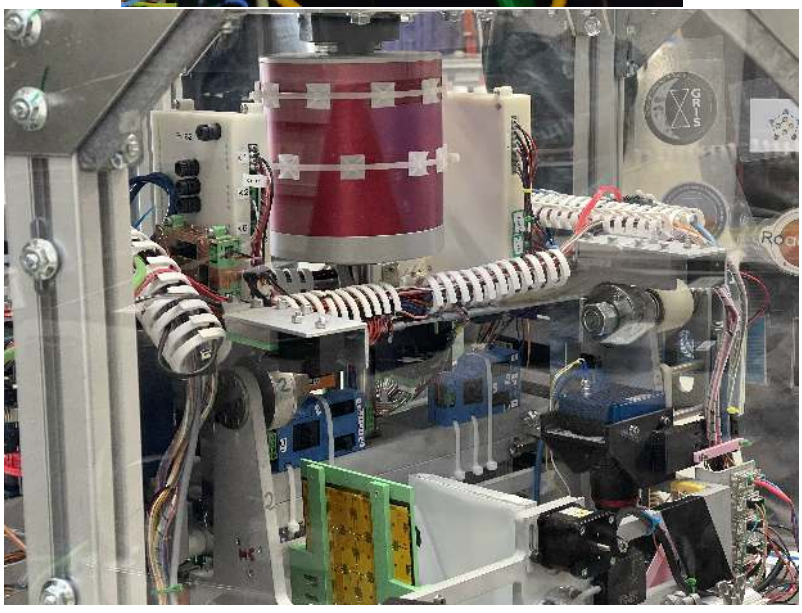
In September, the MSS had the special opportunity to take part in a parabolic flight campaign to conduct two innovative experiments in weightlessness and under reduced gravity. Preparations began with an integration week from September 9 to 13, during which the experiments were installed and tested in 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

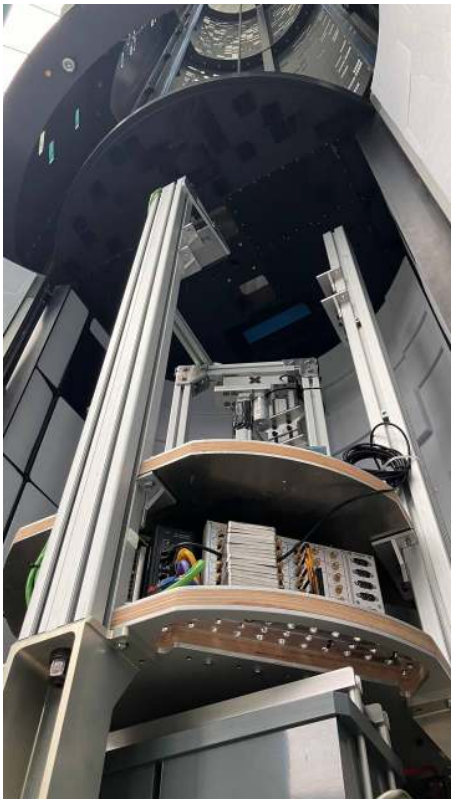

Zero G
FAU
MSS





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

“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: 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

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: J. Anthony (Leeds, UK), Sebastien Aumaitre (Saclay, France), Michael Berhanu (Paris, France), E. Clement (Paris, France), D. Durian (U. Pennsylvania, USA), E. Falcon (Paris, France), S. Fauve (Paris, France), A. Garcimartin (Pamplona, Spain), Y. Garrabos (Bordeaux, France), M. Hou (Beijing, China), X. Jia (Marne, France), C. Lecoutre (Bordeaux, France), S. Luding (Twente, Netherlands), D. Maza (Pamplona, Spain), T. Pöschel (Erlangen, Germany), M. Sperl (Cologne, Germany), N. Vandewalle (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 (KONWIHRIV)
Applicants: Dr. Alberto Leonardi, Prof. Thorsten Pöschel

“Framework for Gas Hydrate Agglomeration under Multiphase Flow”
Emerging Talents Initiative (ETI)
Applicant: Dr. Carlos L. Bassani

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

“Kinetic Pathways of Lower Symmetry Nanocrystal Habit”
EAM Starting Grant 2023/2024
Funded by: Advanced FAU Competence Center Engineering of Advanced Materials.
Applicant: Dr. Carlos L. Bassani

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

11. Publications

Scientific Papers Published by the MSS in Peer-Reviewed Journals in 2024

1. A. A. Ameen, A. Sack, T. Pöschel, TSS-ConvNet for electrical impedance tomography image reconstruction. *Physiological Measurement* **45**, 045006, DOI 10.1088/1361-6579/ad39c2 (2024).

2. M. Bagheri, S. Roy, T. Pöschel, Approximate expressions for the capillary force and the surface area of a liquid bridge between identical spheres. *Computational Particle Mechanics* **11**, 2179–2190, DOI 10.1007/s40571-024-00772-5 (2024).

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. M. Bagheri, S. Roy, T. Pöschel, Comparison of bulk properties of wet granular materials using different capillary force approximations. *EPJ Web Conf.*, in press (2024).

5. M. Bagheri, T. Pöschel, S. Roy, presented at the Conference Proceedings "Traffic and Granular Flow 2024", in press.

6. C. L. Bassani, M. Engel, A. K. Sum, Mesomorphology of clathrate hydrates from molecular ordering. *The Journal of Chemical Physics* **160**, 190901, DOI 10.1063/5.0200516 (2024).

7. C. L. Bassani, G. van Anders, U. Banin, D. Baranov, Q. Chen, M. Dijkstra, M. Dimitriyev, E. Efrati, J. Faraudo, O. Gang, N. Gaston, R. Golestanian, G. I. Guerrero-Garcia, M. Grünwald, A. Haji-Akbari, M. Ibáñez, M. Karg, T. Kraus, B. Lee, R. V. Lehn, R. Macfarlane, B. M. Mognetti, S. Osat, O. Prezhdo, G. Rotskoff, L. Saiz, A.-C. Shi, S. Skrabalak, I. Smalyukh, M. Tagliazucchi, D. Talapin, A. Tkachenko, S. Tretiak, D. Vaknin, A. Widmer-Cooper, G. Wong, X. Ye, S. Zhou, E. Rabani, M. Engel, A. Travesset, Nanocrystal Assemblies: Current Advances and Open Problems. *ACS Nano* **18**, 14791–14840, DOI 10.1021/acsnano.3c10201 (2024).

8. M. Blank, P. Nair, T. Pöschel, Surface tension and wetting at free surfaces in smoothed particle hydrodynamics. *Journal of Fluid Mechanics* **987**, A23, DOI 10.1017/jfm.2024.410 (2024).

9. F. Buchele, M. Blank, T. Pöschel, P. Müller, Model geometries of random porous materials. *International Journal of Heat and Mass Transfer* **234**, 126074, DOI 10.1016/j.ijheatmasstransfer.2024.126074 (2024).

10. S. Cavalli, R. F. Alves, C. L. Bassani, M. A. M. Neto, A. K. Sum, R. E. M. Morales, Modulation of slug flow characteristics observed in three-phase solid-liquid-gas flow measurements. *Chemical Engineering Science* **300**, 120596, DOI 10.1016/j.ces.2024.120596 (2024).

11. S. Duverger, V. Angelidakis, S. Nadimi, S. Utili, S. Bonelli, P. Philippe, J. Duriez, Investigation techniques and physical aspects of the angle of repose of granular matter. *Granular Matter* **26**, DOI 10.1007/s10035-023-01378-z (2024).

12. A. Enriquez, A. Sack, O. D'Angelo, Acoustically propelled winged macroparticles. *Journal of Applied Physics* **136**, DOI 10.1063/5.0227364 (2024).

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

14. A. Madanchi, F. Aghaei, S. H. E. Rahbari, M. R. R. Tabar, T. Pöschel, Non-monotonic dynamic correlation explored via active microrheology. *Journal of Statistical Mechanics: Theory and Experiment* **2024**, 103205, DOI 10.1088/1742-5468/ad8222 (2024).

15. A. Madanchi, F. Aghaei, S. H. E. Rahbari, M. R. R. Tabar, T. Pöschel, Exploring Positional Variations in Glass Viscosity Through Active Microrheology. *Journal of Statistical Mechanics: Theory and Experiment* **2024** (2024).

16. P. Müller, A. Sack, J. Dümler, M. Heckel, T. Wenzel, T. Siegert, S. Schuldt-Lieb, H. Gieseler, T. Pöschel, Automated Tomographic Assessment of Structural Defects of Freeze-Dried Pharmaceuticals. *AAPS PharmSciTech* **25**, 103205, DOI 10.1208/s12249-024-02833-7 (2024).

17. P. Müller, A. Panchenko, W. T. Ku, T. Pöschel, Particle size segregation in granular pipe flow. *Chaos*, in press (2024).

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

19. 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).

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21. S. Roy, H. Xiao, V. Angelidakis, T. Pöschel, Combined thermal and particle shape effects on powder spreading in additive manufacturing via discrete element simulations. *Powder Technology* **445**, 120099, DOI 10.1016/j.powtec.2024.120099 (2024).

22. S. Roy, Fluidization of wet cohesive powder in virtual Couette rheometer. *Particuology*, submitted (2024).

23. S. Roy, T. Pöschel, Shape effects in binary mixtures of PA12 powder in additive manufacturing. *Powder Technology* **448**, 120326, DOI 10.1016/j.powtec.2024.120326 (2024).

24. S. Roy, H. Xiao, V. Angelidakis, T. Pöschel, Structural fluctuations in thin cohesive particle layers in powder-based additive manufacturing. *Granular Matter* **26**, 43, DOI 10.1007/s10035-024-01410-w (2024).

25. S. Roy, T. Weinhart, The of granular matter in additive manufacturing. *Granular Matter* **26**, DOI 10.1007/s10035-024-01473-9 (2024).

26. A. Santarossa, O. D'Angelo, A. Sack, T. Pöschel, All-terrain granular gripper. *Authorea*, submitted, DOI 10.22541/au.173437408.86018701/v1 (Dec. 2024).

27. A. Santarossa, T. Pöschel, Enhanced interlocking in granular jamming grippers through hard and soft particle mixtures. *Granular Matter* **26**, DOI 10.1007/s10035-024-01475-7 (2024).

28. C. Shi, Z. Cheng, A. Leonardi, Y. Yang, M. Engel, M. R. Jones, Y. Han, Preserving surface strain in nanocatalysts via morphology control. *Science Advances* **10**, eadp3788, DOI 10.1126/sciadv.adp3788 (2024).

29. A. P. Singh, V. Angelidakis, T. Pöschel, S. Roy, Shear zones in granular mixtures of hard and soft particles with high and low friction. *Soft Matter* **20**, 3118–3130, DOI 10.1039/d4sm00100a (2024).

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31. N. R. Varela-Rosales, M. Engel, Tuning the stability of a model quasicrystal and its approximants with a periodic substrate. *Soft Matter* **20**, 2915–2925, DOI 10.1039/d4sm00191e (2024).

32. D. E. Wolf, T. Pöschel, Fractal packing of nanomaterials. *arXiv*, DOI 10.48550/ARXIV.2312.03117 (2023).

Other publications published by MSS in 2024 and submitted manuscripts

33. C. L. Bassani, M. Engel, Kinetically Trapped Nanocrystals with Symmetry-Preserving Shapes. *arXiv*, DOI 10.48550/ARXIV.2410.09787 (2024).

34. A. Nazemi, A. Sack, H. Torres, T. Pöschel, H. Xiao, Understanding the propulsion of a scallop-like swimmer in granular media. *Bulletin of the American Physical Society* (2024).

35. N. R. Varela-Rosales, M. Engel, Computational Self-Assembly of a Six-Fold Chiral Quasicrystal. *arXiv*, DOI 10.48550/ARXIV.2408.01984 (2024).

36. H. Xiao, H. Torres, A. Sack, T. Pöschel, Locomotion of a Scallop-Inspired Swimmer in Granular Matter. *arXiv*, DOI 10.48550/ARXIV.2412.05266 (2024).

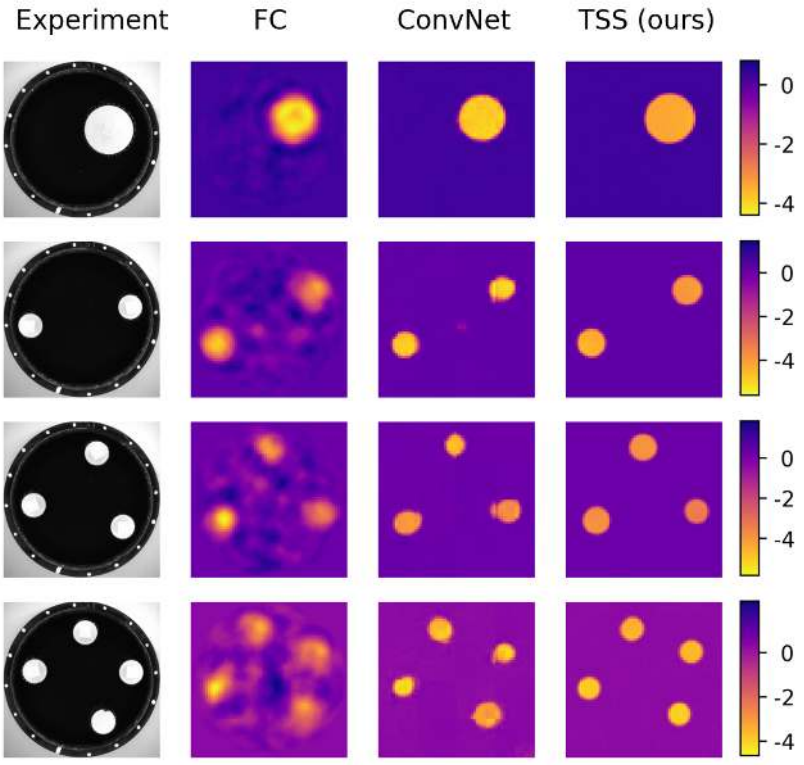
Patent Application

37. O. D'Angelo, A. Sack, T. Pöschel, Resilient deployable structure with programmable mechanical properties. DE 10 2023 130 608.1 (2023).

TSS-ConvNet for Electrical Impedance Tomography Image Reconstruction

Ayman Ameen, Achim Sack, Thorsten Pöschel

Abstract:
Objective. The objective of this study was to propose a novel data-driven method for solving ill-posed inverse problems, particularly in certain conditions such as time-difference electrical impedance tomography for detecting the location and size of bubbles inside a pipe. Approach. We introduced a new layer architecture composed of three paths: spatial, spectral, and truncated spectral paths. The spatial path processes information locally, whereas the spectral and truncated spectral paths provide the network with a global receptive field. This unique architecture helps eliminate the ill-posedness and nonlinearity inherent in the inverse problem. The three paths were designed to be interconnected, allowing for an exchange of information on different receptive fields with varied learning abilities. Our network has a bottleneck architecture that enables it to recover signal information from noisy redundant measurements. We named our proposed model truncated spatial-spectral convolutional neural network (TSS-ConvNet). Main results. Our model demonstrated superior accuracy with relatively high resolution on both simulation and experimental data. This indicates that our approach offers significant potential for addressing ill-posed inverse problems in complex conditions effectively and accurately. Significance. The TSS-ConvNet overcomes the receptive field limitation found in most existing models that only utilize local information in Euclidean space. We trained the network on a large dataset covering various configurations with random parameters to ensure generalization over the training samples.



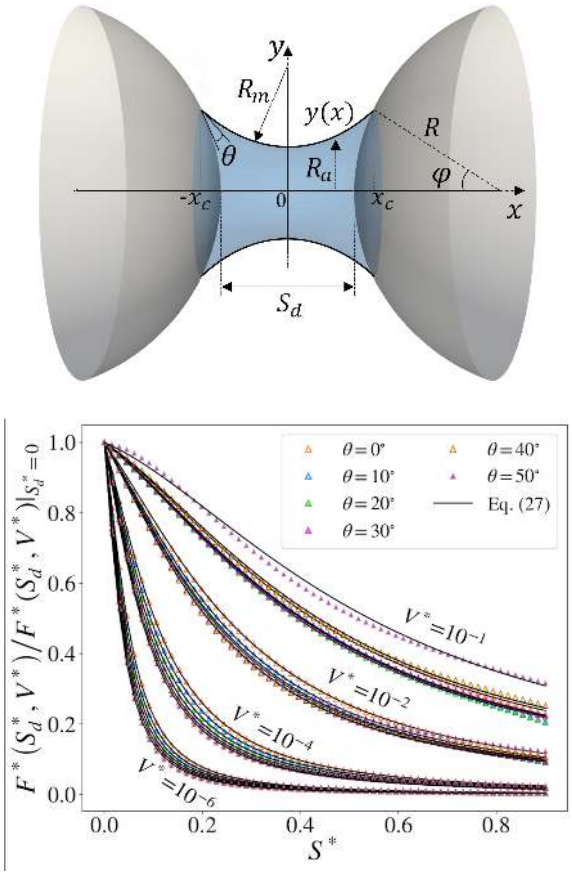
The reconstructed images from four different experimental cases with one to four objects using different deep learning methods.

1. A. A. Ameen, A. Sack, T. Pöschel, TSS-ConvNet for electrical impedance tomography image reconstruction. *Physiological Measurement* **45**, 045006, DOI 10.1088/1361-6579/ad39c2 (2024).

