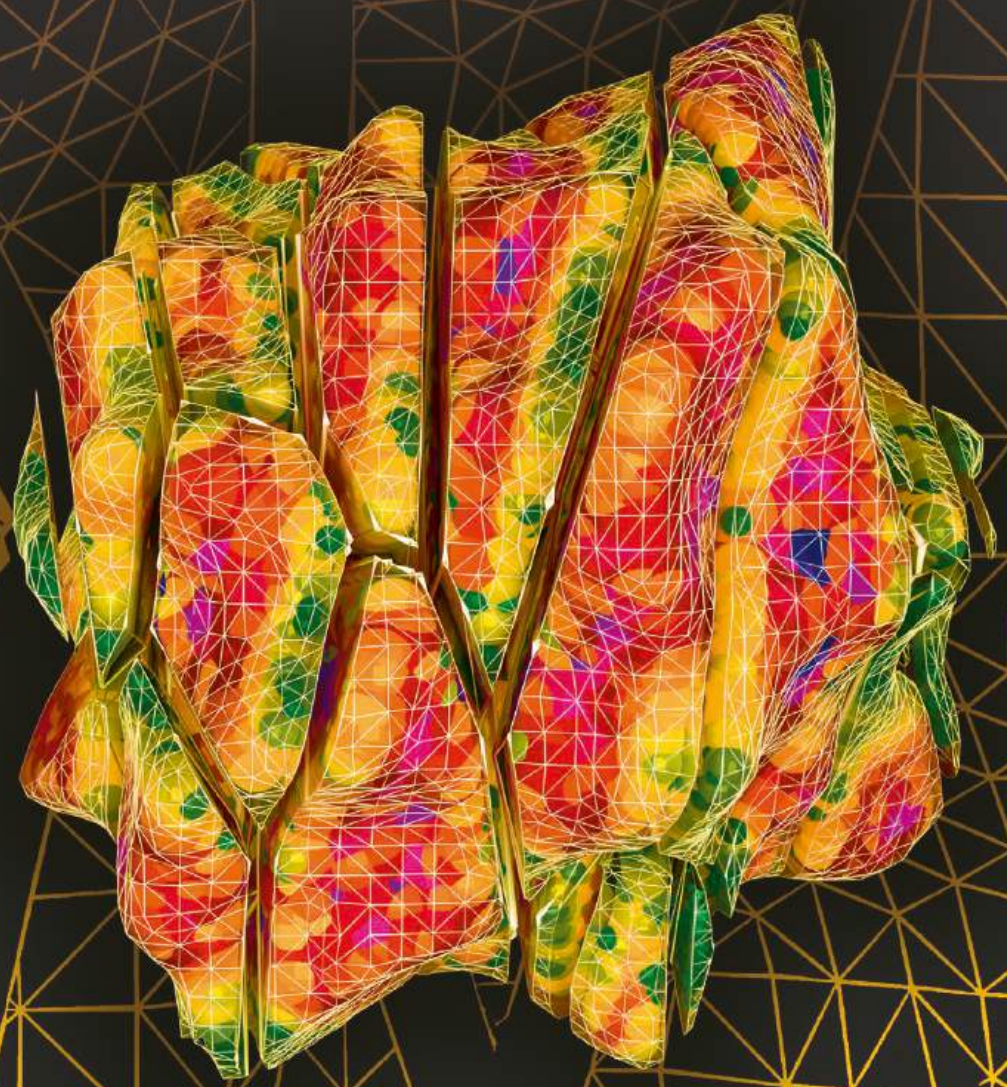
DEM9

9th International Conference on Discrete Element Methods



September 17–21 2023 • Erlangen/Germany

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Institute for Multiscale Simulation
MSS

FAU
Friedrich-Alexander-Universität Erlangen-Nürnberg

DEM9 Book of Abstracts

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9th International Conference on Discrete Element Methods (DEM9)
September 17–21, 2023
dem9.fau.de | mss-dem9@fau.de

Institute for Multiscale Simulation
Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen, Germany
mss.tf.fau.de

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Emergency Phone Numbers

- **Ambulance & Fire Department**: 112
- **Police**: 110
- **Medical Emergency Practice**: +49 9131 81-6060*
- **Medical On-Call Service**: 116 117
- **University Control Center**: +49 9131 85-27777
- **Credit-Card Loss**: 116 116

DEM9 Venue

DEM9 is hosted at the Technical Faculty of the Friedrich-Alexander-Universität Erlangen-Nürnberg. The conference venue is the **Felix Klein building** at **Cauerstraße 11, Erlangen**.

Transportation

The time-schedules of all train and bus routes are available at the **website** (www.bahn.com/en) and **mobile application** of Deutsche Bahn. Information on public transport in the Erlangen-Nürnberg area can also be found at www.vgn.de/en.

Trains

Erlangen is linked to Nuremberg via regional train routes **RE19**, **RE42**, **RE49** and suburban train route **S1**. Various intercity trains connect the two cities, namely routes **IC95**, **ICE1501**, **ICE501**, **ICE503**, **IC2068**, **ICE505**, **ICE507**, **ICE509**, **ICE1601**, **ICE1711**, **ICE603**, **ICE1605**, **ICE803**. The Erlangen central train station (Erlangen Hauptbahnhof) is linked to the DEM9 venue via frequent buses.

Buses

Bus travel is the most economical option to reach Erlangen and Nuremberg from the DEM9 venue:

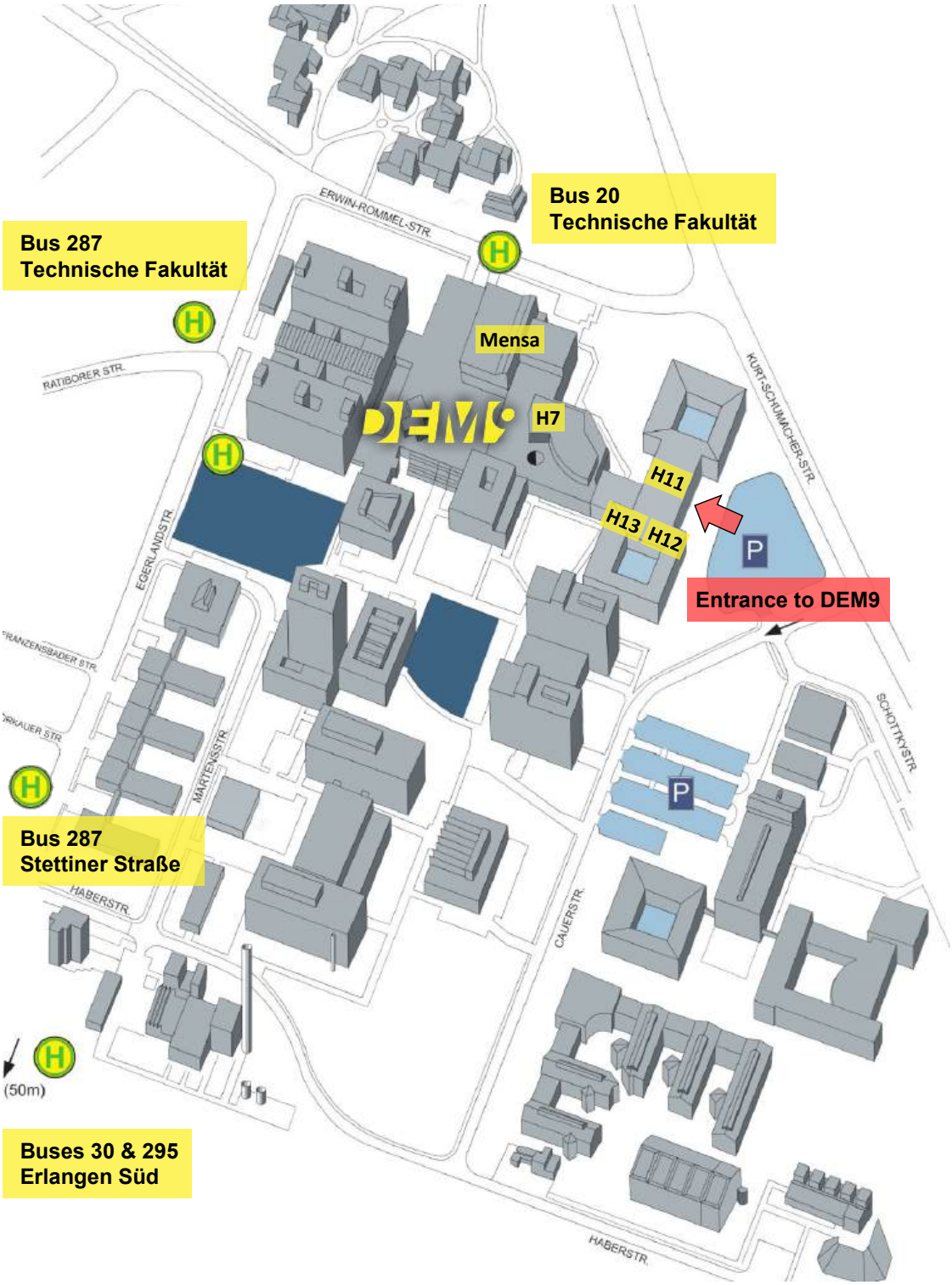
- **Bus 20** connects the DEM9 venue to Erlangen (bus stop: *Technische Fakultät* in direction *Busbahnhof*) and Nuremberg (bus stop *Technische Fakultät* in direction *Am Wegfeld, Nürnberg*).
- **Bus 287** connects the DEM9 venue to Erlangen (bus stop: *Technische Fakultät* or *Stettiner Straße* in direction *Lindnerstraße, Erlangen*).
- **Bus 30** connects the DEM9 venue to Erlangen (bus stop: *Erlangen Süd* in direction *Arcaden/Huggennotenplatz*) and Nuremberg Airport (bus stop *Erlangen Süd* in direction *Nordostbahnhof, Nürnberg*).
- **Bus 295** connects the DEM9 venue to Erlangen (bus stop: *Erlangen Süd* in direction *Huggennotenplatz*).

*Bauhofstraße 6, 91052 Erlangen - Opening hours: Monday, Tuesday, Thursday 18:00-21:00; Wednesday, Friday 13:00 - 21:00; Weekends/Holidays 09:00 - 21:00

Taxis

Taxis are rather expensive in Germany. Some service numbers:

- **Taxi Service Erlangen**: +49 16077-90077
- **Taxi-Zentrale-Erlangen**: +49 09131-19410
- **Taxi24**: +49 17599-92226



About

DEM9 Conference

DEM9 addresses the latest advancements in the simulation of particulate systems using discrete element methods, including coupled simulations, particle fragmentation, non-spherical particles, multiscale and multiphase systems.

DEM Conference Series

DEM is the leading series of conferences in the field of Discrete Element Simulation. Its history ranges back more than 30 years:

- DEM-1 Golden (Colorado), United States, 1989
- DEM-2 Cambridge (Massachusetts), United States, 1993
- DEM-3 Santa Fe (New Mexico), United States, 2002
- DEM-4 Brisbane, Australia, 2007
- DEM-5 London, United Kingdom, 2010
- DEM-6 Golden (Colorado), United States, 2013
- DEM-7 Dalian, China, 2016
- DEM-8 Twente, The Netherlands, 2019
- DEM-9 Erlangen, Germany, 2023

Institute for Multiscale Simulation (MSS)

DEM9 is organized by the Institute for Multiscale Simulation (MSS) at the Friedrich-Alexander-Universität Erlangen-Nürnberg, in Erlangen, Germany. The research and teaching work of the group is focused on particulate and other discrete systems by means of experiments and simulations.

DEM9 Activities

Student Support Grant

DEM9 provides a *Student Support Grant* to enhance the participation of students in the event and to increase the visibility of their work within the DEM research community. The grant is awarded to 35 early-stage researchers.

Video Competition

DEM9 hosts a video competition. The videos are inspired by contributions to the conference and include submissions of both technical and non-technical content. The best videos will be awarded a prize.

Artistic Image Competition

DEM9 hosts an artistic image competition. The non-technical contributions are inspired by science and their content is related to particulate systems. The best images will be awarded a prize.

Special Issues in Scientific Journals

Selected presentations of DEM9 will be published in topical issues of *Powder Technology* and *Granular Matter*:

- Emerging trends in the DEM modelling of granular systems. Powder Technology. Editors: Vasileios Angelidakis (Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany), Bruno Chareyre (3SR-LAB, Grenoble Institute of Technology, Grenoble, France).
- Simulation of particle processes in additive manufacturing. Granular Matter. Editors: Sudeshna Roy (Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany), Thomas Weinhart (Department of Fluid and Thermal Engineering, University of Twente, The Netherlands).

Partners and Sponsors

DEM9 is supported by the FAU Competence Center Engineering of Advanced Materials (FAU EAM), the Research Training Group GRK 2423 Fracture Across Scales (FRASCAL), the FAU Competence Center on Scientific Computing (FAU CSC), the Institute for Multiscale Simulation, and the University of Twente.