Approximate Expressions for the Capillary Force and the Surface Area of a Liquid Bridge between Identical Spheres

Meysam Bagheri, Sudeshna Roy, Thorsten Pöschel

Abstract:
We consider a liquid bridge between identical spheres and present approximate expressions for the capillary force and the exposed surface area of the liquid bridge as functions of the liquid bridge's total volume and the sphere separation distance. The radius of the spheres and the solid-liquid contact angle are parameters that enter the expressions. These expressions are needed for efficient numerical simulations of drying suspensions.



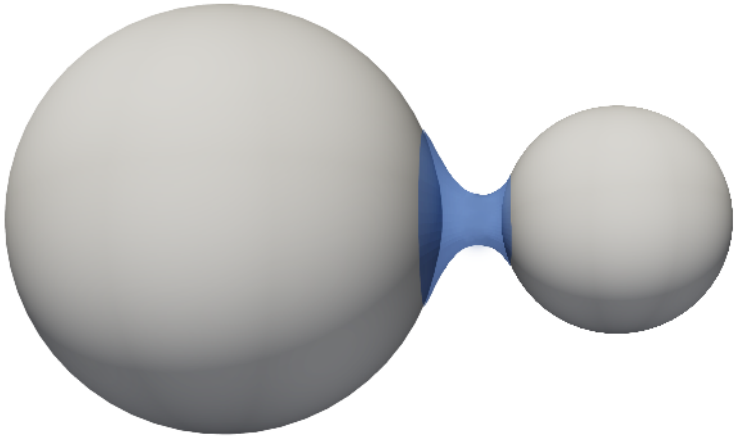
(a) The shape of a liquid bridge between two identical spheres of radius R and distance S_d is a solution of the Young-Laplace equation with the solid-liquid contact angle, θ, and the half-filling angle, φ. (b) Capillary force due to a liquid bridge spanning between two spheres as a function of the normalized distance, S^*, for a range of volumes, $V^* \in \{10^(-6), 10^(-4), 10^(-2), 10^(-1)\}$, and contact angle, $\theta \in \{0^o, 10^o, 20^o, 30^o, 40^o, 50^o\}$.

2. M. Bagheri, S. Roy, T. Pöschel, Approximate expressions for the capillary force and the surface area of a liquid bridge between identical spheres. *Computational Particle Mechanics* **11**, 2179–2190, DOI 10.1007/s40571-024-00772-5 (2024).

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.



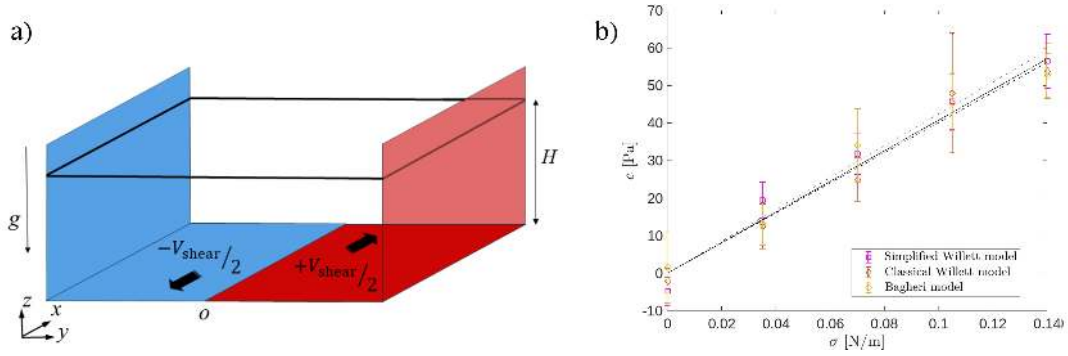
Capillary bridge spanning between two unequal-sized particles.

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).

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

Meysam Bagheri, Sudeshna Roy, Thorsten Pöschel

Abstract:
We simulate wet granular materials using capillary force models in MercuryDPM, comparing the simplified Willett, classical Willett, and Bagheri approximations. Split-bottom shear cell simulations show bulk cohesion increases linearly with liquid surface tension across all models, while macroscopic friction coefficients are weakly dependent on surface tension.



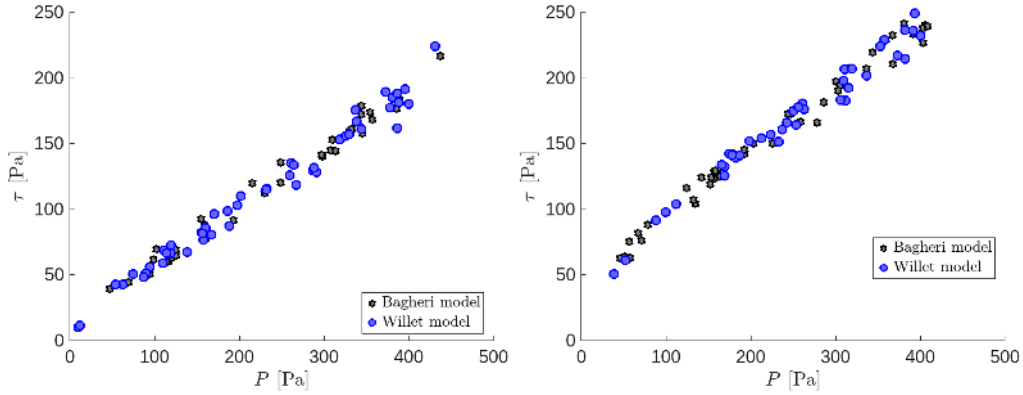
(a) Linear split-bottom shear cell (b) Bulk cohesion c as a function of the surface tension of liquid σ for liquid bridge volume 20 nl.

4. M. Bagheri, S. Roy, T. Pöschel, Comparison of bulk properties of wet granular materials using different capillary force approximations. *EPJ Web Conf.*, in press (2024).

Shear flow of wet granular matter: Influence of the capillary bridge description using MercuryDPM

Meysam Bagheri, Sudeshna Roy, Thorsten Pöschel

Abstract:
In this study, we utilize the previously implemented two-particle capillary force approximations in MercuryDPM to perform bulk simulations of wet granular materials. We compare the performance of the Bagheri and Willett approximations in simulating capillary bridges. Bulk simulations are conducted within a split-bottom shear cell to analyze and compare the resulting bulk cohesion and macroscopic friction coefficients. Our findings show that bulk cohesion increases linearly with liquid surface tension and is consistent for both approximations. In contrast, the macroscopic friction coefficient remains independent of surface tension for both approximations.



Shear stress τ plotted against normal stress P for wet granular materials simulated using different capillary force approximations for liquid surface tension (a) $\gamma = 0.035\,\mathrm{N/m}$ and (b) $\gamma = 0.140$ N/m.

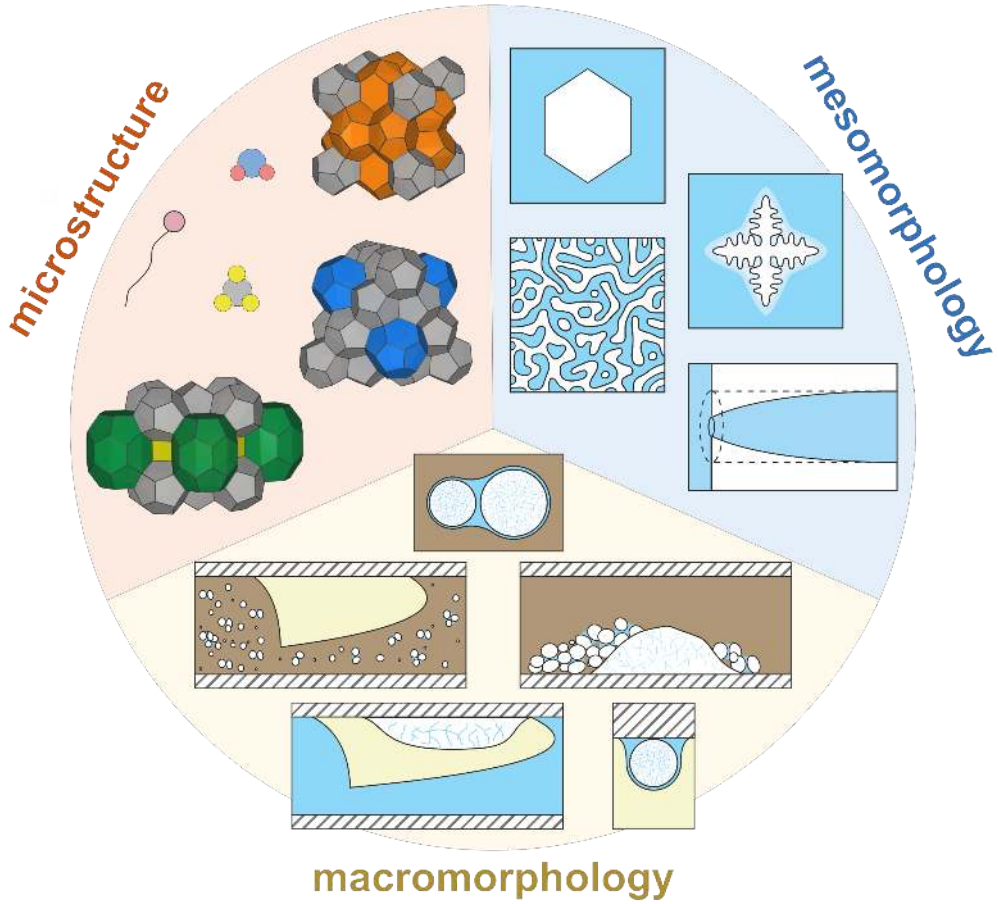
5. M. Bagheri, T. Pöschel, S. Roy, presented at the Conference Proceedings “Traffic and Granular Flow 2024”, in press.

Mesomorphology of clathrate hydrates from molecular ordering

Carlos L. Bassani, Michael Engel, Amadeu K. Sum

Abstract:

Clathrate hydrates are crystals formed by guest molecules that stabilize cages of hydrogen-bonded water molecules. Whereas thermodynamic equilibrium is well described via the van der Waals and Plateeuw approach, the increasing concerns with global warming and energy transition require extending the knowledge to non-equilibrium conditions in multiphase, sheared systems, in a multiscale framework. Potential macro applications concern the storage of carbon dioxide in the form of clathrates, and the reduction of hydrate inhibition additives currently required in hydrocarbon production. We evidence porous mesomorphologies as key to bridging the molecular scales to macro applications of low solubility guests. We discuss the coupling of molecular ordering with the mesoscales, including (i) the emergence of porous patterns as a combined factor from the walk over the free energy landscape and 3D competitive nucleation and growth, and (ii) the of molecular attachment rates in crystallization-diffusion models that allow predicting the timescale of pore sealing. This is a perspective study that discusses the use of discrete models (molecular dynamics) to build continuum models (phase field models, crystallization laws, transport phenomena) to predict multiscale manifestations at a feasible computational cost. Several advances in correlated fields (ice, polymers, alloys, nanoparticles) are discussed in the scenario of clathrate hydrates, as well as the challenges and necessary developments to push the field forward.



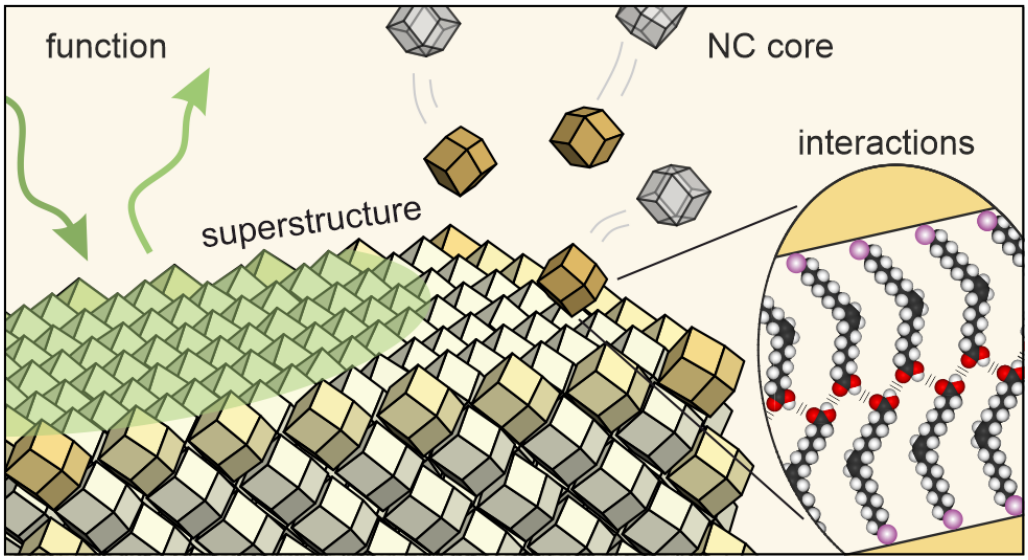
6. C. L. Bassani, M. Engel, A. K. Sum, Mesomorphology of clathrate hydrates from molecular ordering. *The Journal of Chemical Physics* **160**, 190901, DOI 10.1063/5.0200516 (2024).

Nanocrystal Assemblies: Current Advances and Open Problems

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

Abstract:

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

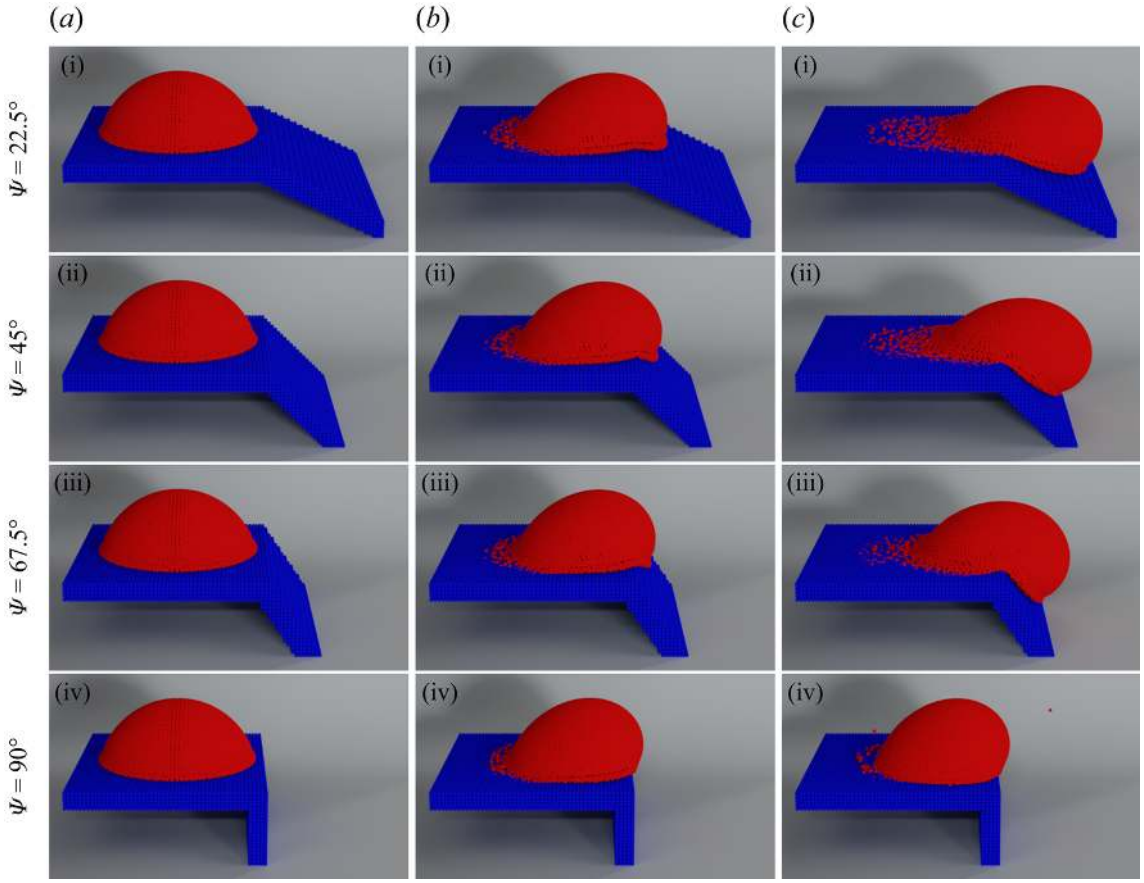


7. C. L. Bassani, G. van Anders, U. Banin, D. Baranov, Q. Chen, M. Dijkstra, M. Dimitriyev, E. Efrati, J. Faraudo, O. Gang, N. Gaston, R. Golestanian, G. I. Guerrero-Garcia, M. Grünwald, A. Haji-Akbari, M. Ibáñez, M. Karg, T. Kraus, B. Lee, R. V. Lehn, R. Macfarlane, B. M. Mognetti, S. Osat, O. Prezhdo, G. Rotskoff, L. Saiz, A.-C. Shi, S. Skrabalak, I. Smalyukh, M. Tagliazucchi, D. Talapin, A. Tkachenko, S. Tretiak, D. Vaknin, A. Widmer-Cooper, G. Wong, X. Ye, S. Zhou, E. Rabani, M. Engel, A. Travesset, Nanocrystal Assemblies: Current Advances and Open Problems. *ACS Nano* **18**, 14791–14840, DOI 10.1021/acsnano.3c10201 (2024).

Surface tension and wetting at free surfaces in smoothed particle hydrodynamics

Michael Blank, Prapanch Nair, Thorsten Pöschel

Abstract:
Surface tension and wetting are dominating physical effects in microscale and nanoscale flows. We present an efficient and reliable model of surface tension and equilibrium contact angles in smoothed particle hydrodynamics for free-surface problems. We demonstrate its robustness and accuracy by simulating several three-dimensional free-surface flow problems driven by interfacial tension.



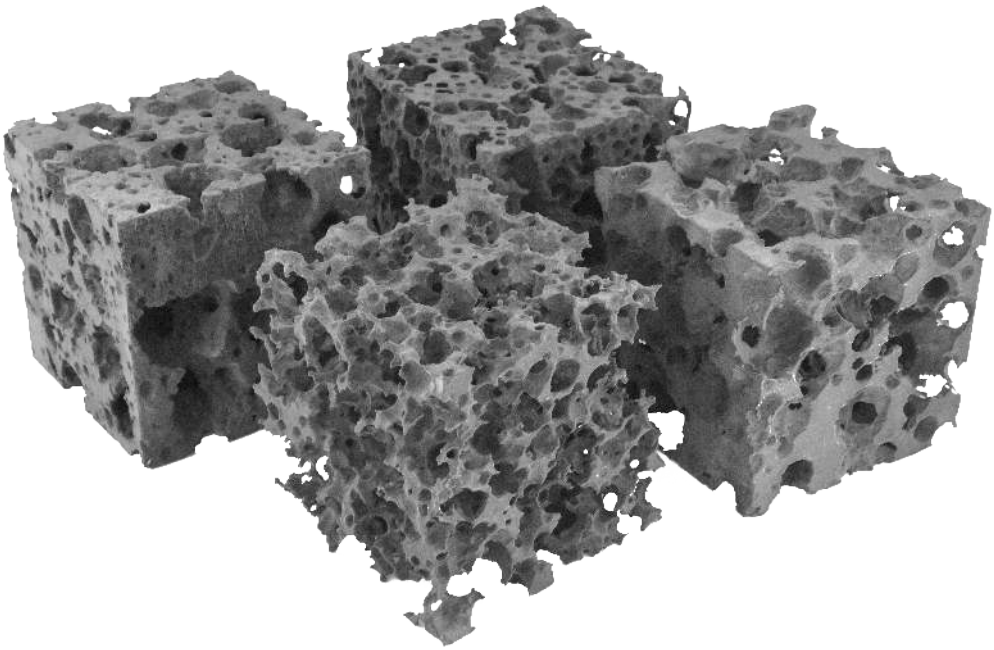
Simulation snapshots of droplets that are accelerated towards the contact line of two planes with different inclinations. Panel (a i–iv) shows the droplets at time $t = 50$ ms resting in equilibrium on a horizontal solid plane with the equilibrium contact angle $\theta_\infty = 50^o$. Panel (b i–iv) shows the droplets at time $t = 100$ ms when approaching the contact line under the action of acceleration f_b. Panel (c i–iv) at time $t = 150$ ms: For $\psi \in \{22.5^o, 45^o, 67.5^o\}$ the contact angle exceeds the threshold, thus the drop passed over the surface discontinuity. For $\psi = 90^o$, the contact angle is below the threshold, thus the drop remains pinned.

8. M. Blank, P. Nair, T. Pöschel, Surface tension and wetting at free surfaces in smoothed particle hydrodynamics. *Journal of Fluid Mechanics* **987**, A23, DOI `10.1017/jfm.2024.410` (2024).

Model geometries of random porous materials

Felix Buchele, Michael Blank, Thorsten Pöschel, Patric Müller

Abstract:
We describe a method for modeling the geometry of random porous materials. The approach enables the independent selection of crucial parameters, including porosity, pore size distribution, pore shape, and connectivity. Consequently, it can effectively model a wide range of porous systems. Due to the diverse and systematic variation possibilities, the method is suitable for developing and optimizing porous structures. The geometries can be exported as triangular meshes, facilitating their immediate use in numerical simulation and further digital processing. We showcase the method's capabilities by minimizing the foam structure's thermal conductivity through geometry optimization.



Exemplary open porous geometries resulting from the sphere packing algorithm.

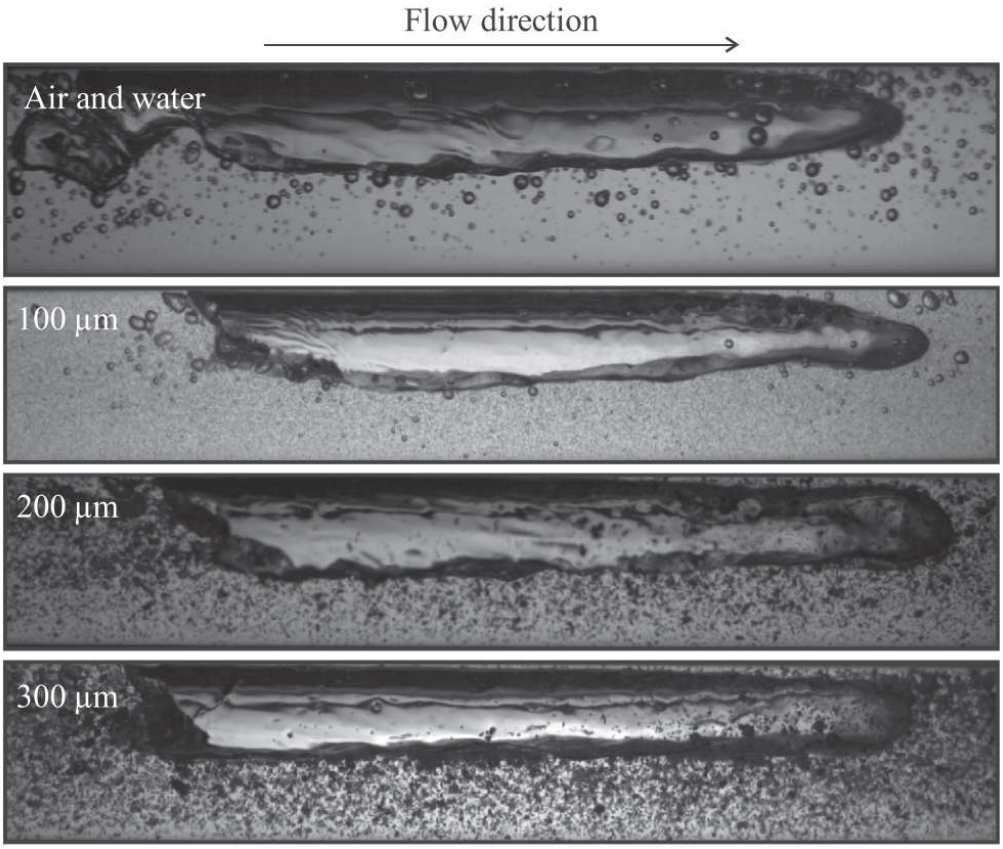
9. F. Buchele, M. Blank, T. Pöschel, P. Müller, Model geometries of random porous materials. *International Journal of Heat and Mass Transfer* **234**, 126074, DOI 10.1016/j.ijheatmasstransfer.2024.126074 (2024).

Modulation of slug flow characteristics observed in three-phase solid-liquid-gas flow measurements

Stella Cavalli, Rafael F. Alves, Carlos L. Bassani, Moises A. Marcelino Neto, Amadeu K. Sum, Rigoberto E.M. Morales

Abstract:

The formation and agglomeration of gas hydrates represent a critical issue in flow assurance. This research aims to evaluate the transport and impact of particles on the slug flow pattern. Experimental investigations were conducted using inert polyethylene particles, mimicking gas hydrates, with four different particle sizes (100 µm, 200 µm, 300 µm, and 400 µm) and three volumetric concentrations (1 %, 2.5 %, and 5 %) with air and water as working fluids. The measurements show a relationship between slug flow characteristics and particle attributes, showing a nonlinear behavior influenced by both particle size and concentration, potentially explained via turbulence modulation. The particle size relative to the turbulent eddy size can either promote or damp the turbulence intensity, with impact on the peak velocity of the flow, and consequences in the elongated bubble velocity. In the case of lower mixture velocities and higher liquid loadings, particles also influence the slug flow formation.

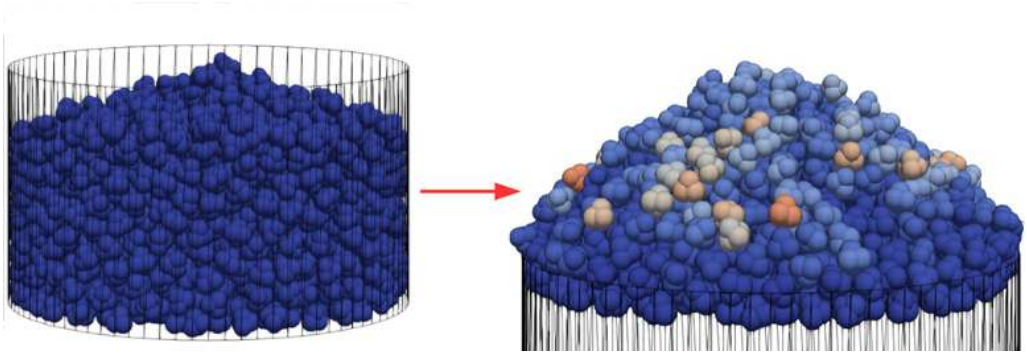


10. S. Cavalli, R. F. Alves, C. L. Bassani, M. A. M. Neto, A. K. Sum, R. E. M. Morales, Modulation of slug flow characteristics observed in three-phase solid-liquid-gas flow measurements. *Chemical Engineering Science* **300**, 120596, DOI 10.1016/j.ces.2024.120596 (2024).

Investigation techniques and physical aspects of the angle of repose of granular matter

Sacha Duverger, Vasileios Angelidakis, Sadegh Nadimi, Stefano Utili, Stéphane Bonelli, Pierre Philippe, Jérôme Duriez

Abstract:
The repose of granular materials is investigated via two different Discrete Element Method (DEM) implementations in comparison with an experimental reference from a recently proposed benchmark setup. On a methodological standpoint, a rigorous measurement method of the angle of repose (AOR) is first proposed for plane-strain and axisymmetric conditions as encountered in the reference experiments. Additionally, two systematic procedures are designed in order to also determine the void ratio of the heap, as a fundamental property of granular matter possibly influencing the AOR. A physical discussion is then developed on the of particle shape, considering the non-spherical nature of reference particles with a convexity value of C=0.954. Adopting non-convex multi-spheres aggregates (i.e. clumps), the first DEM modeling approach successfully predicts the AOR within an 8% tolerance. After a convex simplification that neglects local concavities, another approach based on potential particles underestimates to a greater extent the AOR, bringing it down from 35.95±0.88° to 31.26±0.95°. For the loading setup(s) at hand, the AOR is eventually shown to bear no constitutive nature. It is, for instance, independent of initial void ratio but is still different than the critical friction angle. The latter may actually serve as a lower bound for the process-dependent AOR. These conclusions are drawn from a statistical analysis of a large set of results, accounting for the random nature of the microscopic arrangement in the studied process.



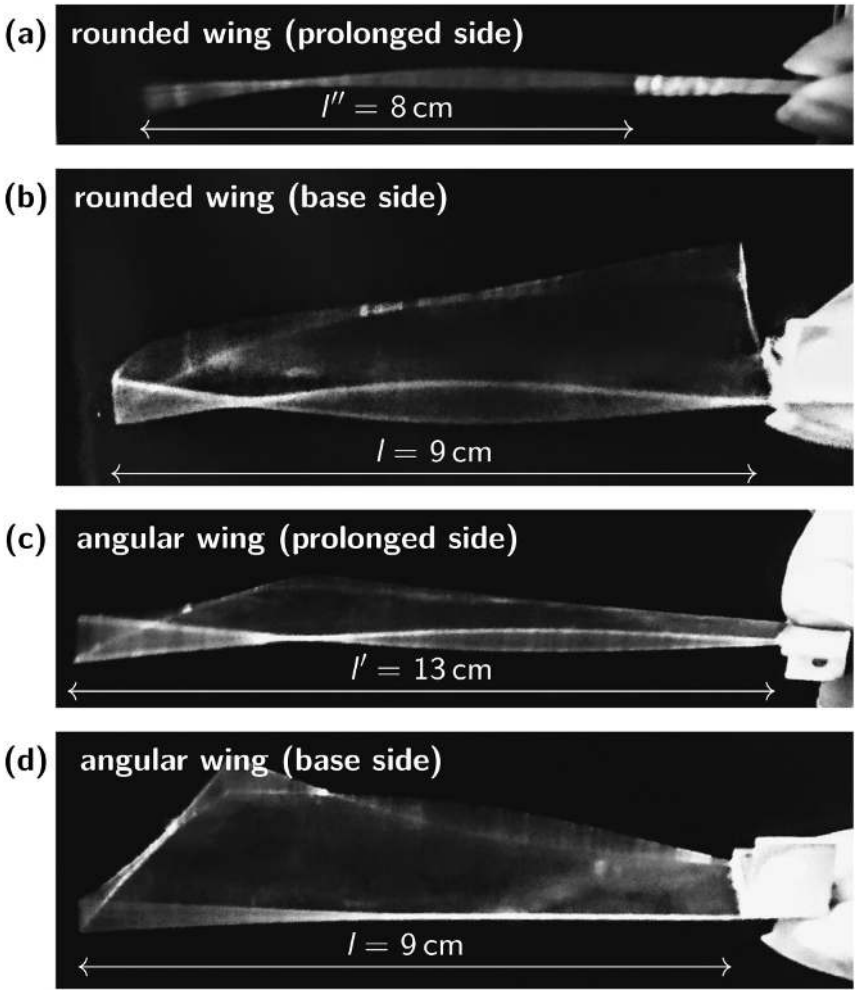
Initial (left) and final (right) states of the heap in the axisymmetric configuration.

11. S. Duverger, V. Angelidakis, S. Nadimi, S. Utili, S. Bonelli, P. Philippe, J. Duriez, Investigation techniques and physical aspects of the angle of repose of granular matter. *Granular Matter* **26**, DOI 10.1007/s10035-023-01378-z (2024).

Acoustically propelled winged macroparticles

Adriana Enriquez, Achim Sack, Olfa D'Angelo

Abstract:
Self-propelled particles harvest and harness energy from their environment, transforming it into a controlled force that propels their motion. We present a mechanism to propel active macroparticles using low frequency noise (10–200 Hz). Thin polymer plates (wings) are acoustically excited at their second natural frequency; the mass of air displaced generates a counter-force, which propels the macroparticles. We show that the magnitude and direction of the propelling force can be tweaked through the wing's shape, dimensions, and orientation. Finally, we design a macroparticle with bidirectional rotation: its rotation direction can be inverted by changing the frequency at which it is excited.



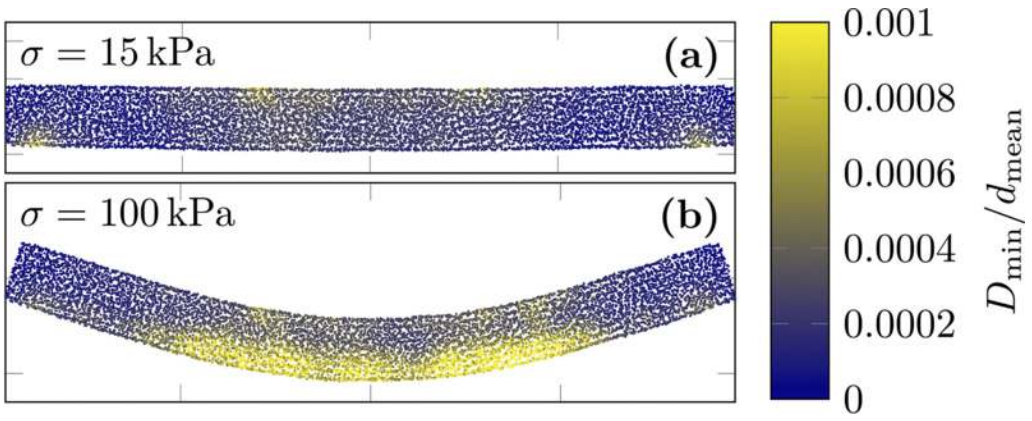
Motion amplitude of asymmetric wings. Rounded wing in two different positions (flipped) to illustrate oscillation of each side: (a) prolonged (l00) and (b) base (l) (both acoustically excited at 90 dB and 32 Hz). Angular wing in two different positions: (c) prolonged (l0) and (d) base (l) (both acoustically excited with 90 dB and 49 Hz). The lengths depicted correspond to the sides at rest, which provide a scale for each image.

12. A. Enriquez, A. Sack, O. D'Angelo, Acoustically propelled winged macroparticles. *Journal of Applied Physics* **136**, DOI 10.1063/5.0227364 (2024).

Structural features of jammed-granulate metamaterials

Holger Götz, Thorsten Pöschel, Olfa D'Angelo

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



D_{min}/d_{mean} of the beam. Examples are displayed for systems with the particles' stiffness E_P=100 MPa and friction coefficient μ_pp=0.3 and external stress values of (a) σ= 15 kPa and (b) σ=100 kPa.