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Monash Uni., AU

Programme

Sunday, September 17

6:30 pm	**Welcome reception & Registration** Location: Reception area

Monday, September 18

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9:55 am	**Morning break** Location: Reception area		
10:25 am	**Granulate-structure interaction** Location: H11	**Coupled methods I** Location: H12	**Mini-symposium: Packings and jamming: a journey through scales** Location: H13
12:30 pm	**Lunch** Location: Mensa (1st floor)		
2:00 pm	**Plenary talk - Antonio Munjiza**: Grand challenge of AI-based virtual experimentation using DEM, FDEM, and hybrid simulation technology Location: H11		
2:45 pm	**Afternoon break** Location: Reception area		
3:15 pm	**Polydisperse systems** Location: H11	**Coupled methods II** Location: H12	**Mini-symposium: SALTED: algorithms and applications for static packing problems** Location: H13
6:00 pm	**Conference banquet** Location: Der Redoutensaal		
7:00 pm	**Evening talk - Troy Shinbrot**: Challenges for DEM from the lab and nature Location: Der Redoutensaal		

Tuesday, September 19

9:30 am	**Plenary talk - Nicolin Govender**: Particle shape effects in granular material using GPU DEM: An industry perspective Location: H11		
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10:45 am	**Cohesive and capillary interactions** Location: H11	**Particle-fluid interactions in industrial applications I** Location: H12	**Mini-symposium: Advancements in additive manufacturing processes through the use of the DEM** Location: H13
1:00 pm	**Lunch** Location: Mensa (1st floor)		
2:00 pm	**Plenary talk - Yuntian Feng**: The developments of the Energy-Conserving Contact (ECC) theory and contact models for arbitrarily shaped particles Location: H11		
2:45 pm	**Afternoon break** Location: Reception area		
3:15 pm	**Granular metamaterials** Location: H11	**Powder processes & technologies** Location: H12	**Mini-symposium: The applications and algorithms of coupled MPM-DEM** Location: H13
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9:30 am	**Plenary talk - Emilien Azéma**: Exploring the scales in highly deformable grain assemblies when compressed far beyond the jammed state Location: H11		
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10:45 am	**Particle-fluid interactions in industrial applications II** Location: H11	**Mini-symposium: DEM-based hybrid algorithms for particle-laden flows** Location: H12	**Mini-symposium: Advances in open-source DEM software** Location: H13
1:00 pm	**Lunch** Location: Mensa (1st floor)		

2:00 pm	**Plenary talk - Hongyang Cheng**: From granular randomness to predictive digital twins:Integrating data-driven and coupled models for uncertainty quantification Location: H11		
2:45 pm	**Afternoon break** Location: Reception area		
3:15 pm	**Vibrated systems and charged particles** Location: H11	**Powder processes technology: Additive Manufacturing** Location: H12	**Mini-symposium: The future of open-source DEM - Discussion** Location: H13
5:20 pm	**Poster session** Location: Reception area		
6:50 pm	**Evening talk - Dirk Helbing**: The Wonderful World of Pedestrians Location: H11		

Thursday, September 21

9:30 am	**Plenary talk - Zeynep Karatza**: ON THE VALIDATION OF DEM MODELS: Bridging the gap between simulation and reality through full-field experimental data Location: H7		
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10:45 am	**Fracture and fragmentation** Location: H7	**Performance analysis & Machine Learning** Location: H12	**Mini-symposium: DEM for understanding complex flows in gas-particle systems** Location: H13
1:00 pm	**Lunch** Location: Mensa (1st floor)		
2:00 pm	**Plenary talk - Eric Parteli**: Particle-based simulations of dry cohesive granular materials Location: H7		
2:45 pm	**Afternoon break** Location: Reception area		
3:15 pm	**Geomaterials** Location: H7	**Flow of non-spherical particles** Location: H12	
5:20 pm	**Concluding remarks** Location: H7		

Plenary Talks

Monday, September 18
9:10 am - Mikio Sakai
2:00 pm - Antonio Munjiza

Tuesday, September 19
9:30 am - Nicolin Govender
2:00 pm - Yuntian Feng

Wednesday, September 20
9:30 am - Emilien Azéma
2:00 pm - Hongyang Cheng

Thursday, September 21
9:30 am - Zeynep Karatza
2:00 pm - Eric Parteli

Mikio Sakai
The University of Tokyo, Japan

What technologies are essential in development of the DEM-based digital twin?

The remarkable development of information and communication technology makes it possible to realize the “Fourth Industrial Revolution”. The industrial revolution drastically changes manufacturing by introducing the digital twin or the Cyber-Physical System. In the digital twin, cyber and physical spaces are highly integrated by digital technologies. The role of modeling and simulation becomes extremely important in the digital twin. Digital twin-based manufacturing will be positively used in powder products. The Discrete Element Method (DEM) will be employed to construct a cyber-space in a powder process. What technologies are essential in the development of the DEM-based digital twin? Probably, a flexible wall boundary model to reflect the minute change, a scaling-law model to reduce the calculation time, accurate modeling for multi-phase flows, verification & validation, analytical models for calculation results (big data), and a reduced order model would be important. To realize the digital twin for the powder processes, the author’s group has developed several valuable technologies such as signed distance function-based wall boundary model, coarse-grained DEM, DEM coupled with Volume of Fluid, and Proper Orthogonal Decomposition. The adequacy of these technologies has been proved through the validation tests. A combination of the above models and analytical approaches will contribute to the realization of the digital twin.

Acknowledgement
This author acknowledges the financial support from Japan Society for the Promotion of Science KAKENHI (Grant No. 21H04870, 21K19760 and 17KK0110).

Antonio Munjiza
University of Split, Croatia

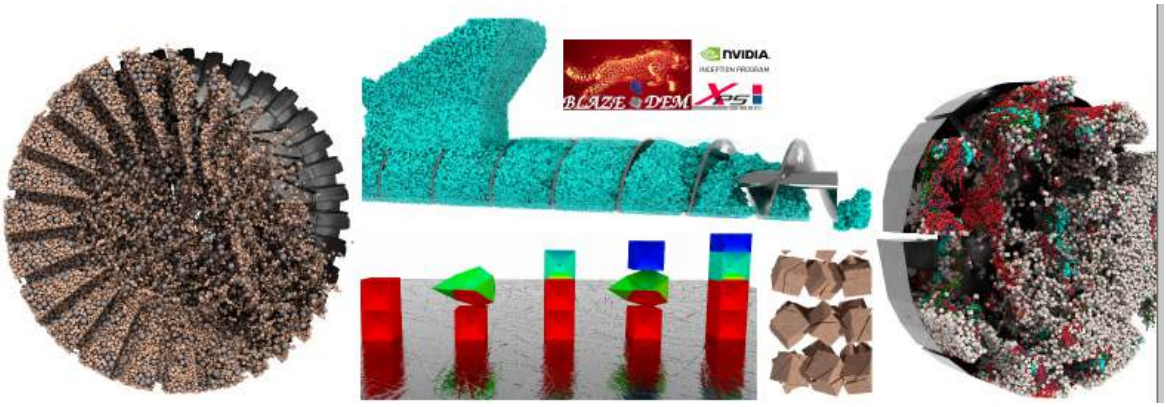
Grand Challenge of AI-based Virtual Experimentation using DEM, FDEM, and Hybrid Simulation Technology

In the last few years significant developments and scientific breakthroughs have been made in DEM-related discontinua simulation methods; particularly in hybrid continuum/discontinuum simulation technologies, such as the combined finite-discrete element method (FDEM). These developments include novel approaches to fluid-solid integrated solvers, large scale parallelization, next generation algorithmic solutions, and application in applied/fundamental research. These advances are typically applied in the context of virtual experimentation, which complements both theoretical and experimental research methods. The next step is the integration of these into artificial intelligence (AI)-based scientific contexts that opens the door for machine-based discovery, enhancing and complementing human input. In this publication, we provide an overview of some of the key recent developments and highlight promising research efforts that illustrate the usage of FDEM-based virtual experimentation results.

Nicolin Govender
University of Johannesburg, South Africa;
Research Center Pharmaceutical Engineering GmbH, Austria

Particle shape effects in granular material using GPU DEM: An industry perspective

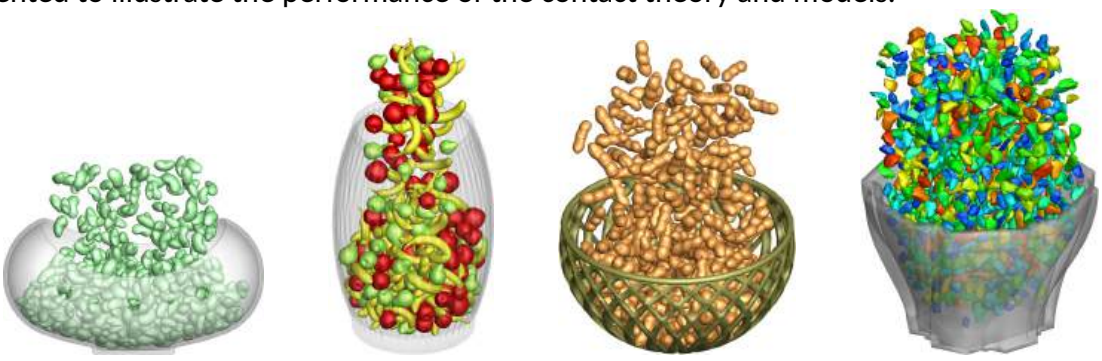
Particle shape plays a crucial role in the resulting macroscopic behavior of granular material yet the majority of DEM simulations use simple spheres with non-physical constructs such as rolling friction without fully understanding the implications thereof. While there have been shape studies using super quadric's and ellipsoids over the years, they still have the same single point contact resolution as spheres. The majority of industrially relevant granular materials are however non-curve linear and have shapes that is best captured by polyhedral shapes. Apart from mechanical behavior, thermal conduction as well as cohesion between these particles occurs over a finite-contact area that is more faithfully captured by polyhedra. In this talk the role of particle shape will be explored for a number of industrial cases such as mixers, screw feeders and silos along with prescriptions for when shape and size simplifications can be used. The underlying theme of the talk will be on the use of GPU computing in the past decade to advance the physics fidelity of DEM simulations along with reduced run-times. Finally an outlook to the future of using high fidelity DEM to generate data for statistical models and physics informed neural networks that can provide answers in the age of digital twins will be presented.



Yuntian Feng
Swansea University, United Kingdom

The Developments of the Energy-Conserving Contact (ECC) Theory and Contact Models for Arbitrarily Shaped Particles

Developing contact theories and models for non-spherical particles in general and arbitrarily shaped particles in particular has been a major research theme in DEM for the last thirty years. In this keynote lecture, the focus will be on the development of an energy-conserving contact theory and associated models for arbitrarily shaped particles. The lecture will begin by reviewing the major developments in the field and highlighting the key challenges and issues that have hindered progress in discrete element modelling of arbitrarily shaped particles [1]. Next, the development of the energy-conserving theory [2] will be presented, which includes 1) introducing the sole assumption that the contact state of two particles is fully described by a contact energy function/potential; 2) imposing the energy-conserving principle that the total kinetic energy must be conserved for an elastic impact; and 3) automatically deriving a general normal contact model in terms of the three contact features: contact normal, contact point, and force magnitude. Such a contact model guarantees to be energy-conserving for any elastic impact, leading to more robust and stable contact models for any contact scenarios. Three energy conserving contact models are established by carefully choosing the contact energy function: the contact area/volume based model [3], the overlap based model [4] and the contact boundary based model. The first model obtains the three contact features from the intersection line(s) of the two particles, while the second model proposes a generic overlap-based contact model by introducing the Minkowski-difference overlap, which unifies the definition of overlap for both convex and concave particles. The third model defines a contact potential using the contact boundary, and its discretised versions cover some existing contact models. Finally, numerical examples are presented to illustrate the performance of the contact theory and models.



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[2] Y. T. Feng (2021). An energy-conserving contact theory for discrete element modelling of arbitrarily shaped particles: Contact volume based model and computational issues. Computer Methods in Applied Mechanics and Engineering. 373:113493.

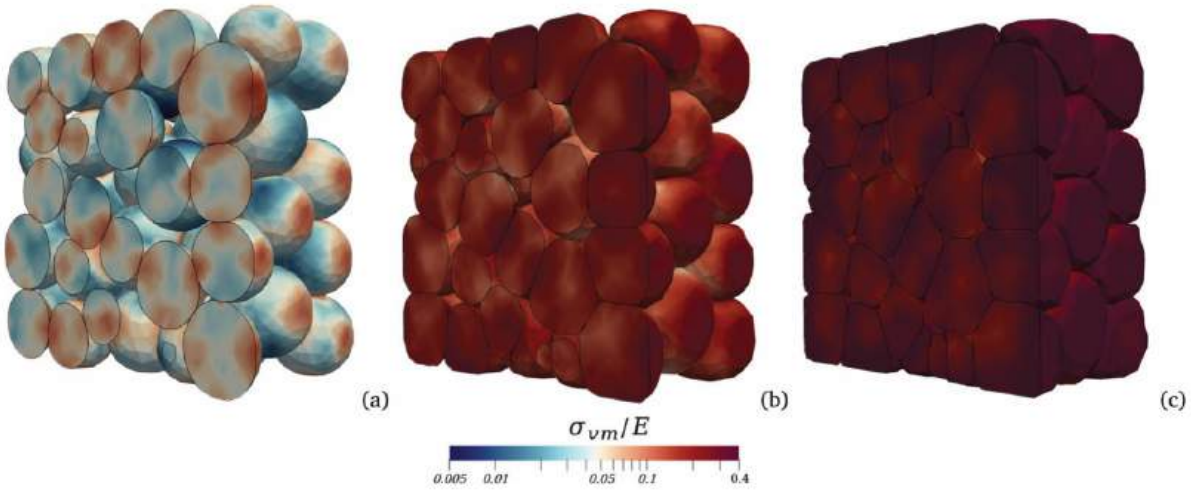
[3] Y. T. Feng (2021). An energy-conserving contact theory for discrete element modelling of arbitrarily shaped particles: Basic framework and general contact model. Computer Methods in Applied Mechanics and Engineering. 373:113454.

[4] Y. T. Feng, Y. Tan (2021). The Minkowski overlap and the energy-conserving contact model for discrete element modelling of convex nonspherical particles. International Journal for Numerical Methods in Engineering, 122(22): 6476-6495.

Emilien Azéma
Université de Montpellier, France

Exploring the scales in highly deformable grain assemblies when compressed far beyond the jammed state

When hard grains (i.e., with high stiffness relatively to the applied stress) are compressed inside a box, they tend to rearrange themselves in a more compact way until a permanent contact forces network is reached, meaning the end of the compression. This “jammed state” depends on the morphology of the grain and the inter-grain friction. What happens now if we consider grains that can deform when the applied stress becomes significant? The compression continues beyond the jammed state, mainly due to the change in shape of the grains and, to a lesser extent, due to their rearrangements. As a result, the solid fraction exceeds that of the Random Close Packing, and it would even be possible to entirely fill the space. By means of coupled finite-discrete elements methods (the non-smooth contact dynamics method NSCD) and experiments using high-resolution imaging coupled with a dedicated DIC algorithm, we analyze the compressive behavior, beyond the jammed state, of two- and three-dimensional granular assemblies made of soft (hyperelastic) grains of different shapes and soft/rigid grain mixtures. We characterize the evolution of the main mechanical observables, from the global scale down to the strain field inside each deformable grain. At the microscopic scale, different power-law relations are evidenced between the local grain structure and contacts, and the packing fraction. We develop an equation that describes the evolution of the packing fraction as a function of the applied pressure. This latter is derived from the granular stress tensor, its limit to small deformations, and the evolution of the connectivity. This compaction equation provides good predictions from the jamming point up to very high densities without the need for tuning any parameters both for numerical and experimental data.