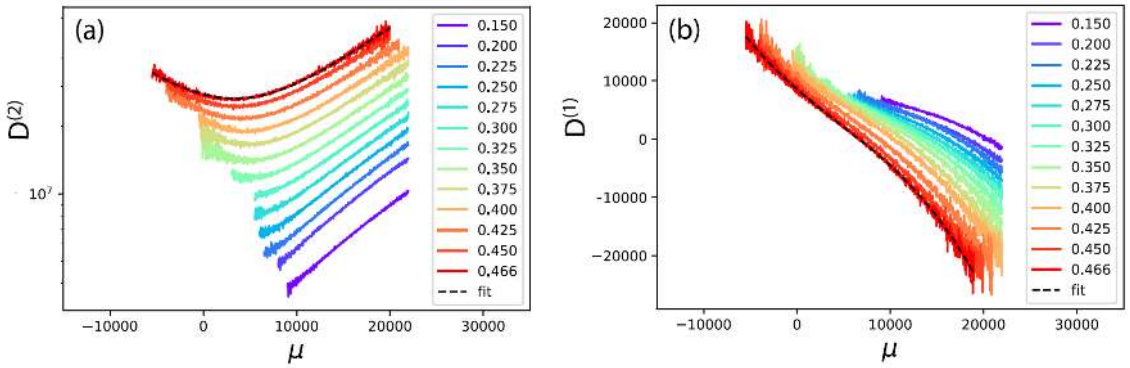
13. H. Götz, T. Pöschel, O. D'Angelo, Structural features of jammed-granulate metamaterials. *Physical Review Research* **6**, DOI 10.1103/physrevresearch.6.013061 (2024).

Non-monotonic dynamic correlation explored via active microrheology

Ata Madanchi, Fatemeh Aghaei, Siamak Rahbari, Mohammad Reza Rahimi Tabar, Thorsten Pöschel

Abstract:

In the study of local and heterogeneous structures in supercooled liquids, microrheology plays a crucial, offering a closer examination of the mechanical properties at a local level. We concentrate on active microrheology, where an external force drives a probe particle. This technique is employed in the study of a Kob–Andersen mixture, using extensive molecular dynamics simulations. Through active microrheology, we analyze the positional dependence of viscosity, observing how probe particles respond to activation velocity. Utilizing advanced stochastic analysis, we disentangle the deterministic and stochastic components of the local viscosity time series, characterizing its nonlinear and intermittent properties, which indicate heterogeneity. We construct a Langevin equation to model the dynamics of local viscosity and derive its drift and diffusion coefficients from simulation data. Additionally, we investigate the temperature-dependent variations of viscosity dynamics, unveiling their multiplicative and nonlinear nature. We elaborate on how the existence of multiplicative dynamics in viscosity results in the characteristic emergence of heterogeneity within viscosity dynamics. We derive a dynamic correlation length from local viscosity. Moreover, this correlation length shows a non-monotonic dependence on temperature with a maximum at about the Kauzmann temperature.



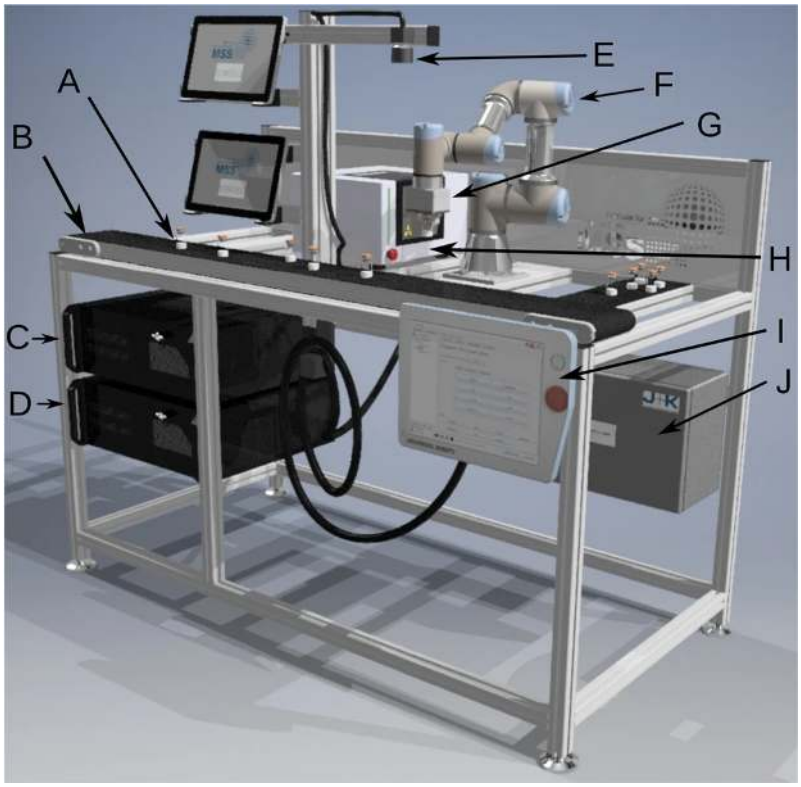
Ensemble-averaged drift and diffusion coefficients of viscosity variability measured by active microrheology. The estimated ensemble-averaged drift terms (a) and diffusion coefficients (b) at various temperatures for a probe velocity of U = 0.008. The pronounced (nonlinear) cubic behavior of the drift function is clearly observable at elevated temperatures.

14. A. Madanchi, F. Aghaei, S. H. E. Rahbari, M. R. R. Tabar, T. Pöschel, Non-monotonic dynamic correlation explored via active microrheology. *Journal of Statistical Mechanics: Theory and Experiment* **2024**, 103205, DOI 10.1088/1742-5468/ad8222 (2024).

Automated Tomographic Assessment of Structural Defects of Freeze-Dried Pharmaceuticals

Patric Müller, Achim Sack, Jens Dümler, Michael Heckel, Tim Wenzel, Teresa Siegert, Sonja Schuldt-Lieb, Henning Gieseler, Thorsten Pöschel

Abstract:
The topology and surface characteristics of lyophilisates significantly impact the stability and reconstitutability of freeze-dried pharmaceuticals. Consequently, visual quality control of the product is imperative. However, this procedure is not only time-consuming and labor-intensive but also expensive and prone to errors. In this paper, we present an approach for fully automated, non-destructive inspection of freeze-dried pharmaceuticals, leveraging robotics, computed tomography, and machine learning.



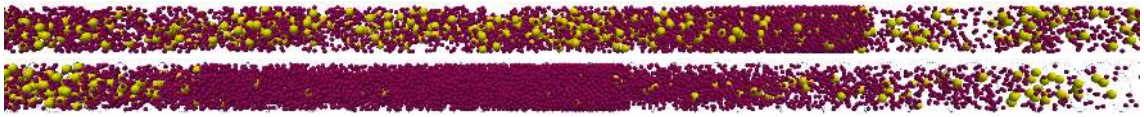
Apparatus for the automated tomographic assessment of structural defects of freeze-dried pharmaceuticals.

16. P. Müller, A. Sack, J. Dümler, M. Heckel, T. Wenzel, T. Siegert, S. Schuldt-Lieb, H. Gieseler, T. Pöschel, Automated Tomographic Assessment of Structural Defects of Freeze-Dried Pharmaceuticals. *AAPS PharmSciTech* **25**, 103205, DOI 10.1208/s12249-024-02833-7 (2024).

Particle size segregation in granular pipe flow

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

Abstract:
The flow of granular material through pipes is characterized by significant variations in solid fraction (density waves) along the pipe. Previously, it has been shown that this intermittent flow behavior can be mitigated by adding a texture to the pipe's inner wall. This work shows that adding surface roughness can lead to particle size segregation as a side effect in polydisperse systems. Using particle simulations, we characterize the parameter ranges in which segregation occurs.



Snapshots of the DEM simulation of a binary mixture through a pipe without (a) and with (b) helical texture. Small particles are drawn in red color and large particles in yellow.

17. P. Müller, A. Panchenko, W. T. Ku, T. Pöschel, Particle size segregation in granular pipe flow. *Chaos*, in press (2024).

Rigid clumps in the MercuryDPM particle dynamics code

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

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

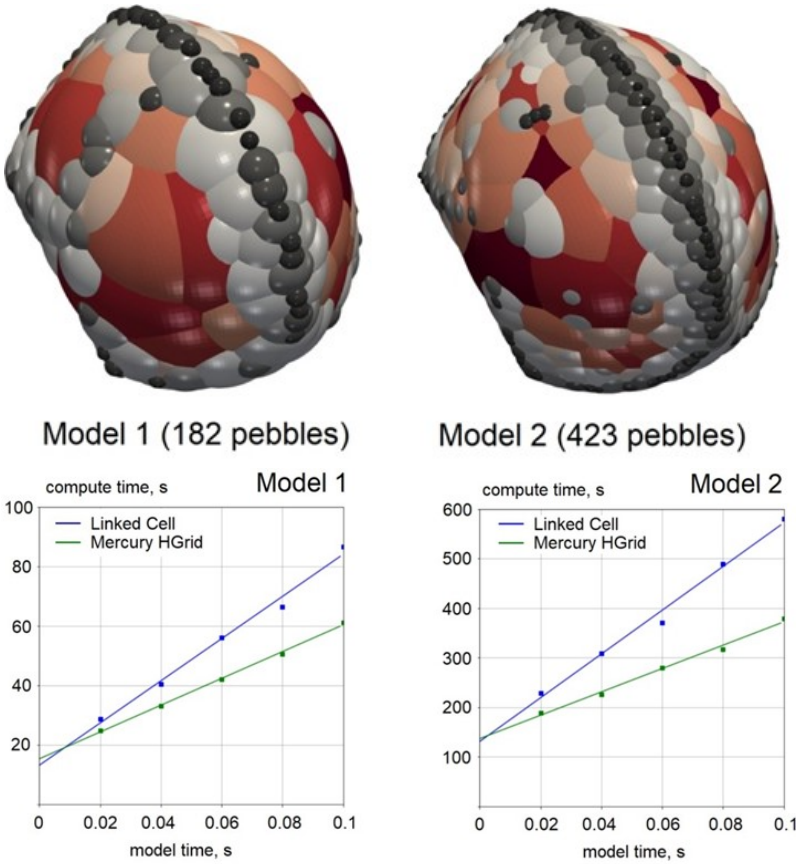


Illustration of the effect of multiple grid levels on computational performance. (A) Clumps used in model 1 and model 2, (B) Dependence of compute time and model time for two models and contact detection approach used.

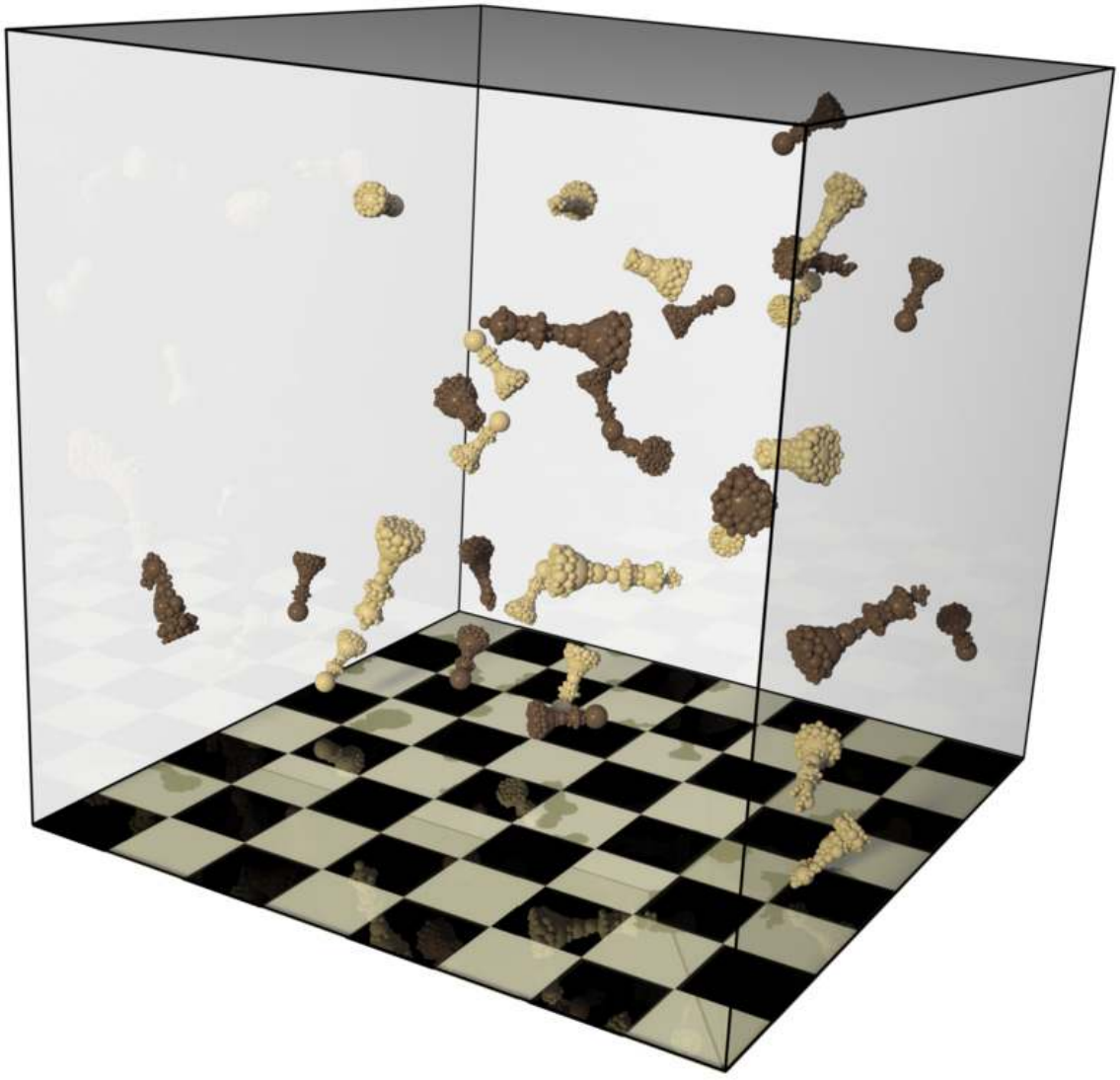
18. I. Ostanin, V. Angelidakis, T. Plath, S. Pourandi, A. Thornton, T. Weinhart, Rigid clumps in the MercuryDPM particle dynamics code. *Computer Physics Communications* **296**, 109034, DOI 10.1016/j.cpc.2023.109034 (2024).

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

Carlos Andrés 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.



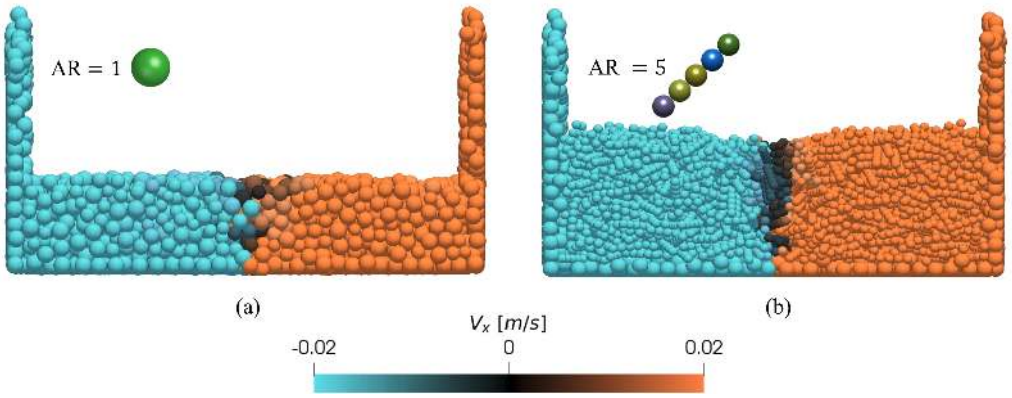
Snapshot of a simulation of non-spherical particles (chess pieces modeled as multi-spheres) bouncing in a box. The elastic Hertz contact force describes particle-particle and particle-wall collisions.

19. 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).

Alignment-induced depression and shear thinning of anisotropic granular media

Huzaif Rahim, Vasileios Angelidakis, Thorsten Pöschel, Sudeshna Roy

Abstract:
When granular materials of shape-anisotropic grains are sheared in a split-bottom shear cell, a localized shear band is formed with a depression at its center. This effect is closely related to the alignment of the particles with aspect ratio (AR), which, in turn, influences the local packing density, the stress distribution, and the system's overall bulk rheology. Particles with large AR tend to align with the shear direction, which increases the packing density in the shear band and affects rheological properties like stress, macroscopic friction coefficient, and effective viscosity. A scaling law correlates particle AR to macroscopic friction and effective viscosity, revealing shear-thinning behavior in bulk and near the surface.



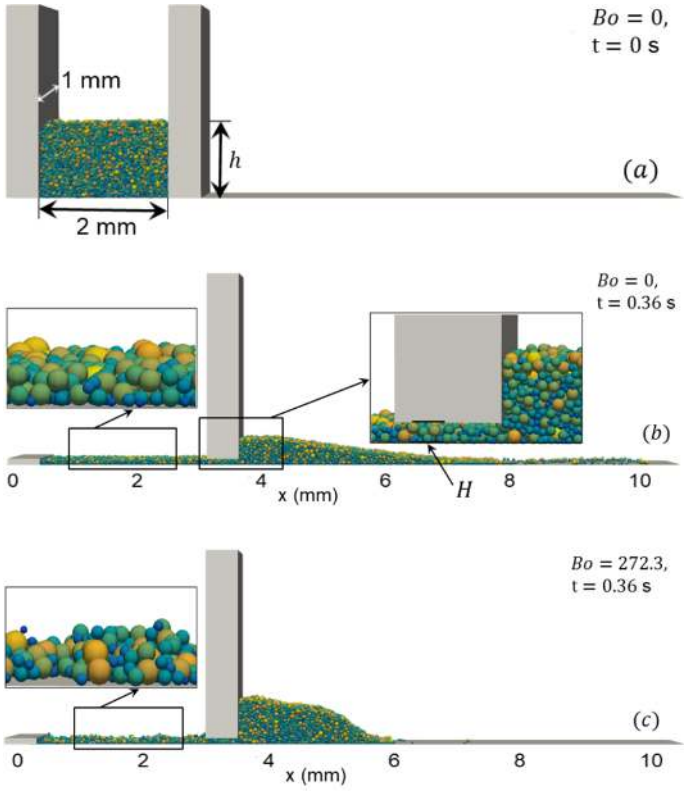
The shear cell filled with (a) spherical particles ($AR = 1$), showing a flat surface, and (b) elongated particles ($AR = 5$), showing a depression on the surface of the shear band.

20. H. Rahim, V. Angelidakis, T. Pöschel, S. Roy, Alignment-induced depression and shear thinning in granular matter of nonspherical particles. *Physical Review Fluids* **9**, DOI 10.1103/physrevfluids.9.114304 (2024).

Combined thermal and particle shape effects on powder spreading in additive manufacturing via discrete element simulations

Sudeshna Roy, Hongyi Xiao, Vasileios Angelidakis, Thorsten Pöschel

Abstract:
The thermal and mechanical behaviors of powders are crucial for additive manufacturing. In powder bed fusion, capturing temperature profiles and packing structures before melting is challenging due to diverse heat transfer pathways and powder properties. This study tackles this challenge with a discrete element model simulating non-spherical particles with thermal properties during powder spreading. Thermal conduction and radiation are integrated into a multisphere particle formulation to model heat transfer among irregular-shaped powders with temperature-dependent elastic properties. The model is utilized to simulate the spreading of pre-heated PA12 powder over a hot substrate representing the part under manufacturing. Variances in temperature profiles are observed in the spreading cases based on particle shapes, spreading speed, and temperature-dependent elastic modulus. Particle temperature beneath the spreading blade is influenced by the kinematics of the particle heap and temperature-dependent properties.



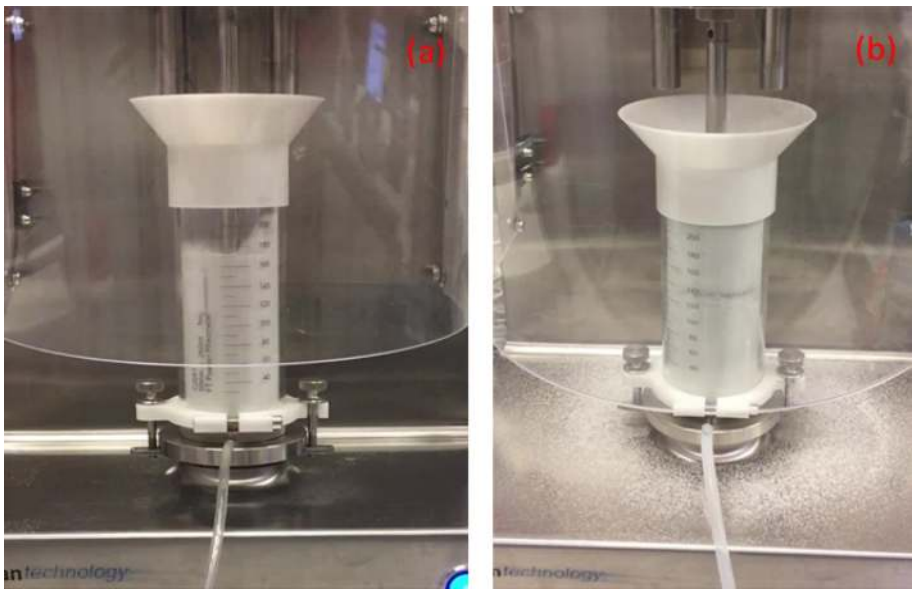
Powder spreading setup showing (a) side view during initial particle deposition, (b) side view during spreading, and (c) deposited powder layer structure after 0.07 s of the powder spreading process with a blade velocity v = 50 mm/s.

21. S. Roy, H. Xiao, V. Angelidakis, T. Pöschel, Combined thermal and particle shape effects on powder spreading in additive manufacturing via discrete element simulations. *Powder Technology* **445**, 120099, DOI 10.1016/j.powtec.2024.120099 (2024).

Fluidization of wet cohesive powder in virtual Couette rheometer

Sudeshna Roy

Abstract:
We use a virtual Couette rheometer to study the behaviour of dry and wet granular materials in aerated beds. A typical fluidization curve for dry powders exhibits a fixed bed characterized by a linear increase in pressure drop with increasing air velocity. This is followed by a fluidized bed at a constant pressure drop with further increases in air velocity. However, wet powders display different aeration behavior due to the inhomogeneous gas flow through the bed. The fluidization behaviour of the powder upon addition of small amounts of silicon oil liquid has been tested for two different grain sizes. We distinguish different regimes of fluidization for wet powders with different saturation of silicon oil and different grain sizes. Further, we compare the hysteresis effects in fluidization and de-fluidization cycles of the materials. We also compare the shear stresses and study the rheology of the materials under different fluidized conditions.



Snapshots of experiments for particle size $d_p \approx 150-212\,\mu$m tests in VCR showing (a) fluidization of weakly cohesive powder ($S^* = 0.005\%$) and (b) cohesive powder ($S^* = 0.019\%$) that is not fluidized.

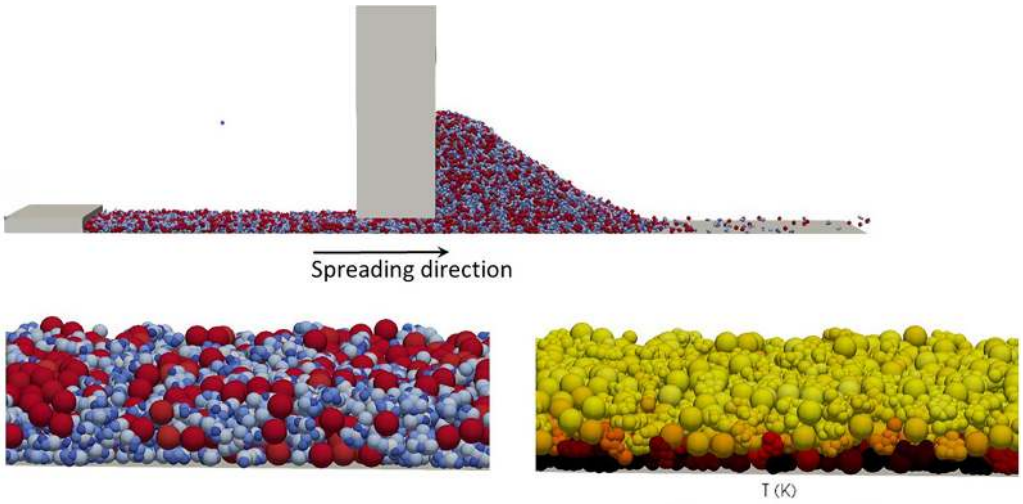
22. S. Roy, Fluidization of wet cohesive powder in virtual Couette rheometer. *Particuology*, submitted (2024).

Shape effects in binary mixtures of PA12 powder in additive manufacturing

Sudeshna Roy, Thorsten Pöschel

Abstract:

The quality of powder spread in additive manufacturing devices depends sensitively on particle shapes. Here, we study powder spreading for mixtures of spherical and irregularly shaped particles in Polyamide 12 powders. Using DEM simulations, including heat transfer, we find that spherical particles exhibit better flowability. Thus, the particles are deposited far ahead of the spreading blade. In contrast, a large fraction of non-spherical particles hinders the flow. Therefore, the cold particles are deposited near the front of the spreading blade. This results in a temperature drop of the deposited particles near the substrate, which cannot be seen with spherical particles. The particles of both shapes are homogeneously distributed in the deposited powder layer.



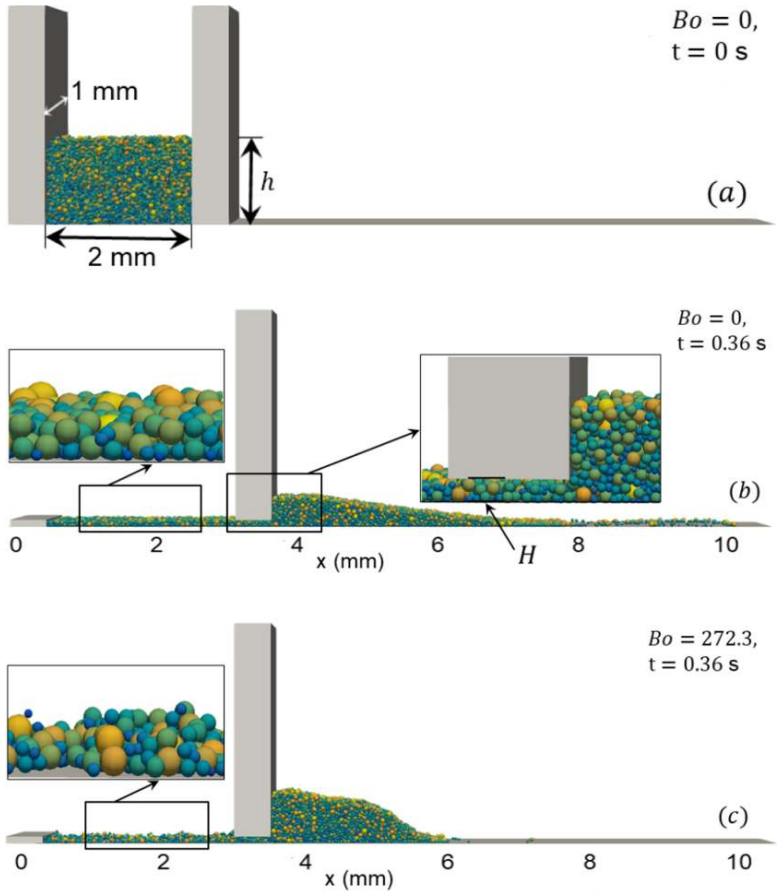
Numerical setup: (a) A powder mixture of volume fraction $\alpha = 0.6$ of spherical particles is spread. (b) deposited powder layer. Non-spherical particles are shown in blue, spherical particles are shown in red. (c) same as (b) but the color codes the temperature after t = 0.05 s of the powder spreading process.

23. S. Roy, T. Pöschel, Shape effects in binary mixtures of PA12 powder in additive manufacturing. *Powder Technology* **448**, 120326, DOI 10.1016/j.powtec.2024.120326 (2024).

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

Sudeshna Roy, Hongyi Xiao, Vasileios Angelidakis, Thorsten Pöschel

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



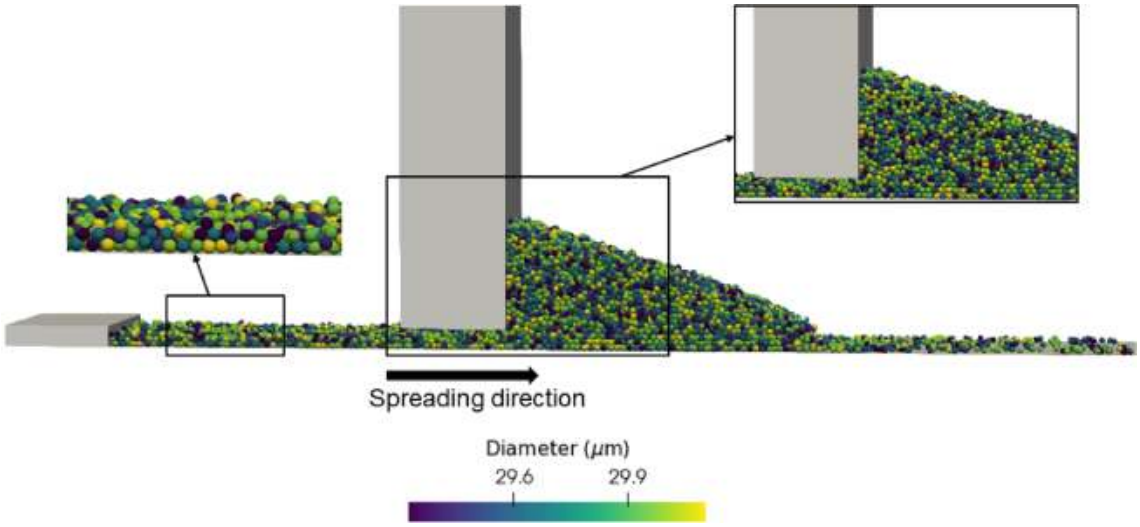
Numerical setup for powder spreading on a planar substrate showing (a) initial configuration and during spreading for (b) cohesionless powders after 0.36 s, and (c) cohesive powders after 0.36 s.

24. S. Roy, H. Xiao, V. Angelidakis, T. Pöschel, Structural fluctuations in thin cohesive particle layers in powder-based additive manufacturing. *Granular Matter* **26**, 43, DOI 10.1007/s10035-024-01410-w (2024).

The role of granular matter in additive manufacturing

Sudeshna Roy, Thomas Weinhart

Abstract:
Additive manufacturing, particularly in granular systems, has revolutionized industries such as aerospace, medical engineering, and automotive manufacturing by enabling complex, customized designs. A critical aspect of additive manufacturing is powder handling, which involves challenges related to deposition, packing density, and safety. Numerical simulations, including the discrete element method and smoothed particle hydrodynamics, play an essential in optimizing these processes. Inspired by the DEM9 conference, where several authors were invited to contribute, this editorial highlights ongoing granular research on additive manufacturing. Previously not extensively covered in Granular Matter, this topical collection showcases novel work to establish additive manufacturing more prominently within the journal. Through contributions on powder spreading, material structure, and innovative computational models, this issue enhances the understanding of additive manufacturing processes and their industrial applications.



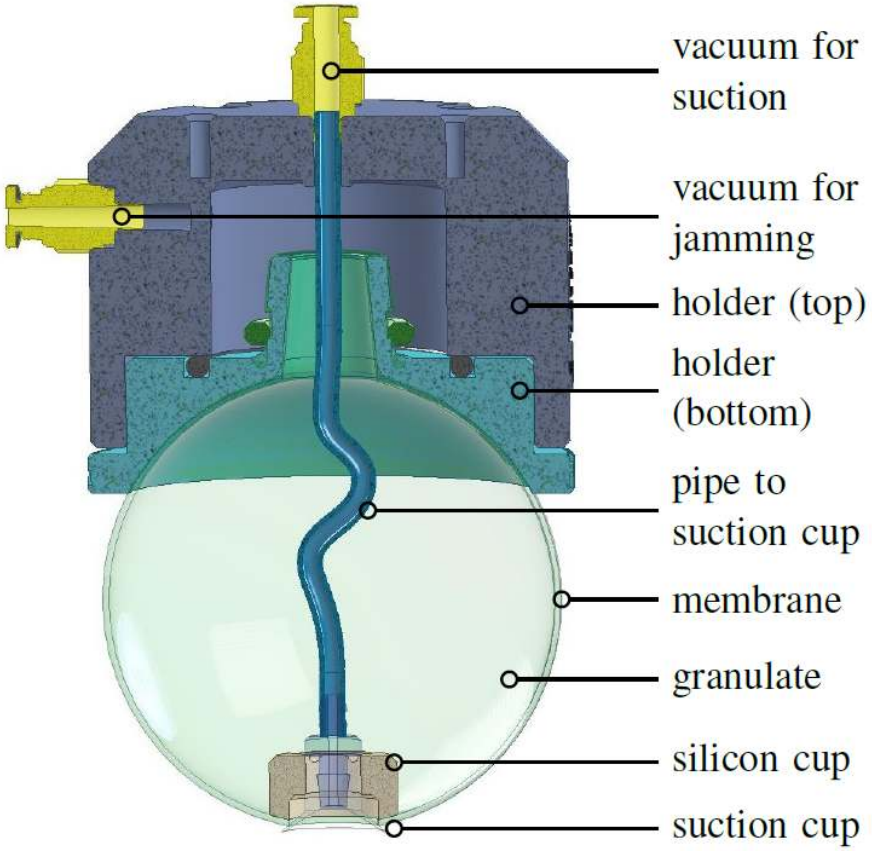
Simulation of powder spreading in an additive manufacturing process. The main image shows the distribution of particles, colored according to their diameter, as they are spread by a blade. The left inset provides a close-up view of the packed powder layer immediately behind the blade, highlighting the uniformity of particle arrangement. The right inset zooms in on the powder pile forming in front of the blade, showing the variation in particle distribution. The color bar represents the particle diameters in micrometers (μm). The arrow indicates the spreading direction.

25. S. Roy, T. Weinhart, The of granular matter in additive manufacturing. *Granular Matter* **26**, DOI 10.1007/s10035-024-01473-9 (2024).

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 on 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.