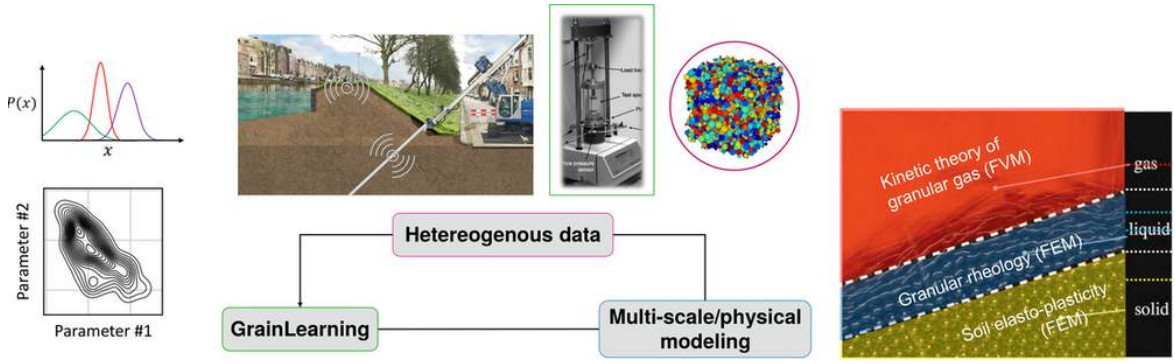


Cross-section of the von Misses stress field inside each grains and for different packing fractions ν= 0.66 (a), ν= 0.86 (b) and ν= 0.96 (c) in an assembly of 100 grains. The color intensity is proportional to the von Mises stress scaled by the Young’s modulus.

Hongyang Cheng
University of Twente, The Netherlands

From Granular Randomness to Predictive Digital Twins: Integrating Data-Driven and Coupled Models for Uncertainty Quantification

Granular materials exist in various sizes and shapes and are often subject to complex motions, ranging from quasi-static to free-flowing. Predicting the bulk behavior of granular materials is difficult because of the randomness in their microstructure and particle-scale properties. Although advanced laboratory testing is making observations of particles more accessible, the data typically characterize physical processes at a given length scale (e.g., particle or continuum). Starting from the particle-scale modeling of granular materials using the discrete element method (DEM), the particle-scale uncertainty can be quantified using Bayesian inference. In an effort of minimizing the variance, uncertainty quantification reduces to calibration. Moving to the macroscopic, continuum level, there exist phenomenological constitutive models, well-established for granular materials in solid-like or fluid-like regimes. The emerging methodological challenges are to couple these “best available models” in complex situations where a transition (e.g., from continuum to discrete) occurs [1] and to propagate particle-scale uncertainty to the continuum level [2] and vice versa; both are essential to developing a predictive digital twin. This presentation aims to introduce probabilistic and data-driven techniques that allow efficient integration of data, at both particle and continuum scales and it is split into three parts: (1) the hierarchical Bayesian approach (2) a combination of data-driven and physics-based modeling for uncertainty quantification, and (3) the coupling of best available models (discrete and continuum) as the most accurate and efficient digital representation of granular materials.



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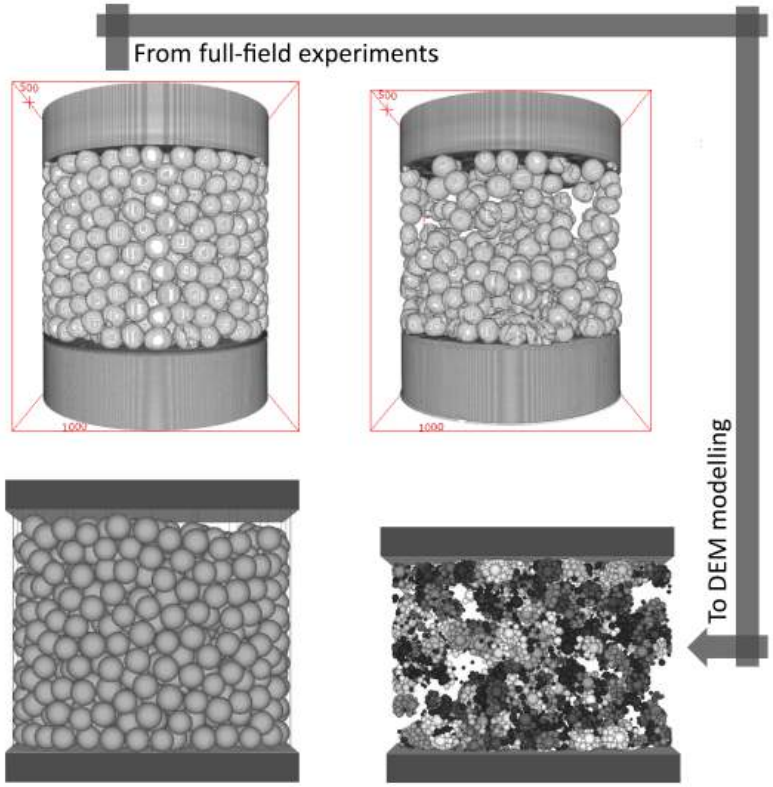
[1] H. Cheng, A.R. Thornton, S. Luding, A.L. Hazel, T. Weinhart. Concurrent multi-scale modeling of granular materials: Role of coarse-graining in FEM-DEM coupling. Comput. Methods Appl. Mech. Eng., 403 (2023), 115651.

[2] H. Cheng, T. Shuku, K. Thoeni, P. Tempone, S. Luding, V. Magnanimo. An iterative Bayesian filtering framework for fast and automated calibration of DEM models. Comput. Methods Appl. Mech. Eng., 350 (2019), pp. 268-294.

Zeynep Karatza
National Technical University of Athens, Greece

On the validation of DEM models: Bridging the gap between simulation and reality through full-field experimental data

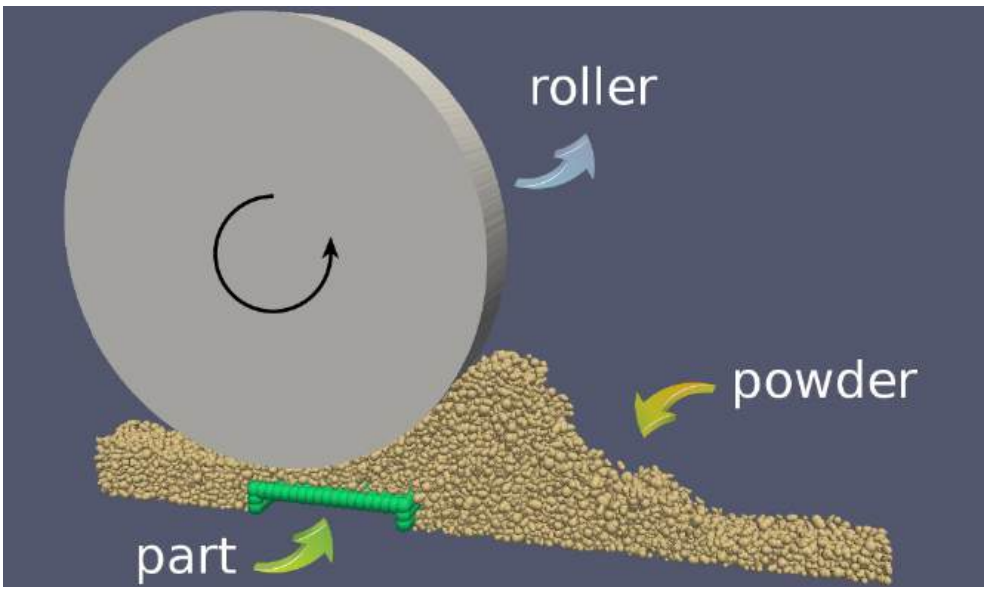
Despite the immense progress of numerical modelling, DEM models still rely on experimental data to provide constraints on material behaviour for the calibration of input parameters and validation of the simulation results. The main limitation of conventional experimental means is that the processes in action are rarely directly observed, and so, often, DEM practitioners resort to empirical curve fitting parameters/techniques that can usually only describe an average response of the simulated material. Since the deformation of a granular assembly is complex and heterogeneous, gathering quantitative full-field information (i.e. a field record of a quantity as opposed to a bulk measurement) is imperative, and has been an essential component of my research using predominantly x-ray computed micro-tomography (XCT). XCT has been growing in popularity in recent years as a research tool in material sciences and engineering. Its success lies in the fact it has enabled the observation and measurement in 3D of the deformation and kinematics of materials during loading. In my research I have focused on studying deformation mechanisms and particularly particle breakage. I developed bespoke loading apparatuses for XCT and algorithms that allowed for the first time to simultaneously track particles and their fragments in to investigate how particle morphology and coordination number affect the different types of breakage. Interestingly, a significant amount of breakage was detected well before the typically defined yielding point, that is often associated with the onset of particle crushing. This information was used to develop a new DEM replacement method, where breakage is simulated by particle replacement (used for primary splitting breakage) and clustering (used for breakage of fragments). The model was validated and calibrated using information from the experiments at multiple scales (particle and whole assembly) and both the particle size distributions and the stress-strain response obtained with the new DEM model matched the experimental results.



Eric Parteli
Universität Duisburg-Essen, Germany

Particle-based simulations of dry cohesive granular materials

In this talk I will present insights into the physics of dry cohesive granular materials from DEM simulations. Such materials play an important role in various technological processes, such as in additive manufacturing. Moreover, dust-sized particles cover the surfaces of Earth, Mars and other celestial bodies of our solar system, thereby exerting profound impact on the geology, climate and geochemistry of their physical environment. However, the representation of dry cohesive particles and their interaction with each other in DEM simulations is still matter of research. As I will show in my presentation, DEM models should consider non-bonded attractive (van der Waals) particle-particle interactions. Neglecting these non-bonded interactions or considering adhesive potentials only at particle-particle contact may lead to incorrect numerical predictions of fine powder behaviour. I will show that it is possible to reproduce quantitatively the packing fraction of strongly polydisperse powders made up of spherical particles as a function of average particle size, provided that the full particle-particle interaction model – including contact and non-bonded attractive van der Waals forces – is considered. Moreover, DEM simulations using this model reproduce quantitatively observed values of the angle of repose from a comprehensive set of experimental measurements, for particle sizes ranging from the micrometre- to the centimetre-scale. Inspired by this quantitative agreement, I obtained an expression for the angle of repose as a function of the Bond number (the ratio of the cohesive force to the gravitational force). As I will show, this expression is simple and further reproduces the angle of repose from numerical simulations within the broad range of gravitational acceleration values from 0.06 to 100 times that of Earth. The future application of this model has the potential to improve the assessment of powder mechanical behaviour for additive manufacturing. In my talk, I will present a DEM model for the powder application process in additive manufacturing that incorporates a representation of complex particle geometric shapes. However, consideration of non-bonded van der Waals interactions is indispensable to reproduce the observed powder behaviour, as I will explain in my talk.



DEM simulation of powder application in additive manufacturing.

Evening Talks

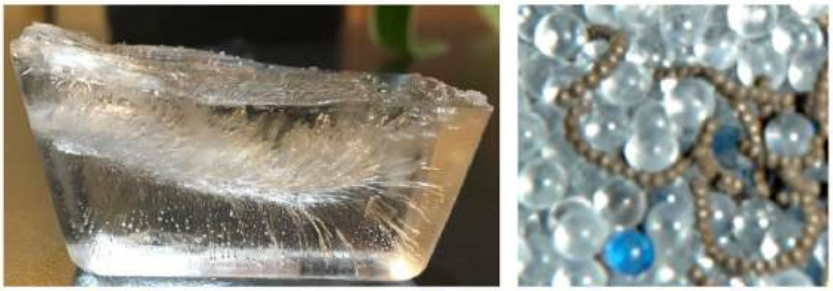
Monday, September 18
7:00 pm - Troy Shinbrot

Wednesday, September 20
6:50 pm - Dirk Helbing

Troy Shinbrot
Biomedical Engineering Department
Rutgers University, NJ, United States of America

Challenges for DEM from the lab and nature

DEM has advanced continuously over the past few decades, and can now simulate large numbers of irregular particles. Nevertheless, many problems are beyond the predictive capacity of current DEM techniques. In this talk, I describe several such problems as a challenge for future DEM analysis. These include examples from the lab as well as from nature. From the lab, I'll discuss a range of simple problems that participants can reproduce on their own, including patterning of air bubbles in ice (water must be very clean) and granular tendril formation (easily produced in fine spices such as thyme). In nature, I'll describe unexplained phenomena including erosional "tafoni" patterns and several exceedingly odd granular patterns seen on Mars and Saturn's moons.



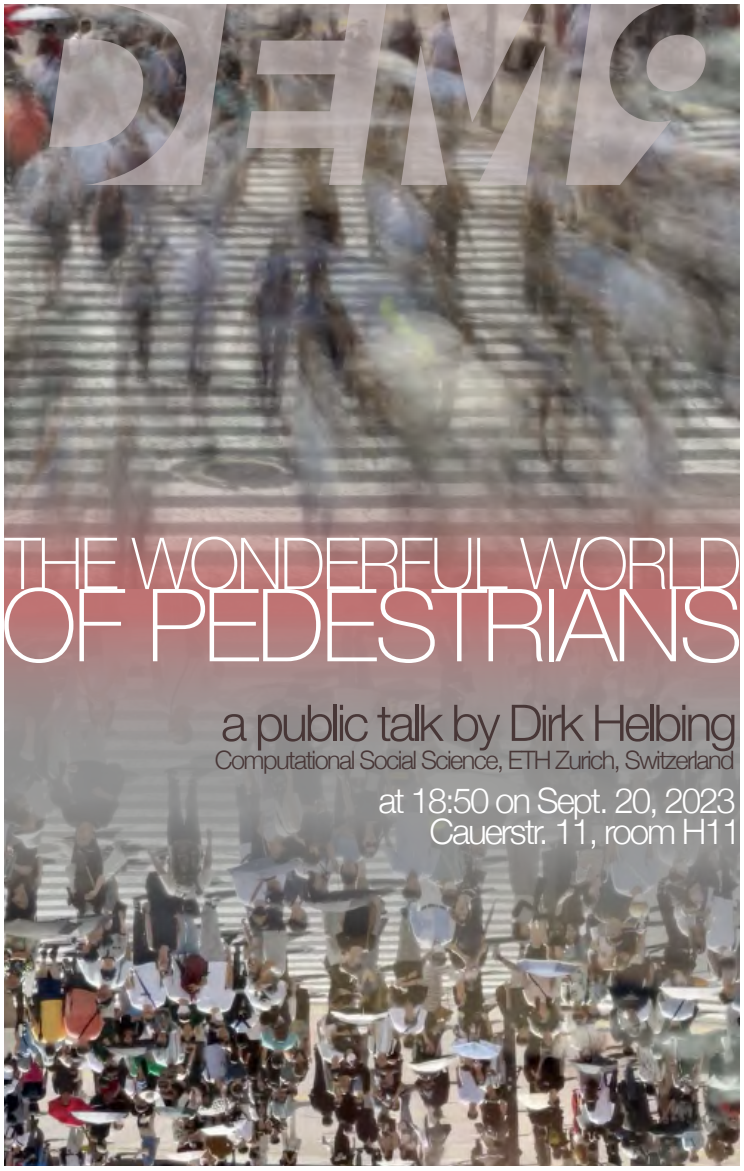
Lab challenges: *patterning of air bubbles in ice; spontaneous tendrils formation in tumbler.*

Nature challenges: *Erosional "tafoni," Martian "flower." Credits: tafoni - S. Morris, flower - NASA*

Dirk Helbing
Computer Science Department, ETH Zurich, Switzerland

The Wonderful World of Pedestrians

In this talk, I am going to look back to how the field of pedestrian, crowd and evacuation dynamics emerged in physics, and how it developed over time. I will give a very personal perspective, with many anecdotes and background stories. Modeling pedestrians and crowds as self-driven many-particle systems has turned out to be a surprisingly powerful approach to model and understand the dynamics of humans moving through space while interacting with others. Besides driven particle and cellular automata models, the Social Force Model is certainly one of the models that was inspired by physics and was able to reproduce several interesting collective patterns of motion, which emerge by self-organization. These patterns include the formation of lanes of uniform walking direction in bidirectional flows, stripe formation in two crossing flows, and oscillatory flows at bottlenecks. Such discoveries, including the faster is slower effect, have inspired improvements in logistics (chip production) and in traffic light control, and it does not stop there. Modern experimental techniques, for example, use Virtual Reality technology combined with multi-agent simulations, to reconstruct crowd disasters as they have happened in the past.