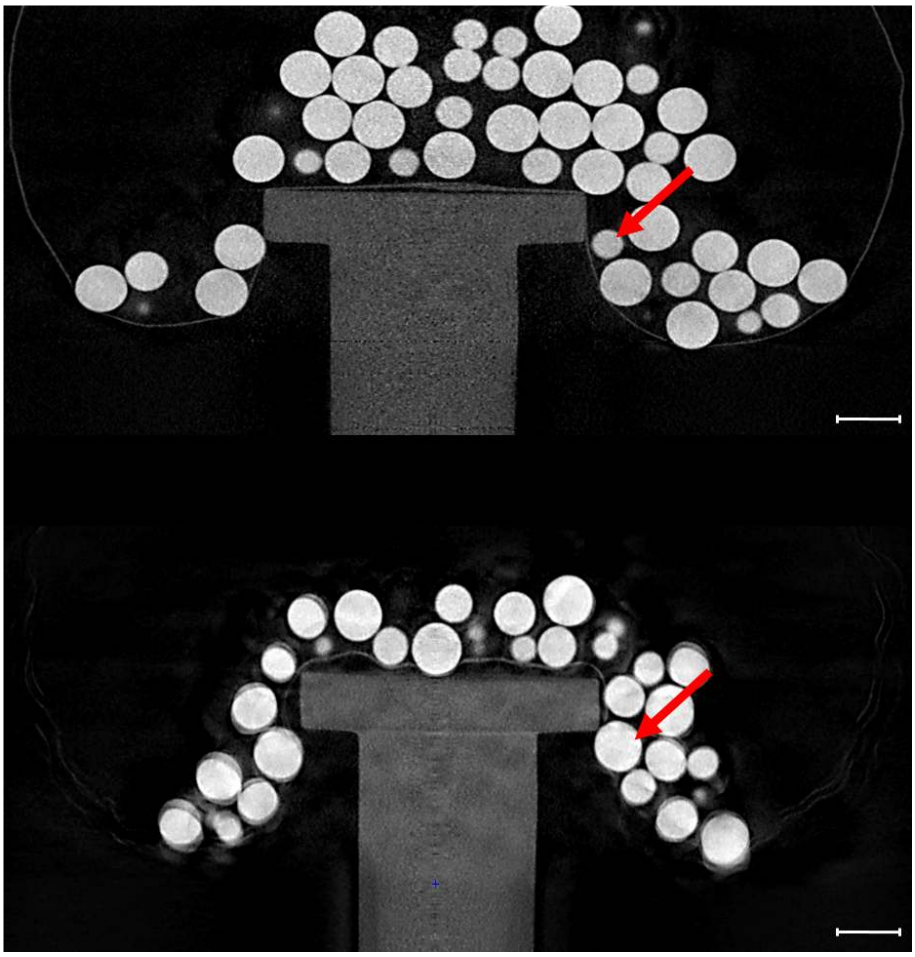
Maximum holding force (a-c) and maximum differential pressure, Δp (d-e) for the studied cases. Colors indicate the employed gripping mechanisms: (I) ordinary granular gripper (jamming only), (II) our gripper where only suction is active (no jamming), and (III) our gripper with both mechanisms, suction and jamming, activated. All data are shown for smooth and rough surfaces. Error bars indicate the standard deviation due to six independent measurements; the heights of the columns show the mean.

26. A. Santarossa, O. D'Angelo, A. Sack, T. Pöschel, All-terrain granular gripper. *Authorea*, submitted, DOI 10.22541/au.173437408.86018701/v1 (Dec. 2024).

Enhanced interlocking in granular jamming grippers through hard and soft particle mixtures

Angel Santarossa, Thorsten Pöschel

Abstract:
We investigate the influence of particle stiffness on the grasping performance of granular grippers, a class of soft robotic effectors that utilize granular jamming for object manipulation. Through experimental analyses and X-ray imaging, we show that grippers with soft particles exhibit improved wrapping of the object after jamming, in contrast to grippers with rigid particles. This results in significantly increased holding force through interlocking. The addition of a small proportion of rigid particles into a predominantly soft particle mixture maintains the improved wrapping but also significantly increases the maximum holding force. These results suggest a tunable approach to optimizing the design of granular grippers for improved performance in soft robotics applications.



X-ray tomograms before evacuation (a) and after (b). The gripper contains a mixture of glass beads 10% and EPS beads. The EPS particles are not visible due to their low X-ray absorbance. The white contour shows the gripper membrane. The red arrows highlight a particle that contributes to interlocking once jamming is induced.

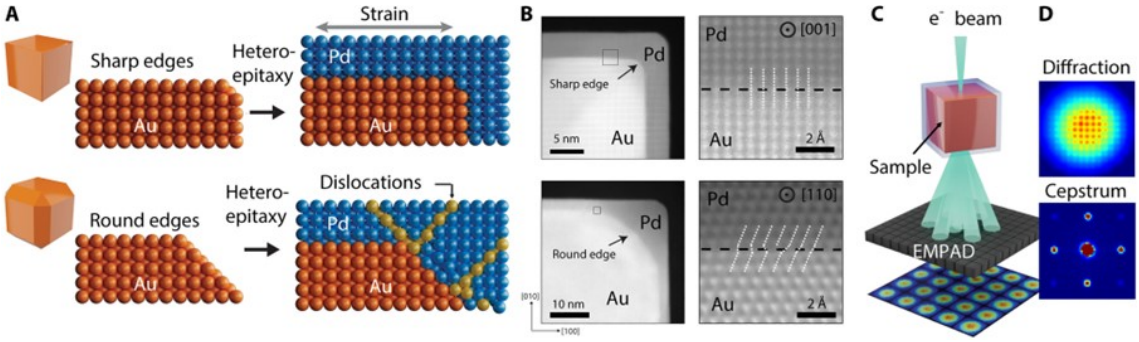
27. A. Santarossa, T. Pöschel, Enhanced interlocking in granular jamming grippers through hard and soft particle mixtures. *Granular Matter* **26**, DOI 10.1007/s10035-024-01475-7 (2024).

Preserving surface strain in nanocatalysts via morphology control

Chuqiao Shi, Zhihua Cheng, Alberto Leonardi, Yao Yang, Michael Engel, Matthew R. Jones, Yimo Han

Abstract:

Engineering strain critically affects the properties of materials and has extensive applications in semiconductors and quantum systems. However, the deployment of strain-engineered nanocatalysts faces challenges, in particular in maintaining highly strained nanocrystals under reaction conditions. Here, we introduce a morphology-dependent effect that stabilizes surface strain even under harsh reaction conditions. Using four-dimensional scanning transmission electron microscopy (4D-STEM), we found that cube-shaped core-shell Au@Pd nanoparticles with sharp-edged morphologies sustain coherent heteroepitaxial interfaces with larger critical thicknesses than morphologies with rounded edges. This configuration inhibits dislocation nucleation due to reduced shear stress at corners, as indicated by molecular dynamics simulations. A Suzuki-type cross-coupling reaction shows that our approach achieves a fourfold increase in activity over conventional nanocatalysts, owing to the enhanced stability of surface strain. These findings contribute to advancing the development of advanced nanocatalysts and indicate broader applications for strain engineering in various fields.



(A) Schematic illustration of strain preservation by a nanoscale morphology with sharp edges. (B) Atomic-resolution ADF-STEM images of the sharp-core (top left) and round-core (bottom left) Au cube@Pd cube NPs. Zoomed-in images from boxed area show a coherent interface (top right) and lattice mismatch (bottom right) between Au and Pd in sharp-core and round-core particles respectively, with the zone axes labeled. (C and D) Schematic showing 4D-STEM with a diffraction pattern (D, top) and an EWPC (D, bottom) from the core-shell NP for precise strain analysis.

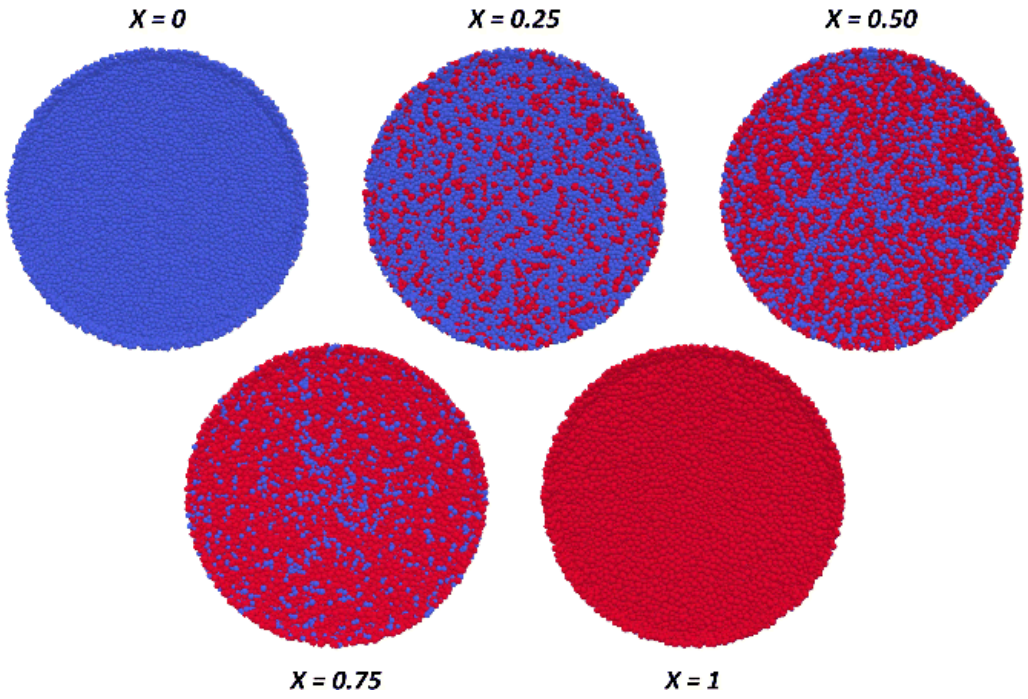
28. C. Shi, Z. Cheng, A. Leonardi, Y. Yang, M. Engel, M. R. Jones, Y. Han, Preserving surface strain in nanocatalysts via morphology control. *Science Advances* **10**, eadp3788, DOI `10.1126/sciadv.adp3788` (2024).

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

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

Abstract:

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



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

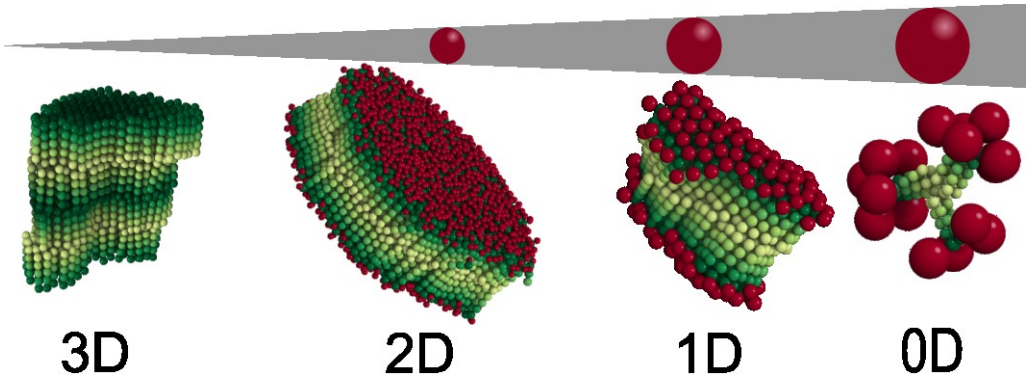
29. A. P. Singh, V. Angelidakis, T. Pöschel, S. Roy, Shear zones in granular mixtures of hard and soft particles with high and low friction. *Soft Matter* **20**, 3118–3130, DOI 10.1039/d4sm00100a (2024).

Geometric Frustration Directs the Self-assembly of Nanoparticles with Crystallized Ligand Bundles

Federico Tomazic, Aswathy Muttathukattil, Afshin Nabiyan, Felix Schacher, Michael Engel

Abstract:

Polymer-grafted nanoparticles are versatile building blocks that self-assemble into a diverse range of mesostructures. Coarse-grained molecular simulations have commonly accompanied experiments by resolving structure formation pathways and predicting phase behavior. Past simulations represented nanoparticles as spheres and the ligands as flexible chains of beads, isotropically tethered to the nanoparticles. Here, we investigate a different minimal coarse-grained model. The model consists of an attractive rod tethered to a repulsive sphere. The motivation of this rod–sphere model is to describe nanospheres with a partially crystallized, stretched polymeric bundle as well as other complex building blocks such as rigid surfactants and end-tethered nanorods. Varying the ratio of sphere size to rod radius stabilizes self-limited clusters and other mesostructures with reduced dimensionality. The complex phase behavior we observe is a consequence of geometric frustration.



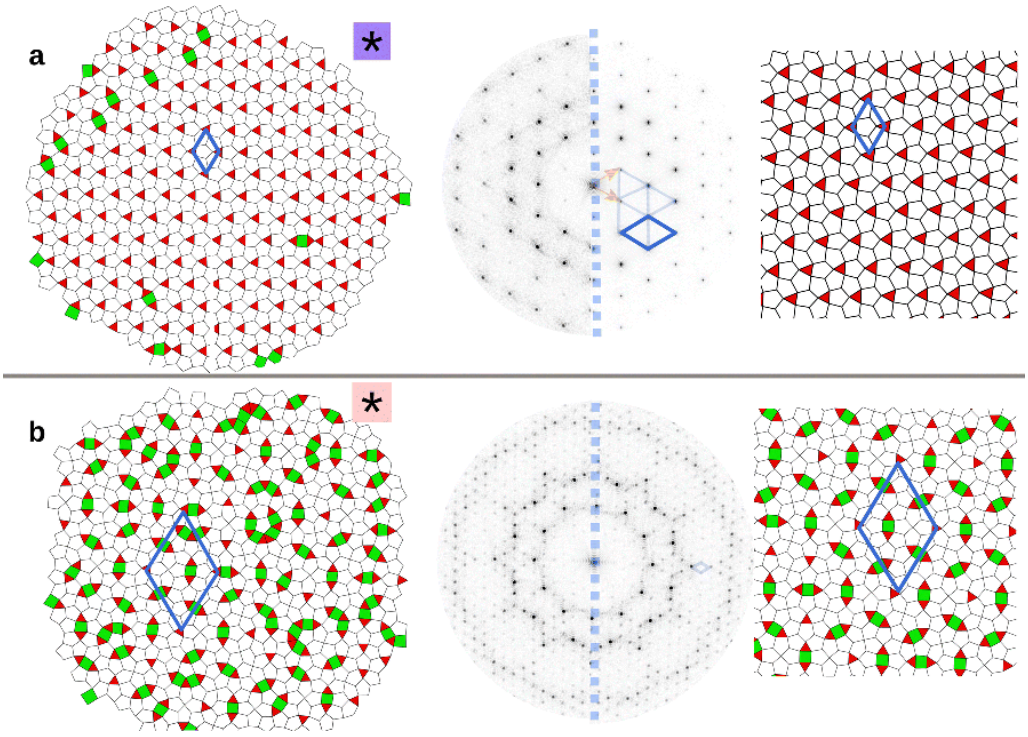
30. F. Tomazic, A. Muttathukattil, A. Nabiyan, F. Schacher, M. Engel, Geometric Frustration Directs the Self-assembly of Nanoparticles with Crystallized Ligand Bundles. *The Journal of Physical Chemistry B* **128**, 11258–11266, DOI 10.1021/acs.jpcb.4c04562 (2024).

Tuning the stability of a model quasicrystal and its approximants with a periodic substrate

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.



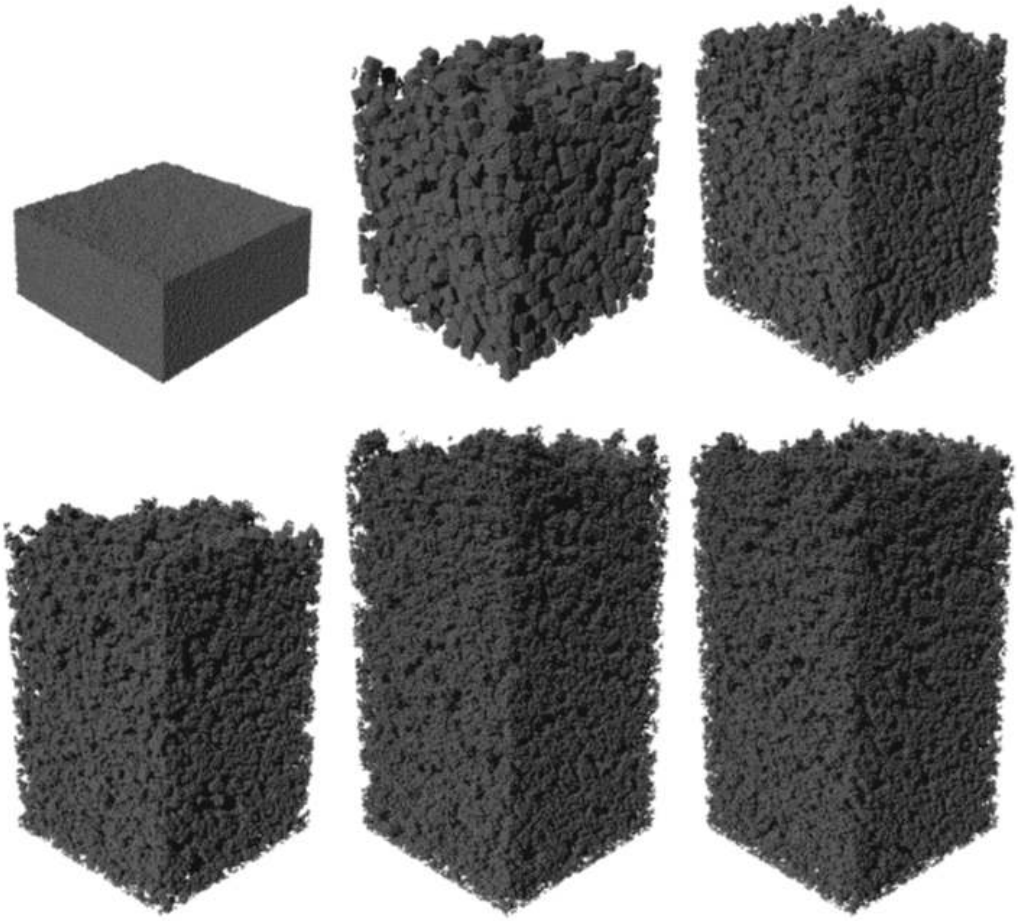
Snapshots from MD simulations at two substrate potential depths. Snapshots are shown in direct space obtained from simulation (left column) and from representative ideal tilings (right column). Diffraction patterns (middle column) are calculated and compared for both snapshots.

31. N. R. Varela-Rosales, M. Engel, Tuning the stability of a model quasicrystal and its approximants with a periodic substrate. *Soft Matter* **20**, 2915–2925, DOI 10.1039/d4sm00191e (2024).

Fractal packing of nanomaterials

Dietrich E. Wolf, Thorsten Pöschel

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



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

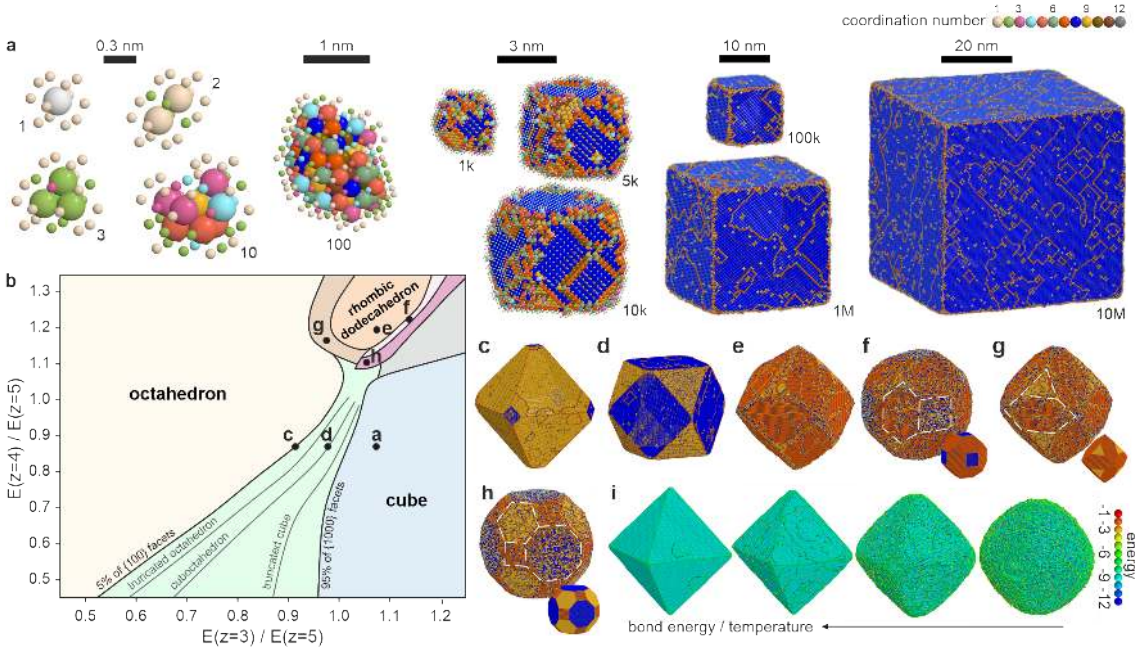
32. D. E. Wolf, T. Pöschel, Fractal packing of nanomaterials. *arXiv*, DOI 10.48550/ARXIV.2312.03117 (2023).

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, mechanical strength, 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.

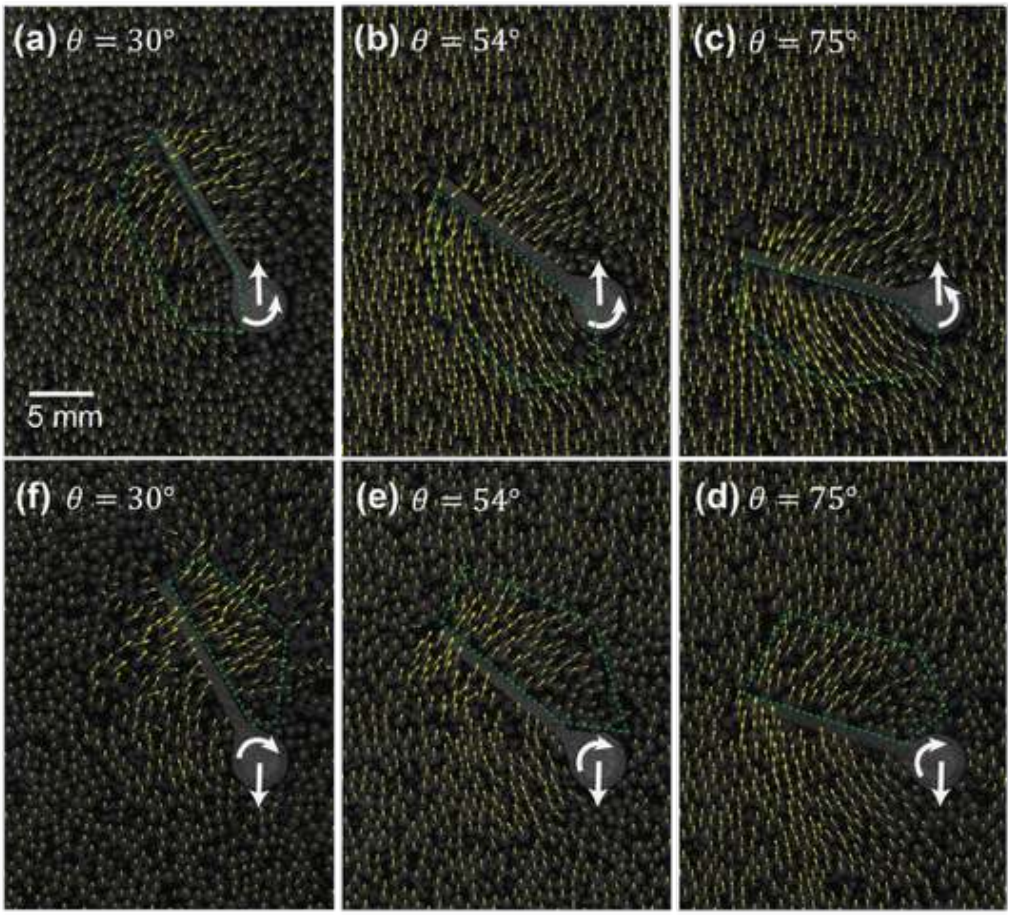


33. C. L. Bassani, M. Engel, Kinetically Trapped Nanocrystals with Symmetry-Preserving Shapes. *arXiv*, DOI 10.48550/ARXIV.2410.09787 (2024).

Understanding the Propulsion of a Scallop-like Swimmer in Granular Media

Amir Nazemi, Achim Sack, Harol Torres, Thorsten Pöschel, Hongyi Xiao

Abstract:
Locomotion in granular media is often complicated due to the soft and yielding nature of granular materials. Simple and reciprocal swimming motions, which typically result in no locomotion in Newtonian liquids, can potentially generate propulsion in granular media. This study aims to examine the mechanisms underlying the locomotion of a swimmer with two flapping wings in granular materials. In both lab experiments and discrete element method (DEM) simulations, we found that the swimmer could generate persistent locomotion by opening and closing its wings reciprocally. For a shallow swimmer, we found that wing rotation led to the formation of heaps and valleys on the free surface, which resulted in hysteresis in the resistive force within a stroke cycle. This, combined with the geometric factors of the scallop, resulted in the generation of propulsion. For a deep swimmer away from the free surface, reversed locomotion direction was observed in DEM simulations, which could possibly be due to a second mechanism involving the jamming of particles near the rotating wings.



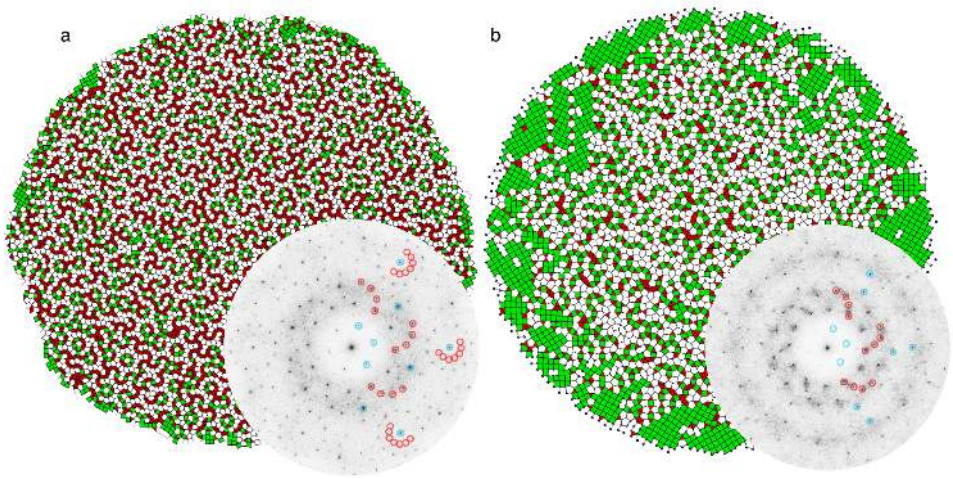
34. A. Nazemi, A. Sack, H. Torres, T. Pöschel, H. Xiao, Understanding the propulsion of a scallop-like swimmer in granular media. *Bulletin of the American Physical Society* (2024).

Computational Self-Assembly of a Six-Fold Chiral Quasicrystal

Nydia Roxana Varela-Rosales, Michael Engel

Abstract:

Quasicrystals are unique materials characterized by long-range order without periodicity. They are observed in systems such as metallic alloys, soft matter, and particle simulations. Unlike periodic crystals, which are invariant under real-space symmetry operations, quasicrystals possess symmetry that requires description by a space group in reciprocal space. In this study, we report the self-assembly of a six-fold chiral quasicrystal using molecular dynamics simulations of a two-dimensional particle system. The particles interact via the Lennard-Jones-Gauss pair potential and are subjected to a periodic substrate potential. We confirm the presence of chiral symmetry through diffraction patterns and order parameters, revealing unique local motifs in both real and reciprocal space. The quasicrystal's properties, including the tiling structure and symmetry and the extent of diffuse scattering, are strongly influenced by substrate potential depth and temperature. Our results provide insights into the mechanisms of chiral quasicrystal formation and the and potential of external fields in tailoring quasicrystal structures.



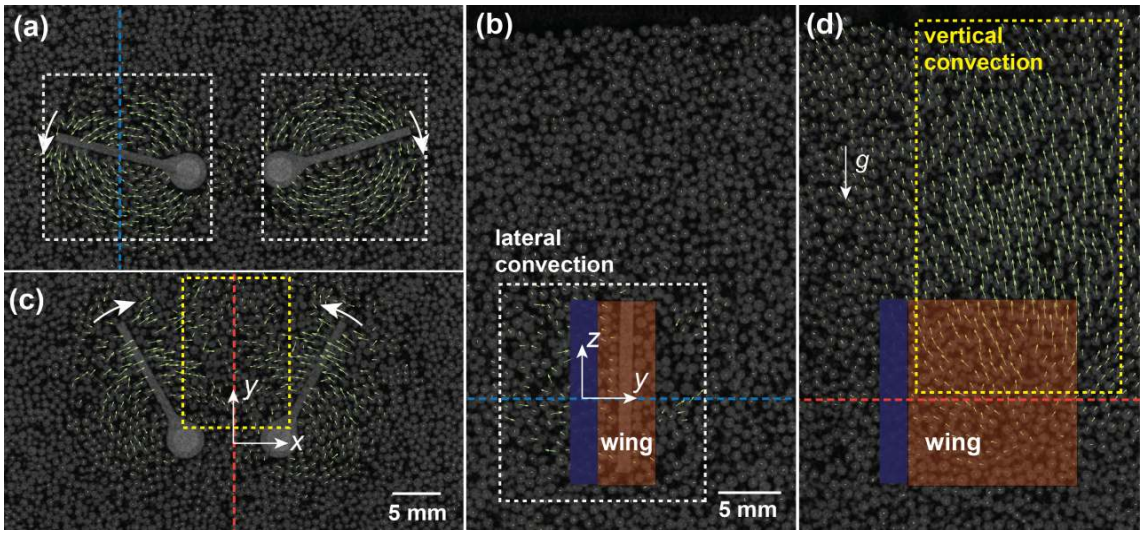
MD simulation snapshots of the CQC at the parameter sets (a) $(T,\varepsilon) = (0.25, 0.5)$ and (b) $(T,\varepsilon) = (0.3, 0.4)$. In these snapshots, nearest-neighbor bonds create a tiling pattern, where triangle tiles are colored red and square tiles are colored green. The insets show diffraction patterns, time-averaged to reduce phonon noise and with chiral symmetry and six-fold symmetry features highlighted using small red and blue circles, respectively. In snapshot (b), the solid-gas interface is wetted by square tiles and diffuse scattering is more pronounced compared to (a).

35. N. R. Varela-Rosales, M. Engel, Computational Self-Assembly of a Six-Fold Chiral Quasicrystal. *arXiv*, DOI `10.48550/ARXIV.2408.01984` (2024).

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.



Cut through X-ray tomograms of the miniature free swimmer in the xy and yz planes with $\theta_c = 20^o$ and $\theta_0 = 80^o$. (a,b) show tomograms for $\theta = 75^o$ during opening, corresponding to $t/T = 0.46$. (c,d) show tomograms for $\theta = 25^o$ during closing, corresponding to $t/T = 0.96$. (b) shows the yz plane at the midpoint of the left wing, indicated by the blue dashed line in (a). (d) shows the *yz* plane at the center of the swimmer, indicated by the red dashed line in (c). The orange and violet regions indicate the projections of the wing and the anchoring rod on the *yz* plane. The white and yellow boxes highlight regions with strong horizontal and vertical convection, respectively. The yellow arrows indicate the displacements (magnified by 2) of the particles between consecutive frames, recorded with delay $T/30$.

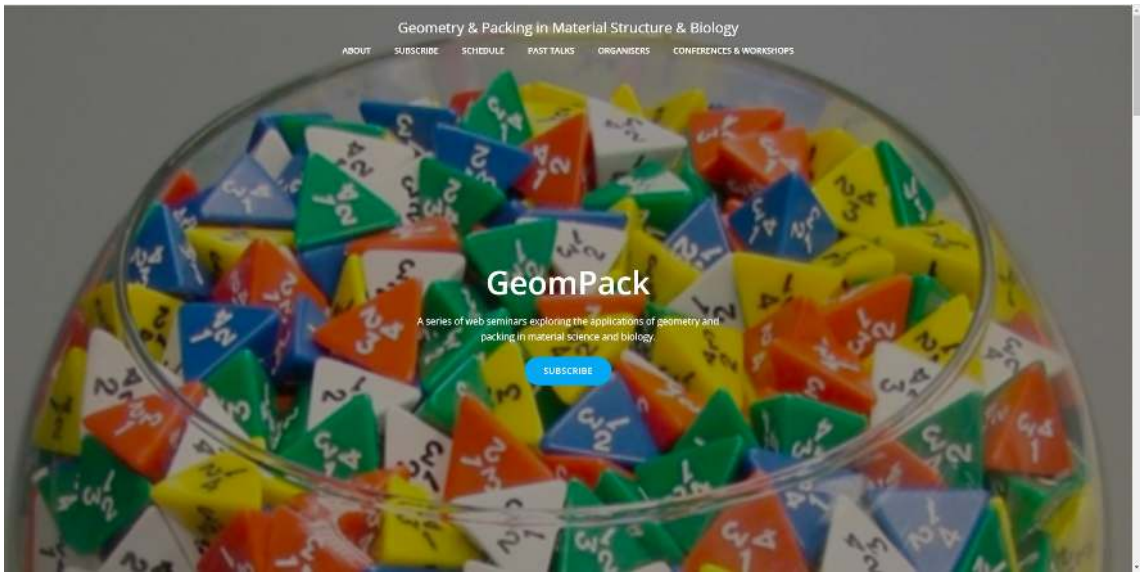
36. H. Xiao, H. Torres, A. Sack, T. Pöschel, Locomotion of a Scallop-Inspired Swimmer in Granular Matter. *arXiv*, DOI 10.48550/ARXIV.2412.05266 (2024).

12. Service for the Scientific Community

GeomPack
Webinar series
Co-organized by Michael Engel

Michael Engel co-organized GeomPack together with Adil Mughal, Greg Grason Miranda Holmes-Cerfon, Reidun Twarock, Joseph D. Paulsen and Daniela Kraft: 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 2024, two webinars took place:

- **6th November 2024**: *"Geometric origin of particle and dislocation dynamics during grain boundary migration"* by Roel P.A. Dullens.
- **20th November 2024**: *"Kinetically Trapped Nanocrystals with Symmetry-Preserving Shapes"* by Carlos L. Bassani.



Space Applications and Low-gravity Research
Mini-session
Co-organized by Olfa D'Angelo

Olfa D'Angelo is co-organizing, with Thomas Voigtmann and Norman Wagner, a mini-session on Space Applications and Low-gravity Research at the Society of Rheology in Austin (TX), Oct. 13-17, 2024. This mini-session offers a platform for rheology and space-related science to meet. Low-gravity research can be used to develop novel rheology experiments, including ones that could not be performed on the ground. Rheology will also be an essential part of future space exploration missions, from granular flows on extraterrestrial planets, to astronauts' physiology, fuel viscosity under different gravity, and 3D printing housing on the Moon. Joining this mini-session will expand your perspective to highlight the rheologists will play in space science and exploration. Besides the exciting lineup of invited speakers who will present during this mini-session and a lunch with a NASA astronaut during which ISS opportunities will be discussed, we offer to highlight posters and presentations related to space applications and low-gravity research within all abstracts submitted to the SoR meeting. Highlight your abstract as part of this topic during submission.