Mini-symposia – Invited Talks

Mini-symposium: Packings and jamming: a journey through scales

Olfa D'Angelo, Patric Müller
Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Granular materials can undergo a jamming transition: from a flowing, liquid-like state, they can develop rigidity and resist finite loads, akin to solids. The emergence of such collective behaviour from the assembly of discrete particles urges us to interrogate the mesoscale, focusing on the geometrical features of dense packings. The mechanical properties of dense granular packings are mediated by both the statistics of the contact network and the properties of individual contacts. DEM simulations provide a valuable tool to link particle properties, the characteristics of the packing and, ultimately, the macroscale mechanical response of the granulate in the jammed state.

In this mini-symposium, we will discuss the latest developments in the DEM-based investigation of packing problems and jamming in particulate systems. Additionally, we will address how these results can be harvested to develop new technologies, notably in soft-robotics.

Invited speakers:

Farhang Radjai, LMGC, CNRS, University of Montpellier, France
Corey O'Hern, Yale University, USA
Joel Clemmer, Sandia National Labs, Sandia National Laboratories, USA
Philipp Schönhöfer, Chemical Engineering, University of Michigan, USA

Fabric and granular plasticity

Farhang Radjai

LMGC, CNRS, University of Montpellier, France (franck.radjai@umontpellier.fr)

Keywords Jamming, fabric state, steric exclusions, plastic behavior

A packing of rigid frictional particles can be found in an infinite number of different metastable fabric states with different levels of connectivity, anisotropy, packing fraction, local order, and long-range order. It seems therefore extraordinary that such a multi-state material is able to exhibit well-defined reproducible behavior under external loading. We discuss this point in the light of particle dynamics simulations, which provide access to the details of microstructure. We show that the fabric states involve a subtle interplay between force balance and steric exclusions. We demonstrate the crucial role of both disorder and steric exclusions in driving the granular microstructure towards steady fabric states that underlie the plastic behavior of granular materials. We also discuss the effects of friction, particle shape, and boundary conditions in this respect.

Structural, vibrational, mechanical properties of jammed packings of deformable particles

Corey O'Hern

Yale University, United States of America (corey.ohern@yale.edu)

Keywords Jamming, deformability, emulsions, packings

We investigate the structural, vibrational, and mechanical properties of jammed packings of deformable particles with shape degrees of freedom in three dimensions (3D). Each 3D deformable particle is modeled as a surface-triangulated polyhedron, with spherical vertices whose positions are determined by a shape-energy function with terms that constrain the particle surface area, volume, and curvature, and prevent interparticle overlap. We show that jammed packings of deformable particles without bending energy possess low-frequency, quartic vibrational modes, whose number decreases with increasing asphericity and matches the number of missing contacts relative to the isostatic value. In contrast, jammed packings of deformable particles with non-zero bending energy are isostatic in 3D, with no quartic modes. These studies underscore the importance of incorporating particle deformability and shape change when modeling the properties of jammed soft materials.

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2. D. Wang, J. D. Treado, A. Bormand, B. Norwick, M. P. Murrell, M. D. Shattuck, and C. S. O'Hern, "The structural, vibrational, and mechanical properties of jammed packings of deformable particles in three dimensions," Soft Matter 17 (2021) 9901.

Pushing the high-pressure limit of jamming in granular matter

Joel T. Clemmer, Joseph M. Monti, Jeremy B. Lechman

Sandia National Laboratories, United States of America (jtclemm@sandia.gov)

Keywords Jamming, elastic deformation, shear, LAMMPS

Applying theoretical insight from the jamming transition to granular applications is often throttled by the complex reality of many industrial and natural processes. Grains are typically not ideal, defect-free spheres and many processes involve non-negligible stresses that can induce significant deformation, damage, or fracture in grains. To address such issues, we use a bonded particle model to explore how traditional expectations of granular behavior near jamming, both in compaction and shear, extend to high pressures. This methodology allows simulations to flexibly capture important mechanisms that emerge at high pressures such as elastic or plastic deformation and fracture. We quantify how both standard metrics of jamming (coordination number, packing fraction, etc.) as well as measures of grain deformation and volumetric strain depend on increasing pressure. Material properties, such as elastic moduli or the strength of friction between grains, are controlled using new nonlocal interaction terms or by carefully arranging bonded particles in a grain. Results are compared to traditional discrete element methods to identify where behavior diverges with increasing pressure. This work leverages open-source capabilities in LAMMPS to run large scale simulations. New capabilities include a streamlined framework for new contact force models, a bonded particle package, support for nonlocal force interactions, and efficient algorithms for contact detection in highly polydisperse systems.

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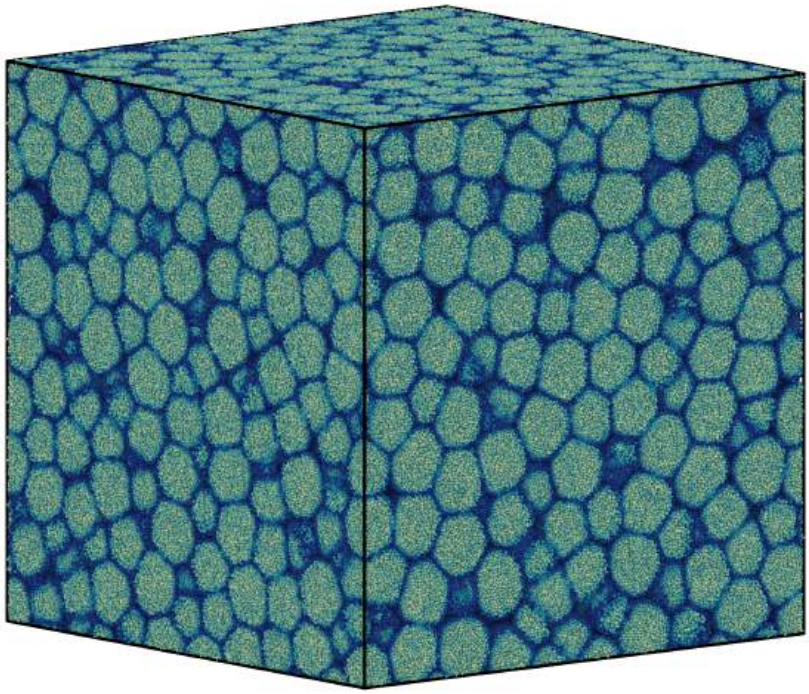

Shape-driven, emergent behavior in active particle systems

Philipp Schönhöfer

University of Michigan, United States of America (pschoenh@umich.edu)

Keywords Active particles, particleshape

It is well established that the collective and self-emergent dynamics of active swarms in biology, colloidal science and modern-day robotics can be traced back mostly to the local interactions between neighbouring particles. While nature and robotics scientists developed intricate strategies/algorithms for organisms/robots to communicate on the local scale and thereby coordinate their global dynamics, we still lack the ability to synthesize colloidal particles with a similar degree of complexity. In that regard, we study how shape and other morphological properties of active particles influence both the local structures and global dynamics in crowded active particle systems. In particular, we demonstrate mechanisms that can control the clustering and collective migration of self-propelled particles by using models of both rigid and deformable particles.

Mini-symposium: SALTED: Simulation of granular packings via sequential particle deposition

Thorsten Pöschel
Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Simulating static packings through numerically solving Newton's equation of motion is notoriously difficult due to the slow convergence of the integration schemes. For cases where the dynamics of the process is much less critical than the packing itself, Sequential Particle Deposition can be a promising alternative. In this mini-symposium, we discuss the idea of generating large packings of highly complex particles through sequential deposition and its limitations, an efficient implementation in a software package, and applications of this simulation method.

Invited speakers:

Nikola Topic, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Vasileios Angelidakis, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Dietrich E. Wolf, University of Duisburg-Essen, Germany
Lothar Brendel, University of Duisburg-Essen, Germany

SALTED - A High Performance Simulator for Granular Packings

Nikola Topic, Thorsten Pöschel

Universität Erlangen-Nürnberg, Germany (nikola.topic@fau.de)

Keywords Sequential ballistic deposition, event-driven, complex-shaped particles

We present an efficient event-driven algorithm for sequential ballistic deposition of complex-shaped rigid particles. In the sequential deposition process, by performing steps of rolling and linear motion, the particles move along the steepest descent in a landscape formed by the boundaries and previously deposited particles. The computer time for the simulation of a deposition process depends on the total number of spheres but only weakly on the sizes and shapes of the particles. The proposed algorithm generalizes the Visscher-Bolsterli algorithm [1] which is frequently used for packing of spheres, to non-spherical particles [2]. The proposed event-driven algorithm allows simulations of multi-million particle systems using desktop computers.

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An Open-Source Software for Sequential Particle Deposition

Vasileios Angelidakis

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(vasileios.angelidakis@fau.de)

Keywords Sequential particle deposition, non-spherical particles, open-source software

The packing of discrete objects is of interest to a variety of applications in science, engineering and everyday life. Numerical simulations can shed light into the properties of packings with diverse properties, such as highly irregular particle shapes. Sequential Particle Deposition has been recently extended to complex particle shapes, and can produce packings with millions of particles within minutes. This contribution presents the algorithmic features of SALTED, an open-source software applying Sequential Particle Deposition for the efficient generation of large static packings of complex objects.

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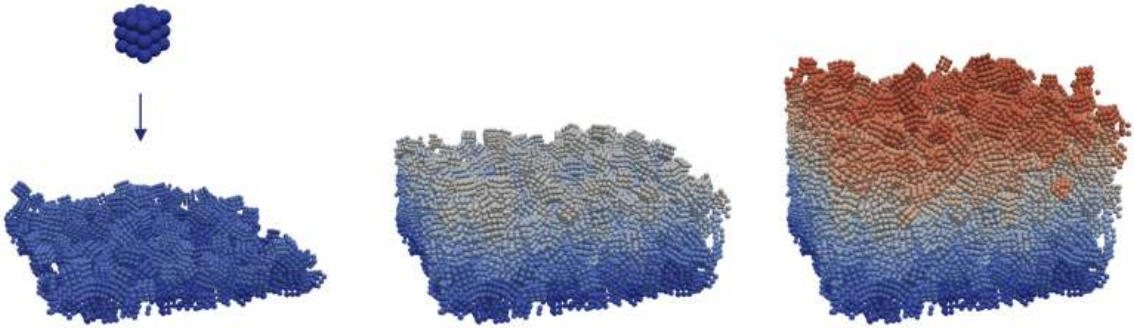

Universal structure of cohesive particle agglomerates after many dispersion-settling cycles

Dietrich E. Wolf

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Keywords Fractals, cluster size distribution, dust, porosity

Cohesive particles form agglomerates that can be very porous. Their geometry, in particular, their fractal dimension, depends on the agglomeration process (diffusion limited or ballistic, growth by adding single particles or by cluster-cluster aggregation). In practice, however, the packing structure changes depending on the mechanical processing of the agglomerate after it has grown. Surprisingly, under certain fixed process conditions, the packing converges to a statistically invariant structure, as shown in [1]-[4], independent of the initial growth process. We consider the repeated fragmentation on a given length scale, followed by ballistic reagglomeration. Examples for the fragmentation are sieving with a given mesh size, or dispersion in a turbulent fluid. We model the reagglomeration by gravitational sedimentation. The converged structure is fractal up to the fragmentation length scale, and the fragments have a power-law size distribution. The power law and the fractal dimension are connected by a scaling relation.

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Evolution of charged agglomerate statistics under continued binary collisions

Florian Führer, Lothar Brendel, Dietrich E. Wolf

University of Duisburg-Essen, Germany (lothar.brendel@uni-due.de)

Keywords Agglomerate collisions, charged particles, cluster size distribution, planet formation

Protoplanetary disks consist of a dilute dispersion of charged dust agglomerates in a turbulent gas. We consider the question, whether binary collisions with possibly a large number of fragments, part of which may reagglomerate, can in the long run lead to a stationary agglomerate size distribution. We developed an efficient simulation model combining a Smoluchowski-like collision kernel with a DEM simulation of the fragmentation and reagglomeration process resulting from a binary collision. The resulting clusters update the agglomerate statistics. We find that this iterative evolution leads to a stationary distribution of the charged agglomerates. It is compared with the charged cluster size distributions obtained by two different mechanisms, the fragmentation of a sediment due to a sudden pressure release [1] and the agglomeration in a freely cooling granular gas [2].

References

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Mini-symposium: Advancements in additive manufacturing processes through the use of the Discrete Element Method (DEM)

Sudeshna Roy[1], Thomas Weinhart[2]
[1] Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany [2] Department of Fluid and Thermal Engineering, University of Twente, The Netherlands

Additive Manufacturing (AM) techniques have revolutionized various industries by enabling the production of complex geometries with unprecedented precision. This minisymposium proposal aims to bring together researchers and experts to discuss the intricate interplay between powder spreading, the application of the Discrete Element Method (DEM), and the dynamic phase change phenomena in additive manufacturing. By exploring these key areas, we aim to foster a deeper understanding of AM processes and pave the way for advancements in process control, material quality, and part performance.

Topics that could be covered during the mini-symposium include, but are not limited to:

- Powder Spreading and material structure
- Phase change dynamics in Additive Manufacturing
- Advanced Simulation Techniques in Additive Manufacturing
- Advanced Process Control and Optimization

Invited speakers:

Yuan Tan, Chair of Process Systems Engineering, Technical University of Munich, Germany
Juan Alvarez Naranjo, University of Twente, Enschede, The Netherlands
Dominic Soldner, LTM, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

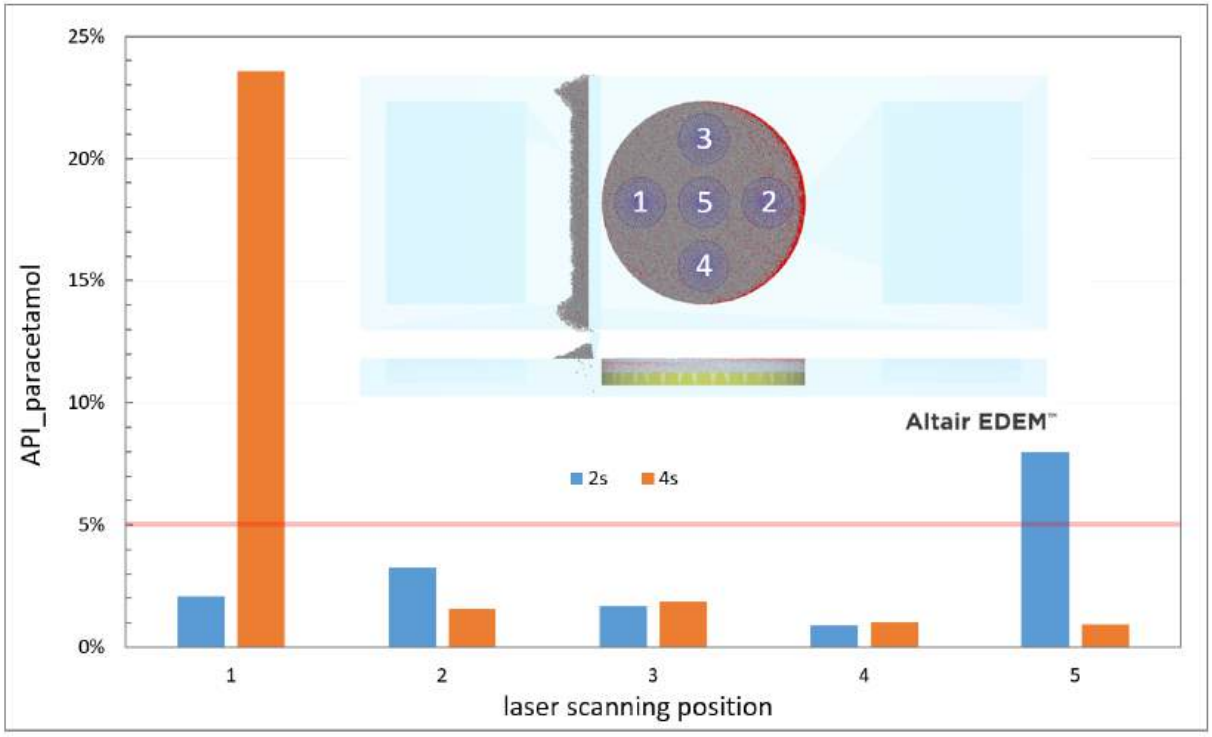
DEM simulation-based study on segregation mechanisms of the powder layer in the selective laser sintering of drug-loaded tablets

Yuan Tan, Daniel Schiochet Nasato, Heiko Briesen

Chair of Process Systems Engineering, Technical University of Munich, Germany (yuan.tan@tum.de)

Keywords DEM, selective laser sintering, drug-loaded tablet, powder spreading, powder segregation

Homogeneous mixing of multi-size and cohesive powders is a major challenge in the additive manufacturing of drug-loaded tablets using selective laser sintering (SLS). Considering the predominant but tiny proportions of active pharmaceutical ingredient (API) in a matrix of much larger constituents in tablets, e.g. drugs containing 5% paracetamol and the rest being matrix material, the consequence of particle segregation can be severe. According to the European Pharmacopoeia, the variance of paracetamol must be within ±1% of the labelled amount. In addition, the inhomogeneity of the powder mixture can be exacerbated after each layer of powder is applied in the special manufacturing process using SLS. However, this phenomenon has not been systematically investigated. The Discrete Element Method (DEM) is used to describe the behaviour of pharmaceutical powders in order to understand the mechanistic details of powder spreading during the preparation phase of SLS. The particle parameters of three pharmaceutical formulations (paracetamol in Kollicoat® IR, PEG and ethyl cellulose) used in the DEM simulation were calibrated using the lifting cylinder test and the shear cell test with a rheometer. The effect of process parameters (spreading direction, spreading speed, layer thickness and layer amount) and particle model properties on the uneven API distribution is quantitatively demonstrated and explained with mechanistic details of powder flow during spreading. The deviations of API concentration in the simulation are up to 10% for different laser scanning positions, in some cases even more than 25%. This study demonstrates that the use of SLS for pharmaceutical development to enable the production of personalised 3D printed drugs on demand requires additional attention to API segregation during powder preparation.



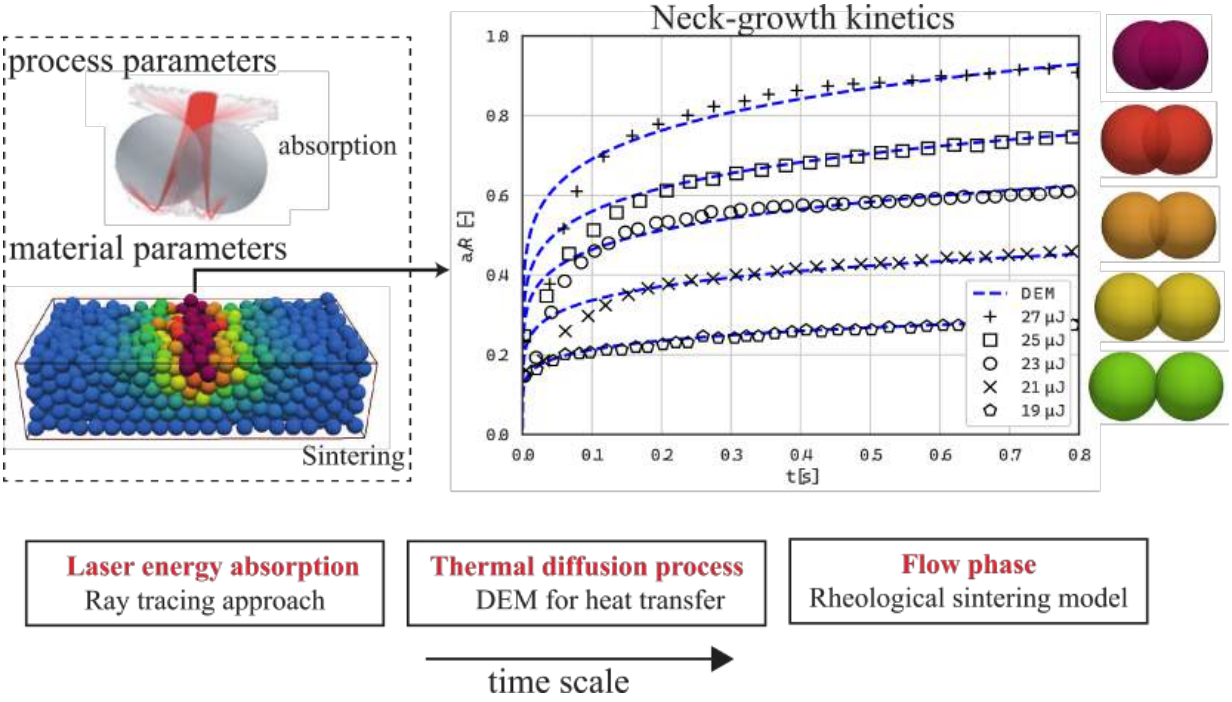
Contact rheology model for visco-elastic powders during laser sintering

Juan E. Alvarez[1], Hongyang Cheng[1,2], Stefan Luding[1], Thomas Weinhart[1]

[1] Multi-scale Mechanics, Faculty of Engineering Technology, MESA+, University of Twente, The Netherlands.; [2] Department of Civil Engineering and Management, Faculty of Engineering Technology, University of Twente, The Netherlands. (j.e.alvareznaranjo@utwente.nl)

Keywords Contact rheology, Laser energy absorption, Multi-physics discrete element method, Sintering, Visco-elastic powders

Laser sintering is a widely used process for producing complex shapes from sintered layers with desirable levels of shrinkage. However, understanding the complex interaction between the laser and the particulate bed is a challenge. This investigation provides new insights into the process by simulating the neck growth and the contact rheology of particle pairs as a function of the laser energy. To achieve this, a multi-physics discrete element method (DEM) framework is developed, encompassing temperature-dependent contact rheological and thermal properties. Moreover, energy transport is implemented using a ray tracing model to calculate laser-irradiated energy absorption. The DEM model is calibrated and validated with experimental data on neck growth and temperature evolution of laser-sintered particle pairs (PS and PA12). The results show that the neck growth and the contact rheology during laser sintering are strongly influenced by the temperature-dependent viscoelastic behaviour of the system, demonstrating the potential applicability of the proposed framework to different cases. As a practical application, the calibrated model predicts the shrinkage of laser-irradiated zones in thin polymer layers. It paves the way for additive manufacturing advancements, as the model accounts for the contact rheology of powders.



Continuum Based Simulation for Additive Manufacturing

Dominic Soldner, Ludwig Herrnböck, Christian Burkhardt, Julia Mergheim, Paul Steinmann

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Keywords Process Simulation, Additive Manufacturing, Homogenization, Thermo-Mechanics

Originating from the area of rapid prototyping, additive manufacturing (AM) has developed to a manufacturing process which is nowadays also used in serial production. The reason for the success of this technology lays in the design freedom of the manufactured parts, the increasing manufacturing accuracy and the possibility of using a vast range of materials. Yet, expensive experimental investigations are usually necessary during the product development, calling for numerical tools to reduce the associated cost. This contribution presents the activities of the Institute of Applied Mechanics at the Friedrich-Alexander-Universität Erlangen-Nürnberg within the Collaborative Research Center 814 – Additive Manufacturing.

The prediction of mechanical properties, as well as geometric accuracy of additively manufactured parts using process simulation represents a major task, since they affect the use- and durability of the produced parts. This calls for investigations on multiple scales using various modeling techniques. This includes continuum based process simulation for the prediction of the thermal field, residual stresses and distortion, as well as investigations of lattice structures accounting for the obtained grain structure using geometrically exact beams and homogenization techniques. Due to the typically high computational demand of detailed process simulation, different physical model reduction techniques and their limitations are demonstrated. In addition, potential links to incorporate DEM-based results in future work are discussed.

Mini-symposium: The applications and algorithms of coupled MPM-DEM

Wen-Jie Xu[1], Jidong Zhao[2], Chuanqi Liu[3]
[1] Institute of Geotechnical Engineering, Department of Hydraulic Engineering, Tsinghua University, Beijing, China
[2] The Hong Kong University of Science and Technology, Hong Kong S.A.R., China
[3] Institute of Mechanics, Chinese Academy of Sciences, Beijing, China

Most of the processes and phenomena in nature and industry (e.g., fluidized beds, marine engineering, geological hazards, etc) involve complex Multi-phase, Multi-process and Multi-scale problems (“3M”). In recent years, with the rapid development of numerical methods and computer hardware, more and more researchers have taken advantage of DEM itself to develop the coupling algorithms with other numerical methods (e.g., FEM, MPM, SPH and LBM, etc.). So that we can better carry out the studies and analysis of these complex processes from the physical and mechanical mechanisms of their “3M” than only one numerical method.

This mini-symposium focuses on the developing coupled MPM-DEM algorithm as well as their application in industry or natural field. The objectives of the presentation include but not limited to:

- Development of the coupled DEM algorithms with MPM and so on.
- The parallel technologies for the algorithms, such as MPI, GPU and so on.
- Case study using the coupled MPM-DEM algorithms, such as the application in the industry fields and natural hazards (landslide, tsunami, debris flow and so on).

Invited speakers:

Yihao Shi, Zhejiang University, China
Sergio Andres Galindo Torres, Westlake University, China

Implementation of coupled material point-discrete element method (MPDEM) in Taichi parallel programing language

Yihao Shi

Zhejiang University, People's Republic of China (shiyh@zju.edu.cn)

Keywords Taichi, Material point method, Discrete element method, High-performance programming, parallel computing

The material point method (MPM) [1] and discrete element method (DEM) [2] are two popular numerical methods in geotechnical engineering in recent decades due to their effectiveness in simulating large deformation problems. In light of their high computational cost, a way to improve the computational efficiency is urgently needed. In the study, an object-oriented numerical simulator based on the coupled material point-discrete element method (MPDEM) and implemented in Taichi language [3] is first proposed for geomechanics applications. Taichi is an open-source package embedded in Python that has been designed to facilitate high-performance and parallel computing on GPUs with enhanced productivity and portability. Both the DEM and MPM components are implemented on GPU and concurrently solved via contact forces exchanging between the two methods. Contrast to existing contact schemes in the literature [4-5], a hybrid point-to-point and point-to-surface contact method is introduced to achieve the trade-off between the efficiency and accuracy of MPDEM. Serval typical benchmark tests are simulated to validate the versatility of the simulator, including column collapse, particle sliding and particle impacting on a granular bed. DEM tests with different particle numbers are conducted and compared with an open-source code based on hybrid CPU-GPU, demonstrating a speedup of approximately 1.7.