Particles 2025
Invited Session
Co-organized by 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`

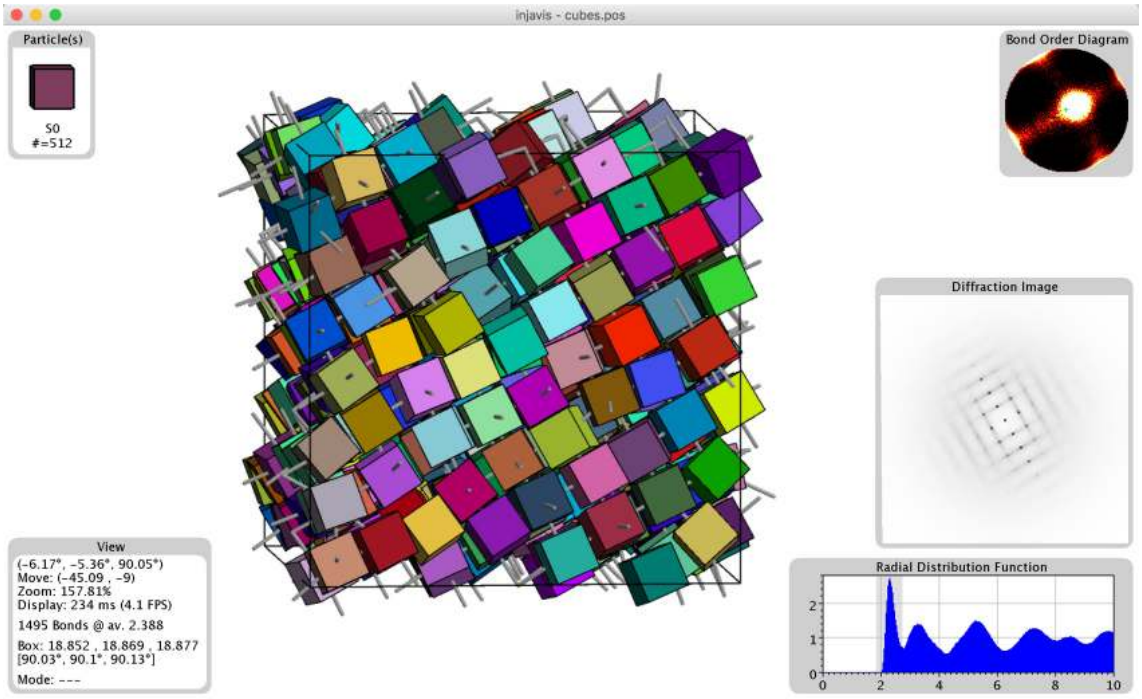
The software package Injavis (acronym for INteractive JAva VISualization) displays, analyzes, and manipulates particle simulation data. An emphasis lies on geometry and structural analysis as well as interactivity. The main input and output file format is .pos, which is a format developed specifically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



Olfa D'Angelo Co-organized a session on Modeling & Simulation

Olfa D'Angelo together with Mikio Sakai, Eric J. R. Parteli and Harald Kruggel-Emden organized a session on "Modeling & Simulation" at the International Powder and Nanotechnology Forum (IPNF) 2024. It took place in Frankfurt, Germany, on June 11 and June 12, 2024 and featured the following keynote lectures:

- *"From droplets to capsules: rheology, capillary interactions, and wetting"*
  Prof. Jens Harting (Helmholtz Institute Erlangen-Nürnberg for Renewable Energy)
- *"Modelling particle processes in the chemical and pharmaceutical industries."*
  Christoph Kloss, Christoph Goniva (German, Simulation)
- *"GRAF: Simulating Diverse Industrial Processes Through a Comprehensive DEM-CFD Based Approach"*
  Mr. Vidura Yashodha Gamage (Kozo Keikaku Engineering Inc.)
- *"DEM/CFD simulation of chemically reacting, thermally thick particles in moving granular assemblies with gas flow: challenges and recent developments."*
  Prof. Viktor Scherer (Ruhr-Universität Bochum)
- *"Advancing Discrete Element Method Simulation: A Comprehensive Verification and Validation Study"*
  Prof. Mikio Sakai (The University of Tokyo)

Olfa D'Angelo – ESA consultant

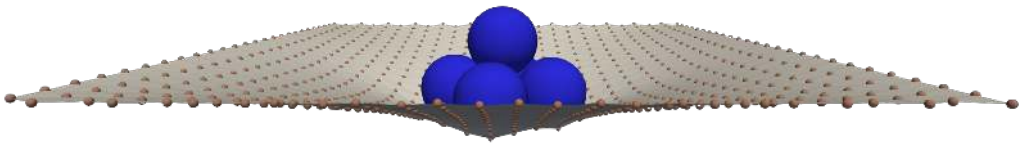
Olfa D'Angelo was selected as a consultant for the European Space Agency Facility Definition Team on defining the post-ISS facility for soft matter science in space. She is in charge of the granular matter sub-group. Thogether they are publishing a document named "Strategic Directions for Space Research in Soft Matter and Biophysics".

Carlos L. Bassani
Workshop on chemical-physics fundamentals of nanomaterials

In October 2024, the iRTG-ParSciTech of CRC 1411 hosted its inaugural Summer School (Summer course of the Collaborative Research Center 1411 on Design of Particulate Products) at the Fraunhofer Forschungscampus in Waischenfeld. Held from October 14 to 17, the event brought the CRC doctoral researchers together for the purpose of exploring the fundamentals of designing particulate products. With over 27 participants, the Summer School featured lectures and workshops led by specialists in various fields. Topics included "Chemical-Physics Fundamentals of Nanomaterials", a seven-hour workshop led by Dr. Carlos L. Bassani (Project D04).

Holger Götz – Developer for MercuryDPM

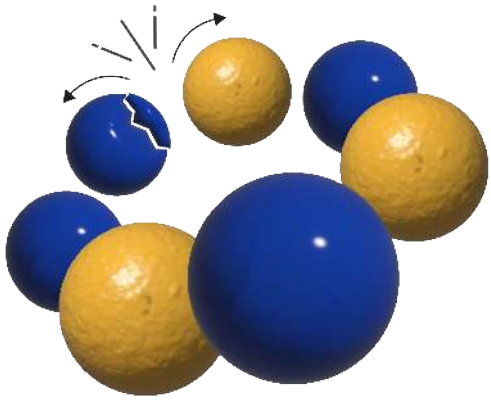
Holger Götz is part of the MercuryDPM team since 2021. He added the mass spring system to the kernel, which has been available in version 1.0 since May 2022.
`https://www.mercurydpm.org/about/team#h.4xjfxeowlicv`



MERCURYDPM

Holger Götz co-organized a training session for MercuryDPM

At the inaugural Conference of the COST Action 'Open Network on Discrete Element Method Simulations' (ON-DEM), Holger Götz co-organized a training session on the open-source DEM software MercuryDPM alongside Dr. Deepak Tunuguntla and Prof. Anthony Thornton. The ON-DEM COST Action aims to promote the use of open-source DEM codes and to drive scientific advances that enable the simulation of more realistic and complex problems. This training session supported these goals by providing hands-on experience with MercuryDPM to the next generation of DEM users, developers, and practitioners. The event took place on May 14 in Espoo, Finland.



ON-DEM

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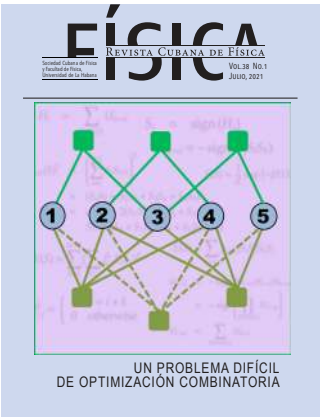
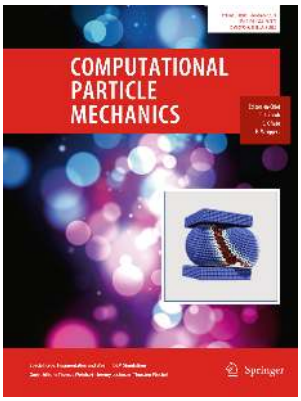


Prof. Thorsten Pöschel
Senior Editor since 2014

Computational Particle Mechanics
Springer/Nature

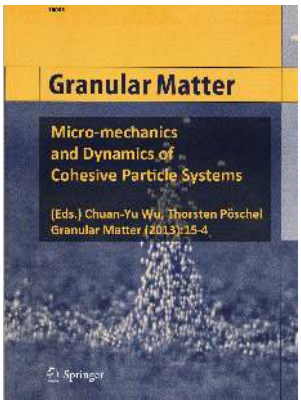
`www.springer.com/journal/40571/`



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

Granular Matter
Springer/Nature

`www.springer.com/journal/10035`



Prof. Thorsten Pöschel
Editor since 2006

13. PhD Graduations

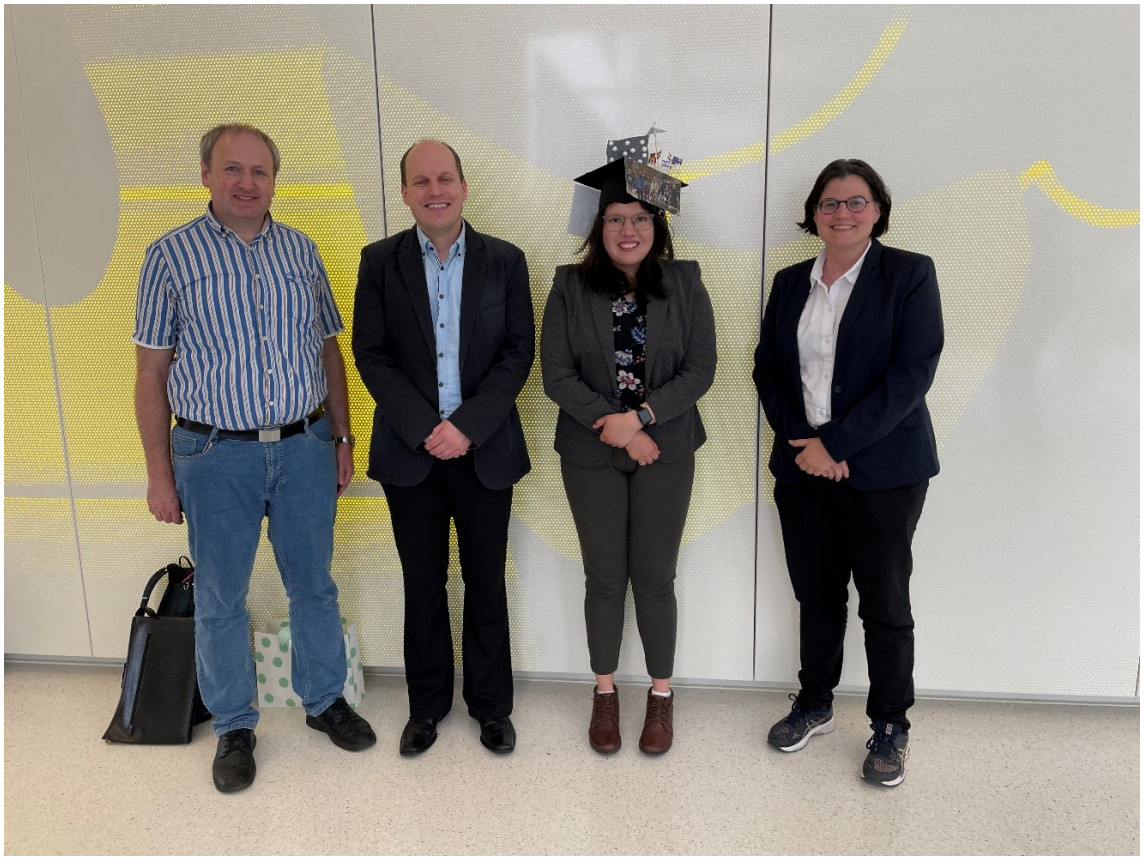
Holger Götz,
Jamming und Konvektion in Granulaten

Faculty: Chemical Engineering / Dr. -Ing.
Date: May 22, 2024
Chairman of the examination committee: Prof. Dr. Michael Wensing
Members of the examination committee: Prof. Dr. Thorsten Pöschel, Prof. Dr. Stefan Heinrich, PD Dr. Sebastian Pfaller

Holger at his PhD defense

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

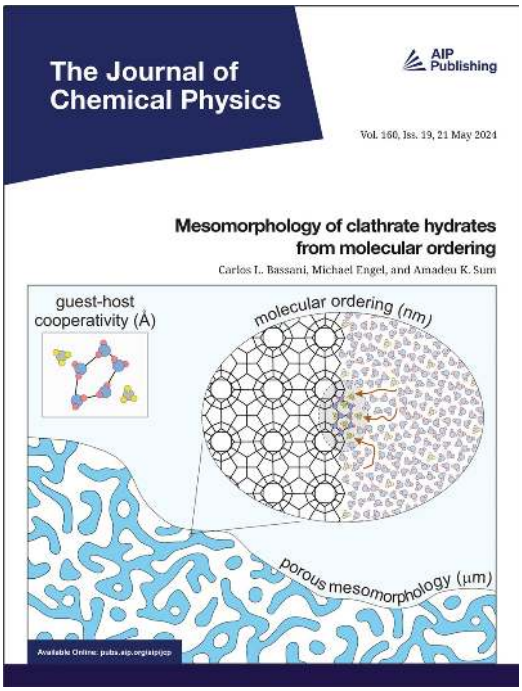
Faculty: Department of Physics / Dr. rer. nat.
Date: June 18, 2024
Chairman of the examination committee: Prof. Dr. Sabine Maier
Members of the examination committee: Prof. Dr. Michael Schmiedeberg, Prof. Dr. Sabine Maier, Prof. Dr. Michael Engel



Nydia at her PhD defense

14. Awards

Cover image of the Journal of Chemical Physics
The Journal of Chemical Physics chose our submission to be featured as the cover image. This particular image is associated with the paper titled "Mesomorphology of clathrate hydrates from molecular ordering," authored by Carlos L. Bassani, Michael Engel, and Amadeu K. Sum.



Meysam Bagheri's Artwork in 2024 EAM Calendar
Meysam Bagheri's artwork, submitted for the DEM9 art contest, has been chosen to be featured in the upcoming 2024 EAM (Engineering of Advanced Materials) calendar. The piece is set to be showcased as the featured image for the month of March.

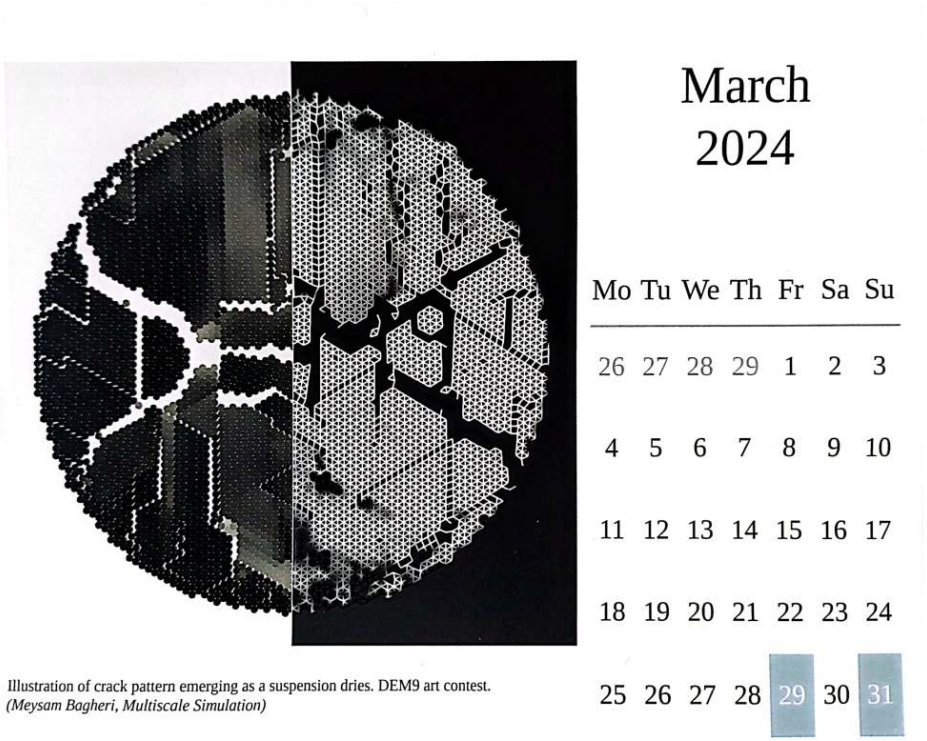


Illustration of crack pattern emerging as a suspension dries. DEM9 art contest.
(Meysam Bagheri, Multiscale Simulation)

Michael Engel among top 2% most widely cited scientists
Michael Engel, professor at MSS, is among the 2% most cited scientists worldwide in 2022. The study by a team of researchers from Stanford University is based on data extracted from Scopus: J. Baas, "October 2023 data-update for 'Updated science-wide author databases of standardized citation indicators.'" Elsevier Data Repository, Oct. 04, 2023. doi: 10.17632/BTCHXKTZYW.6.

15. University Self-Administration

Activities within the University Self-Administration

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

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

16. Public Attention and Public Outreach

MSS goes Girl's day

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

Institute for
Multiscale Simulation

MSS

Friedrich-Alexander-Universität
Erlangen-Nürnberg