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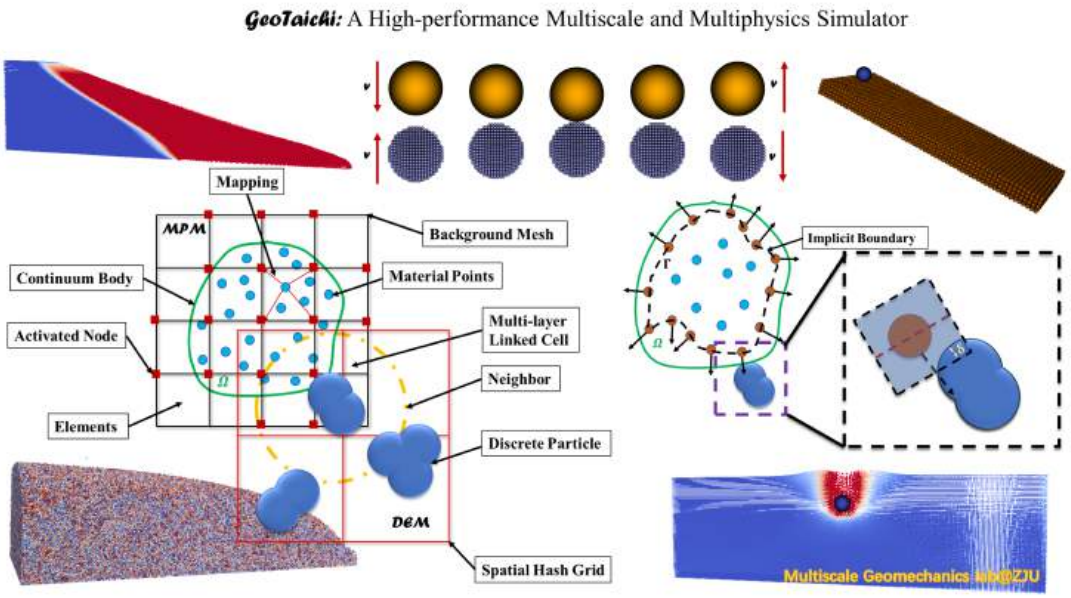

Recent advances in the coupling of discrete element methods with meshless partial differential equation solvers

Sergio Andres Galindo Torres

Westlake University, People's Republic of China (s.torres@westlake.edu.cn)

Keywords Material Point Method, Discrete Element Method, Geological hazard simulation

In this talk, we will introduce some of the recent advances that the Multi-scale Multi-physics Modelling (M3) laboratory at Westlake University has achieved in coupling discrete element modeling (DEM) approaches with meshless solvers such as the Material Point Method (MPM)(Ren et al., 2022) and the Smooth Particle Hydrodynamics method (SPH)(Trujillo-Vela et al., 2020). Firstly, the physics of the coupling will be explained, where we choose to consider the integration nodes as particles with mass. With this assumption, we can simulate the coupling as the interaction between two particles, the DEM and the meshless integration node. We will explain how to impose nonpenetrating conditions and the shear forces in situations where the meshless solver represents either liquids or solids. We will explain how to adapt these approaches for two DEM shape descriptors: the Spheropolyhedron (SDEM) for polyhedral particles(Ren et al., 2023); and the Metaball (MDEM) which can represent realistic grain shapes coming from CT-scan data(YifengZhao et al., 2023). Finally, we will show applications of these methods in critical hazard prevention areas such as debris flow and tsunami modeling.

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Mini-symposium: DEM-based hybrid algorithms for particle-laden flows

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The discrete element method (DEM) has become a popular choice to model processes involving granular materials and particulate systems, providing detailed information about the motion, forces, and interactions among individual particles with arbitrary shapes (e.g. spheres, rods, ellipsoids) and specific physical properties (e.g. charge, surface roughness). In DEM simulations, contact models are essential in describing the interactions (e.g. friction, adhesion, elastic) between particles and between particles and surfaces. In particle-laden flows, DEM is coupled to fluid solvers like the lattice Boltzmann method (LBM), smoothed particle hydrodynamics (SPH), finite volume method (FVM), and direct numerical simulation DNS, to name a few. Furthermore, DEM can be coupled with external fields such as electric and magnetic fields to simulate various complex physics problems involving multiscale, multi-component, and many-body interactions such as electrophoresis, reactive flows, turbulence, multiphase flow, particle transport, inkjet printing, and artificial microswimmers.

This mini-symposium discusses DEM-based approaches for modelling particle-laden flows, emphasising the technical and computational challenges related to industrial and academic scale applications.

The topics of interest of this mini-symposium may include, but are not limited to:

- Hybrid approaches combining DEM with external fields.
- DEM application in renewable energies.
- Porting DEM-based codes to next-generation supercomputing architectures.

Invited speakers:

Qingguang Xie, Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Germany

Gaurav Nath, [1] Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Germany [2] Mechanical Engineering Department, Indian Institute of Technology Delhi, New Delhi, India

Jens Harting, [1] Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Germany [2] Department of Chemical and Biological Engineering and Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Hongyang Cheng, Faculty of Engineering Technology, University of Twente, The Netherlands

Simulations of magnetic anisotropic particles at fluid-fluid interfaces

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Keywords Anisotropic particle, liquid interface, magnetic field, discrete element method, lattice Boltzmann method

Hybrid computational frameworks provide a viable method for numerical simulations of complex fluid comprising multi-component, fluid-solid interaction and external fields. We develop a hybrid approach combining the discrete element, and the lattice Boltzmann (LB) methods to investigate the dynamics of magnetic anisotropic (e.g. ellipsoid, Janus) particles at flat and curved fluid-fluid interfaces interacting with external fields. We apply the Shan-Chen pseudopotential multicomponent LB method for multicomponent fluids. The particles are discretized on the lattice and strongly coupled to fluid species by a bounce-back boundary condition. The orientation of anisotropic particles is specified with quaternions and a lubrication force correction is applied when particles are in close contact. Our in-house code is highly parallelized with MPI and shows good strong scaling with thousands of cores. We apply our methods to investigate the behaviour of magnetic spherical and ellipsoidal Janus particles adsorbed at a fluid-fluid interface interacting with an external magnetic field. The anisotropic particles deform the interface, and generate capillary interactions, and arrange into reconfigurable chain-, hexagonal-lattice-, and ring-like structures, which can be actively controlled by varying the external magnetic field. We develop interface energy models to reveal the underlying mechanism and find good quantitative agreement with simulation results.

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Self-assembly of Amphiphilic Janus Spheres: Lattice Boltzmann-Discrete Element simulations for Soft Matter

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Keywords Fluid-particle coupling, Janus particle, self-assembly

The viability of a coupled DEM-lattice Boltzmann method (DEM-LBM) for soft matter applications is demonstrated. The self-assembly of amphiphilic Janus spheres is achieved in bulk and confined arrangements incorporating full 4-way coupling for the dispersed particles and fluctuating hydrodynamics for the continuous phase. Fluid-particle coupling is done via the native momentum exchange method. The anisotropic interactions between Janus particles are incorporated via a pair potential borrowed from a molecular dynamics (MD) study [1]. Janus particle clusters formed are identified via a distance-based clustering algorithm. Subsequently, the relevant cluster properties like size distribution, mean cluster size and cluster shapes are examined. LBM results show good agreement with corresponding MD results [1,2]. However, the current approach is found to be computationally expensive in the low Reynolds number regime (< 0.1), taking substantial time to reach equilibrium. Nevertheless, the current LBM framework is valid for soft matter problems and can be extended to study problems like active particles.

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Capillary interactions, aggregate formation, and the rheology of particle-laden flows with a hybrid discrete element and lattice Boltzmann method

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Keywords Capillary, aggregate, rheology

The agglomeration of particles caused by the formation of capillary bridges has a decisive impact on the transport properties of a variety of at a first sight very different systems such as capillary suspensions, fluidized beds in chemical reactors, or even sandcastles. Here, we study the connection between the microstructure of the agglomerates and the rheology of fluidized suspensions using a coupled lattice Boltzmann and discrete element method approach. We benchmark a number of effective models to describe the capillary bridges between particles [1] and then address the influence of the shear rate, the secondary fluid surface tension, and the suspending liquid viscosity [2]. The presence of capillary interactions promotes the formation of either filaments or globular clusters, leading to an increased suspension viscosity. Unexpectedly, filaments have the opposite effect on the viscosity as compared to globular clusters, decreasing the suspension viscosity at larger capillary interaction strengths. In addition, we show that the suspending fluid viscosity also has a nontrivial influence on the effective viscosity of the suspension, a fact usually not taken into account by empirical models.

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Wave Propagation in Fluid-Saturated Granular Media using Coupled Lattice Boltzmann-Discrete Element Method

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Keywords Wave propagation, Lattice Boltzmann method, Discrete element method, Fluid-solid coupling, Acoustic source, Biot's theory

Poroelasticity theory predicts wave speeds in saturated porous media by linking solid skeleton deformation with fluid flow. This connection is crucial, particularly at smaller wavelengths where interactions between grains and fluid gain prominence. This study explores how compressional and shear wave speeds depend on pressure and volume fraction in fluid-saturated, random, isotropic, frictional granular materials. To capture particle-fluid interactions, we couple the lattice Boltzmann and discrete element methods. We introduce an acoustic source to generate traveling waves within the saturated medium. By analyzing wave speeds in the wavenumber-frequency space across various pressures and volume fractions, we uncover frequency and wavelength dependencies. Strikingly, in random isotropic granular media, pressure-wave velocity data collapse onto a single curve when properly scaled by volume fraction.

Mini-symposium: Advances in open-source DEM software

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[2] Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

As problems get more and more complicated it is becoming increasingly difficult for PhD students to make progress by developing their own codes from scratch. Therefore, more and more we have to build on the previous generation of work, not only in terms of ideas but also with respect to software. This means going forward, large multi-developer open-source packages will become essential tools to remain at the forefront of the field.

There are many open-source codes for simulating particles, all with their own unique features. This session will serve the dual purpose of bringing together the developers of different open-source codes and also be a one-stop shop for potential new users.

Topics that could be covered during the minisymposium include, but are not limited to:

- Overview of open-source DEM software.
- Advancements in modelling complex granular systems.
- Validation and verification of open-source DEM software.
- Open-source software for DEM-based simulation of industrial processes.

Invited speakers:

Remy Mozul, LMGC (UM-CNRS), France
Anthony Thornton, University of Twente, The Netherlands
Bruno Chareyre, Université Grenoble Alpes, CNRS, Grenoble INP, 3SR, Grenoble, France

LMGC90 : a Python Framework to simulate non smooth mechanical discrete systems

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Keywords NSCD, Non-Smooth, Multi-Physics

LMGC90 is an open-source software dedicated to the mechanical modeling of collections of interacting objects with multiple physics coupling. This software was first designed to gather the knowledge and developments made by J.J. Moreau and M. Jean around the use of the Non Smooth Contact Dynamics (NSCD) method. It allows the modeling of rigid or deformable mechanical bodies in 2D and 3D. The software manages a wide range of shapes for the contact detection and allows to mix as complex as necessary interaction laws (from frictional contact with inelastic shock to cohesive zone models). Furthermore physics couplings (thermal effects, porous, fluids, etc) are progressively taken into account either through strong or weak coupling. LMGC90's modular data model and architecture was made so that it ensures robustness while allowing to add new features. The core of the software is written in Fortran90 to provide computational efficiency while the API is written in Python to make the processing and pre/post-processing steps easer, since these steps are strongly user-depend. Furthermore since there are a lot of accessor on the internal database, it also makes it easier to do weak coupling with any other software. There are entry points within the core of the software to allow to use external libraries for contact detection, material behavior computations or even finite element library. The software may address a wide range of applications, the recent uses are in the domain of railway (ballast) simulation, asteroid (self-gravity accretions), architectural masonry structure (Notre-Dame de Paris restoration work-group) and concrete's fracture under multi-physics loading (chemo/thermal loading for containment building of nuclear power plant). As a research software it is meant to help mainly researchers or advanced users within an R&D teams of industrial actors.

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MercuryDPM: Fast, flexible, particle simulations

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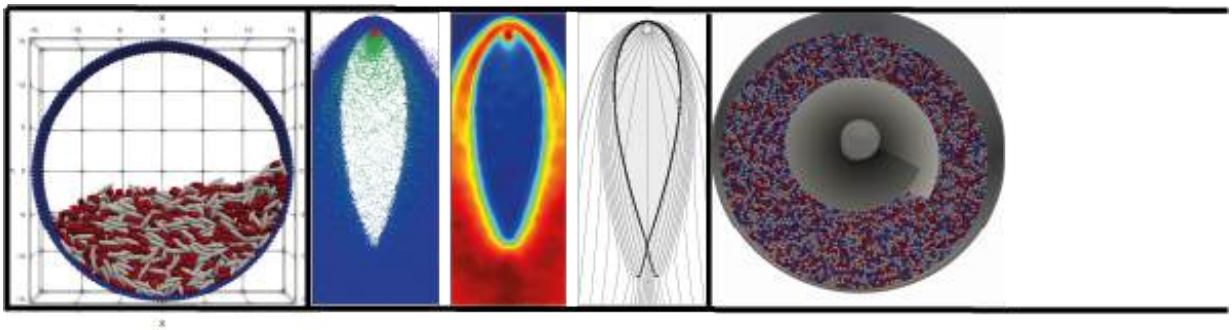
Keywords DEM Open-source Particle Simulations

MercuryDPM is an object-oriented C++ algorithm parallelised using both MPI and OpenMP for simulating particulate systems. Its developers' community has created many features, including moving, wearable, curved walls (polygons, cone sections, helices, screw threads, level-sets, nurbs, triangulated, etc); non-spherical particles (multisphere, superquadric, bonded particles, deformable clusters); state-of-the-art granular contact models (wet, charged, sintered, melting, cohesive, etc); specialised classes for common geometries (inclined planes/chutes, hoppers, etc); general interfaces (particles/walls/boundaries can all be changed with the same set of commands); liquid droplet/spray models; STL readers for industrial geometries; restarting; visualisation (xBalls and Paraview); a large self-test suite; extensive Doxygen documentation; and numerous tutorials and demos.

For efficiency, it uses an advanced contact detection method, the hierarchical grid. This algorithm has a lower complexity than the traditional linked-list algorithm for polydispersed scenarios, which allows large simulations with wide size distributions. It also contains the coarse-graining tool MercuryCG. Coarse-graining is a novel way to extract continuum fields from discrete particle systems. It ensures by definition that the resulting continuum fields conserve mass, momentum and energy, a crucial requirement for accurate coupling with continuum models. The approach is flexible and the latest version can be applied to both bulk and mixtures; boundaries and interfaces; time-dependent, steady and static situations; even experimental data. It is available in MercuryDPM either as a post-processing tool or it can be run in real-time, e.g. to define pressure-controlled walls.

Finally, MercuryDPM is coupled with the open-source FEM solver oomph-lib via the integrated coarse-graining tool. There are many uses of this coupling (in development), including interaction with elastic bodies, both fully and unresolved fluids, and multiscale coupling. We will demonstrate the features of the code via several examples including: (wet) highly-polydisperse mixing in a rotating drum, wear on vibrating sieves, and sack filling.



YADE - An open-source framework for open-science

Bruno Chareyre[1], Vasileios Angelidakis[2], Katia Boschi[3], Karol Brzeziński[4], Robert A. Caulk[1], Carlos Andrés del Valle[5], Jérôme Duriez[6], Anton Gladky[7], Janek Kozicki[8], Gerald Pekmezi[9], Luc Sholtès[10], Klaus Thoeni[11]

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Keywords DEM, open source, open science

When the development of Yade-DEM (Šmilauer et al., 2021) started, almost twenty years ago, making it open-source was a primary objective. It is used nowadays for classical DEM simulations as well as particle-fluid coupling, thermo–hydro-mechanical coupling, interaction with deformable membrane-like structures, cylinders and grids, FEM-coupling, non-spherical particles, deformable particles, and other brittle material simulations. It counts a large, active, and growing community of users and developers. The computationally-intense parts of the source code are written in C++, using flexible object models which allow for easy implementation of new features. A command line interface using Python enables rapid and concise scene construction, simulation control, post-processing, and debugging. A graphical user interface with 3D rendering makes simple basic manipulations, exploring variables, and live visualization even simpler. The software is available as a pre-compiled package for Debian and Ubuntu. It appears that the initial decision of developing under an open-source license was key to a sustained development. Understanding the tools and methods that were used is of interest for every development project in science, and it paves the way to "Open" science.

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Mini-symposium: The future of open-source DEM — Discussion

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Open-source software packages have exhibited rapid growth in recent years. The open availability and transparency of implementation make open-source software appealing to the various communities interested to use them directly or to develop new features on top of well-established and well-verified code. The process of developing open-source software can have many forms, as it can be a voluntary contribution to the scientific community, part of a thesis or other student project, a side hobby, or a full-time job. In the granular world, the developers' teams of open-source codes applying the Discrete Element Method (DEM) have many different sizes and shapes, with some of them organised centrally, some being completely de-centralised, or some even being a two-person job. With this diversity of roles, organisational schemes, expertise and priorities, creating links among different developers' communities is essential in improving the overall quality and usability of open-source software, and dispelling stereotypes about their accuracy and trust-worthiness, via creating mechanisms such as formal or informal cross-code sanity-checks, benchmarking, code peer-review, sharing of good and bad experiences and practices, or direct exchange of technical knowledge. In this mini-symposium discussion session, we will review recent efforts of the open-source DEM community to work together on grants and scientific papers and discuss opportunities for further collaboration.

Invited speakers:

Daniel Barreto, Edinburgh Napier University, United Kingdom

Open Network on DEM simulation

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Keywords Open-source DEM, research network

Considerable progress has been recently made with regards to DEM simulations. There are, however, challenges associated to computational expense, as well as the accuracy, and realism to simulate large (real) scale problems. Using periodic boundary conditions, homogenisation, density scaling, time extrapolation, various computer architectures, modelling of complex particle shapes, and development of (more) realistic contact models, as well as the use of optimisation, inference, Artificial Intelligence (AI) algorithms or surrogate modelling, amongst other approaches have been also suggested to tackle these challenges. However, most of these advances have been developed in discipline "silos" and across different DEM codes.

A large group of DEM researchers across multiple disciplines have recently obtained funding from COST to create a research network to tackle these challenges and unify existing knowledge. The network promotes the use of open-source DEM software.

The ambition is that by tackling the challenges discussed, the network will set the foundation for solving the next generation of problems across disciplines, and set standards and strategies for the future of DEM modelling. The network will be managed by dividing the required the work in the working groups described below:

1. "Passing through time and space scales" for tackling real, and large-scale problems.
2. "Getting closer to physics" to consider more complex phenomena by validating, calibrating, and developing existing/new contact models.
3. "Processing big data and visualization" to better analyse and post-process DEM results.
4. "Working with industry" for widening commercial utilisation of open-source DEM codes.
5. "Disseminating best practices" to promote interoperability and enforce robustness of results.

Currently the research network includes more than sixty participants including academia, industry, and diverse DEM users' groups. It is hoped that this presentation will encourage discussion on the challenges described and increase the network's capability and reach by increasing its membership.

Mini-symposium: DEM for understanding complex flows in gas-particle systems

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[1] Institute of Process Engineering, Chinese Academy of Sciences, Beijing, China
[2] Beijing Institute of Technology, Beijing, China

This symposium aims to bring together leading academic scientists, researchers and research scholars to exchange and share their experiences and research results on all aspects of complex flows in gas-particle systems using DEM related novel computational methods. It also provides a premier interdisciplinary platform for researchers, practitioners, and educators to present and discuss the most recent innovations, trends, and concerns as well as practical challenges encountered and solutions adopted in the fields of gas-particle systems.

- Fully Resolved Computational Methods: FV-DEM, FE-DEM, LBM-DEM, SPH-DEM, etc.
- Unresolved Computational Methods: CFD-DEM, LBM-DEM, MP-PIC, etc.
- Conceptual, Constructive, Empirical, Experimental, or Theoretical Work on Gas-Particle Systems.
- Engineering and Industrial Applications Involving Gas-Particle Flows.

Invited speakers:

Fengxian Fan, University of Shanghai for Science and Technology, China
Chuan-Yu Wu, University of Surrey, United Kingdom
E Dianyu Jiangxi University of Science and Technology, Nanchang, China
Xinxin Tang, UNSW, Sydney, Australia
Ruifeng Hu, Lanzhou University, Lanzhou, China
Kimiaki Washino, Osaka University, Osaka, Japan
Kaiwei Chu, Shandong University, Jinan, China
Yongzhi Zhao, Zhejiang University, Hangzhou, China
Kun Xue, Beijing Institute of Technology, China

Scaling laws on granular capillarity dynamics

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Keywords Granular capillarity, Discrete Element Method (DEM), Phase diagram, Scaling law

When a narrow tube inserted into a static container filled with particles is subjected to vertical vibration, the particles rise in the tube. This phenomenon is termed as granular capillarity, because of its resembling the capillary effect of liquid. As the granular capillarity is driven by the convective motion of the particles in the container induced by the vibrating tube, the dynamics of granular capillarity may be affected the behavior of granular convection. Here we numerically investigated the granular capillarity dynamics using the particle-based Discrete Element Method (DEM). The phase diagram of the granular capillarity is shown in the frequency-amplitude plane. The scaling forms of the dynamics of particles in the phenomena of granular capillarity in terms of steady-state capillarity height , average ascending rate, and convection velocity with the sliding friction coefficient between the tube wall and the particles, the sliding friction coefficient between the container wall and the particles, as well as the container width to particle diameter ratio are explored.

DEM Analysis of Volumetric Expansion of Granular Materials Based on a Microscopic Diffusion Model

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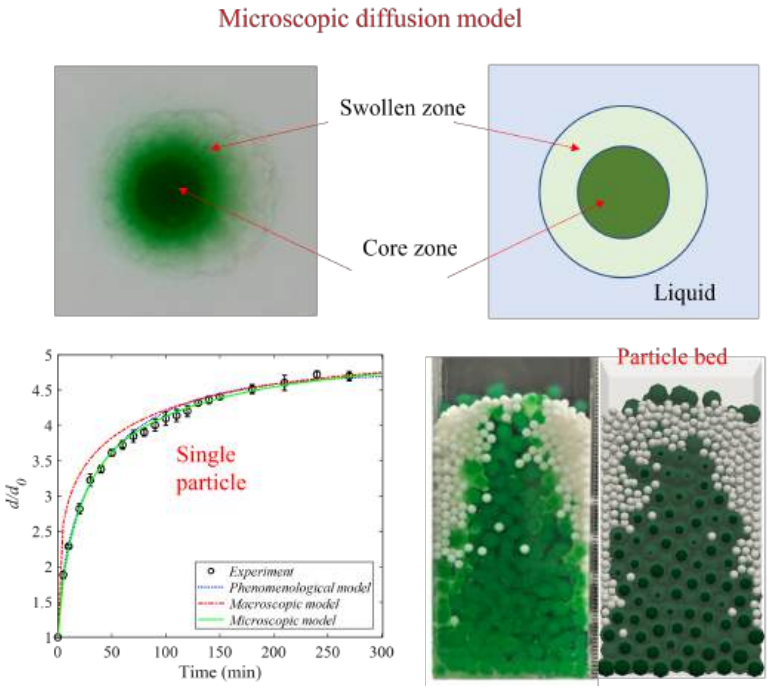
Keywords Particle Swelling, Expansion, Diffusion, Discrete element method, Particle shrinkage

Volumetric expansion or swelling is a prevalent phenomenon in many processes of granular materials. For example, in the Lithium battery, electrode particles will undergo large volume expansions due to Li-ion diffusion during discharging processes, which results in cracks within the battery and finally lead to battery capacity loss (1). For the pharmaceutical tablet, swelling of excipients particles affects the performance of the disintegration of tablets in the patient's body and the efficiency of the oral delivery of drugs (2). Aiming to rigorously model these deformable particles, a microscopic model that considers the microstructural evolution during diffusion is developed for the first time and implemented into the discrete element method (DEM). The robustness of this model is evaluated by comparing its performance with a macroscopic diffusion-induced swelling model and a phenomenological swelling model. The swelling behaviours of a single particle and a particle bed in a rectangular container in water are then investigated experimentally, as well as numerically using the developed models. It is shown that the microscopic swelling model and the phenomenological swelling model can better describe single particle swelling than the macroscopic swelling model. Moreover, the microscopic swelling model can not only reproduce the phenomena of volume expansion of particles as well as but also well predict the microstructural evolution of individual particles, as observed experimentally. Furthermore, the microscopic swelling model is more accurate in predicting expansion of the particle beds. It is hence demonstrated that DEM with the microscopic swelling model, which captures the microscopic physical mechanisms of particle swelling and the microstructural change of swelling particles, could well describe the swelling behaviour of particle systems and could be a useful tool for modelling swellable granular materials in various industrial processes.



Studies on development of a multi-scale and multi-physics-coupled ironmaking blast furnace model and its inner thermochemical behaviors

E Dianyu

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Keywords Ironmaking blast furnace, Multi-scale multi-phase flow, Heat and mass transfer, Simulation and modelling, Process optimization

Ironmaking blast furnace (BF) process, proceeding under a high temperature and a high pressure, is largely operated as a "black box" due to its inner complicated multi-phase flow (gas, liquid, solid and powder etc.) and multi-physics-coupled (force field, temperature field, and chemical composition field). It has been realized that the mathematical model can be taken as an effective method to know, study and further guide practical BF operation based on the fact that the current practice largely depending on empirical experience. This study, based on advanced multi-scale-coupled CFD-DPS approach, aims to develop a multi-phase flow BF model by creatively overcoming various challenges in high-temperature process modeling. Generally, the studies are listed as follows: The present work firstly develops a multi-phase (gas, liquid and solid) and multi-scale-coupled mathematical BF model which considers heat and mass transfer in a solid particle, and then study the theoretical speedup mechanism for the multi-phase transition processes and investigate its inner thermochemical behaviors evolution periodically; Secondly, it will examine the void fraction variations and its related chain reactions due to solid particle shrinkage and degradation, stress change etc. in dry zone, and explore the relations between the cohesive zone profile variation and some key variables such as burden distribution and gas inlet condition, additionally investigate the interactions of gas, liquid and solid in dripping zone, and finally provide scientific support and theoretical basis for improving BF operation efficiency and decreasing energy consumption under some new operation conditions.

Modelling of gas-solid-liquid flow and particle mixing in a rotary drum

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Keywords Rotary drums, CFD-DEM, volume of fluid (VOF), active-passive interface, particle mixing, particle dispersion

Solid-liquid rotary drums have been widely practised in various industries, while the complex multiphase hydrodynamics hinders the understanding and optimisation of these processes. In this work, the computational fluid dynamics-discrete element method (CFD-DEM) coupled with a volume of fluid (VOF) is developed to describe the gas-solid-liquid flow and mixing behaviours in a rotary drum including inter-particle collisions, inter-phase interactions, and interface morphology. A smoothing method is used to link the quantities between the particle and computational grids, allowing the fine grids to resolve flow details such as the gas-liquid interface position and curvature. After model validations, the typical mixing behaviours of gas-solid-liquid flow in a rotary drum are studied. The effects of liquid presence and rotating speed on particle-scale behaviours (e.g., repose angle, active-passive zone depth, solid residence time and contact force chain) and the time-evolved mixing performances (e.g., mixing index and dispersion) are studied. The results show a positive correlation of the active depth, mixing degree, and particle dispersion with the rotating speed. The liquid presence leads to a deeper active depth, prolonged solid residence time in the active zone, and lower contact force. The work sheds light on the design and process optimization of rotary drums.

Coupling DEM with PRDNS: A multiple-time-step algorithm

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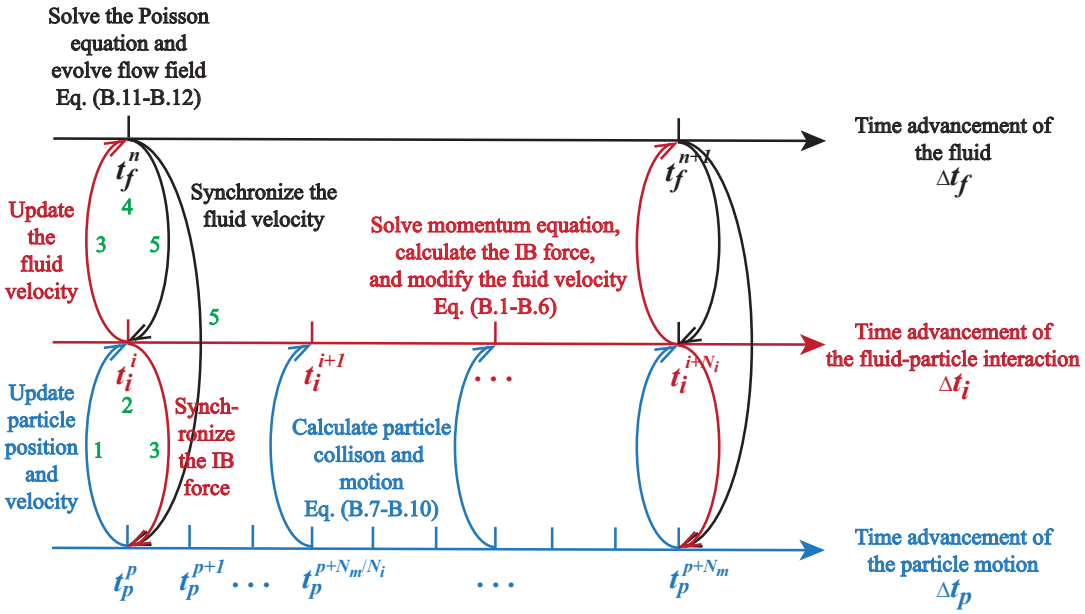
Keywords Particle-Resolved Simulation, Direct-Numerical Simulation, Discrete Element Method, Particle Collision Model

This contribution presents a multiple-time-step algorithm (MTSA) for coupling the discrete element method (DEM) with particle-resolved simulations (PRDNS). In practice, the time step required for resolving a collision process is much smaller than that for a fluid flow, thus the computational cost of the traditional soft-sphere model by reducing the time step is relatively high in particle-resolved simulations. Usually, the collision time is stretched to several times the flow solver time step to adapt to the sudden change in particle motion. However, the stretched collision time is not physical, the hydrodynamic force may be severely underestimated during a stretched collision, and the simulation results of gas-particle systems may be sensitive to the stretched collision time. The proposed MTSA adopts different time steps to resolve fluid flow, fluid–particle interaction, and particle collision. We assessed the MTSA for particle–wall collisions as well as particle–particle collisions, determined the optimal iteration number in the algorithm and obtained excellent agreements with experimental measurements and reference simulations. The computational cost of the MTSA can be reduced to about one order of magnitude less than that using the traditional soft-sphere model with almost the same accuracy. The MTSA was then implemented in a particle-resolved simulation of sediment transport with thousands of particles. By comparing the results obtained using the MTSA and a version of the stretching collision time algorithm (SCTA), we found that stretching the collision time reduced particle stiffness, weakened particle entrainment, and affected some turbulence and particle statistics.



Fully resolved CFD–DEM coupling model for gas-liquid-solid flows with non-spherical particles

Kimiaki Washino, Ei L. Chan, Giang T. Nguyen, Taichi Tsujimoto, Takuya Tsuji, Toshitsugu Tanaka

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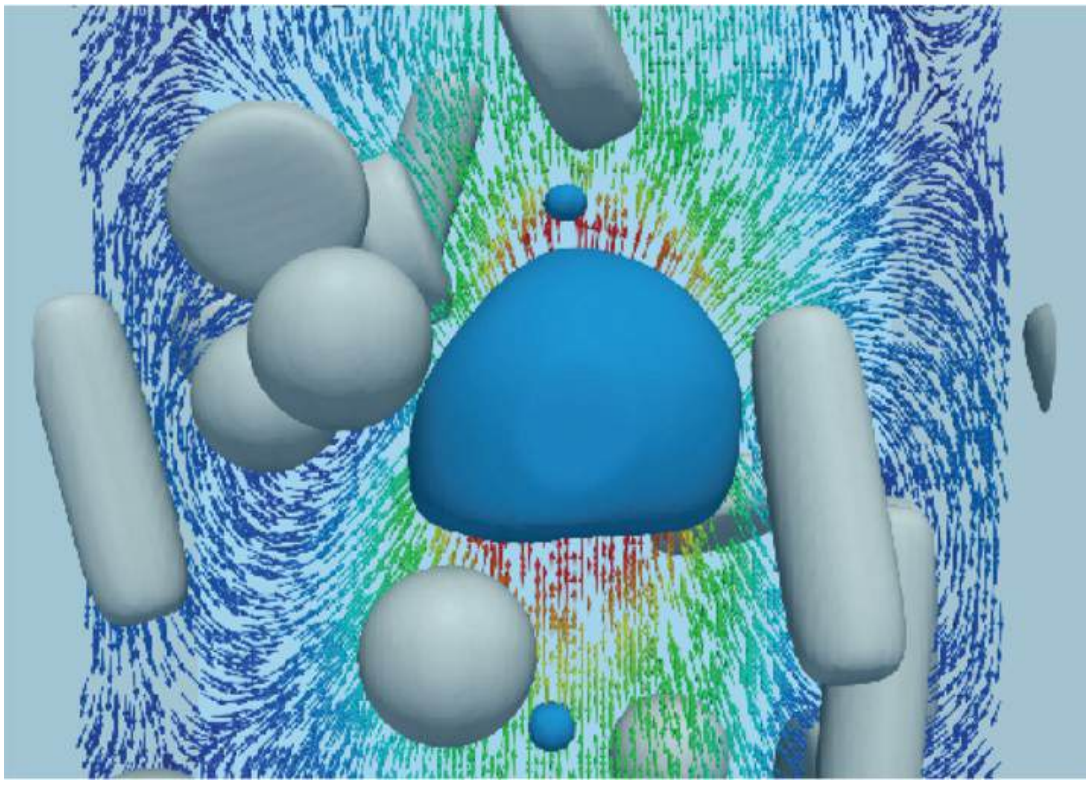
Keywords DEM, CFD, Resolved coupling, Non-spherical particles

In this work, a fully resolved CFD–DEM coupling model is developed to simulate gas-liquid-solid three-phase flows with non-spherical particles. The interface capturing method with a colour function is employed to distinguish the gas and liquid phases with a diffuse interface technique. The Volume Penalisation (VP) method is used to consider the hydrodynamic interactions between the fluid and particles where the permeability is optimally determined to eliminate the model error. The Immersed Free Surface (IFS) method, which artificially extends the gas-liquid interfaces into the interior of the particles while keeping the prescribed contact angle, is employed to take into account the wettability of the particle surface. Finally, the Continuous Capillary Force (CCF) model, that converts the surface tension (i.e., line force) into an equivalent body force, is employed to capture the capillary interactions. Both gas-liquid and fluid-solid interfaces are smoothly represented with a specified thickness so that the interface thicknesses and CFD cell size can be decoupled (i.e., independent of each other). Several test simulations, such as a flow through packed ellipsoids and liquid bridge between a pair of cubic particles, are performed to evaluate the accuracy of the model developed. Some demonstrative simulations are also performed to discuss the applicability of the proposed model to complex fluid-particle flows including a bubbly flow with various particle shapes. It is found that the particle shape can have a significant impact on the fluid-particle interactions and resultant particle movement.



CFD-DEM Study of Complex Particle-Fluid Systems including cohesive and bonded particles

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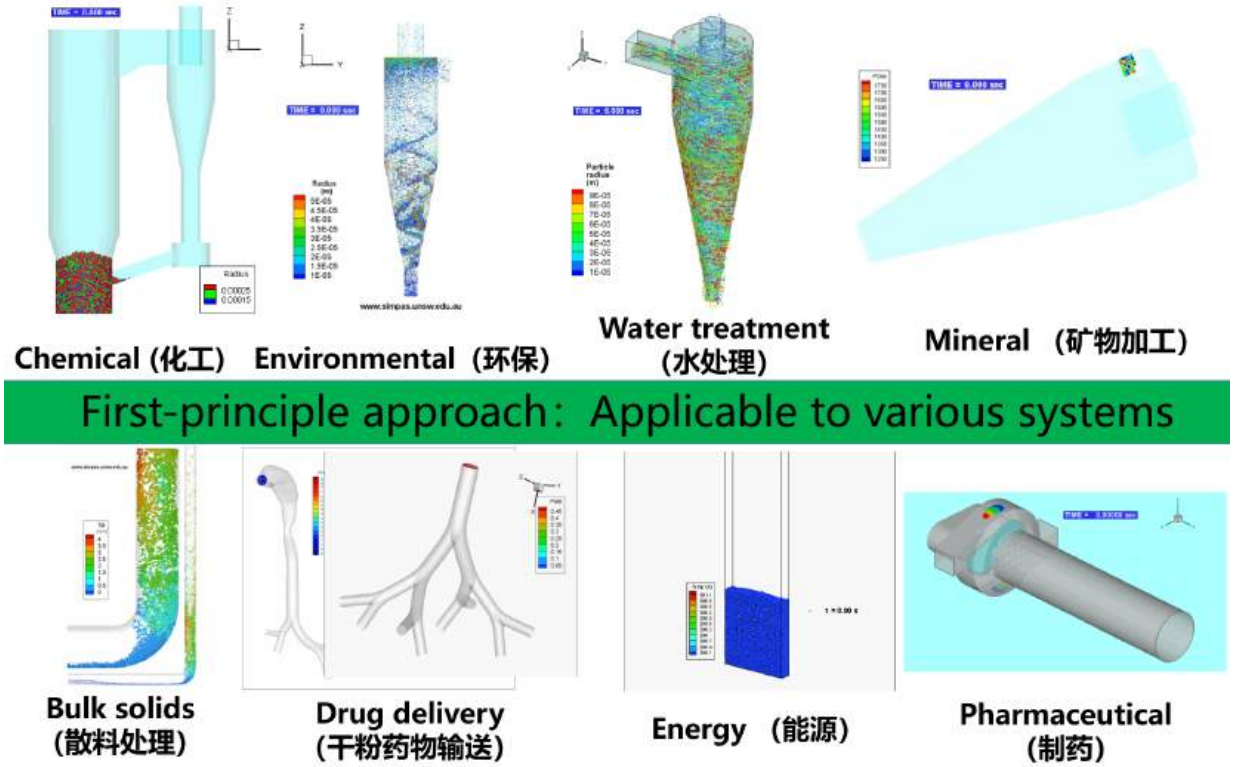
Keywords Particle-fluid system, Computational Fluid Dynamics, Discrete Element Method, coarse-grained, bonded particles

Complex particle-fluid system is ubiquitous in nature and industries, in which "kinematics of particles or granular materials" is one of the 125 most challenging scientific issues in the first quarter of 21th centry [Science, 2005]. Recently, it has been proved that a combined approach of Computational Fluid Dynamics and Discrete Element Method (DEM) (CFD-DEM) is an effective approach to study the fundamentals of particle-fluid systems. This work shows how a CFD-DEM model is developed and generally used to study various complex, three dimensional and large-scale particle-fluid systems. Especially, it shows how a coarse-grained (CG) CFD-DEM approach can be developed and used to significantly reduce the computaitonal cost of DEM simulations. The work includes model development, model validation, model study, data analysis, process innovation, and development of process simulator.



CFD-DEM modelling and simulation of particle-fluid systems containing non-spherical particles

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Keywords Non-spherical particle, Discrete element method, Computational Fluid Dynamics, CFD-DEM

The coupling between fluid and granular materials is commonly encountered in many industrial processes from chemical to energy, agriculture, mining, pharmacy and many other fields. And the shape of granular materials is normally non-spherical. Therefore, investigating the particle-fluid systems containing non-spherical particles for a deeper understanding of their underlying mechanisms and then for improving the performance of the related industrial processes is necessary. For investigating the intricate flow behaviors of particle-fluid systems, the numerical simulation method of coupling DEM (Discrete Element Method) with CFD (Computational Fluid Dynamics) has been widely recognized as a promising tool, and some efforts have been done to the CFD-DEM investigations of non-spherical particles in our laboratory. This talk will introduce the research progress of our laboratory on CFD-DEM investigations for non-spherical particles, including the discrete element modeling of non-spherical particles, the coupling methodologies between CFD and DEM and the use of the non-spherical CFD-DEM coupling model in some applications involving particle-fluid flows. In the end, the outlooks for future investigations of particle-fluid systems containing non-spherical particles by numerical method are given.

Particle jetting induced by the explosive dispersal

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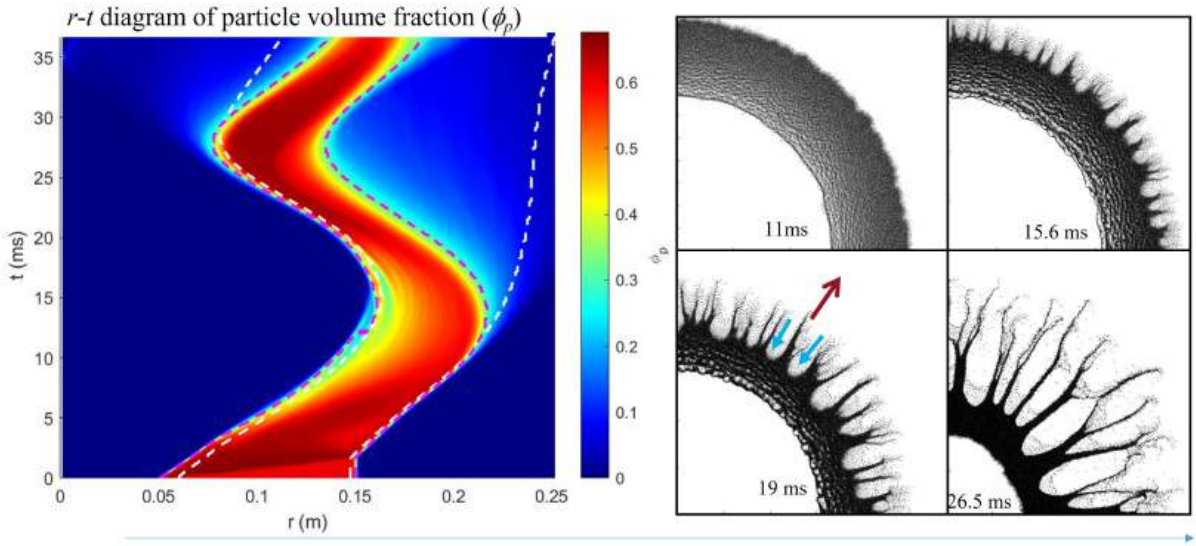
Keywords CCFD-DEM, Particle jetting, multi-scale structure, pattern, infiltration

Jetting structures are widely found in particle rings or shells dispersed by the central explosion. In contrast some explosive dispersal of particles only results in a dispersed cloud without distinctive structures. Employing the coupling method of the compressible computational fluid mechanics and discrete element method (CCFD-DEM), the numerical investigation reveals the underlying physics governing the formation of the jetting structure, which is related with the competition between the shock compaction and gas infiltration, two major processes during the shock interaction with the granular media. If the shock compaction exceeds the gas infiltration, the discernable jetting structures are expected, precipitated by the agglomerates of fast-moving particles induced by the heterogenous network of force chains. Otherwise, particles are uniformly accelerated by the interstitial flows, no distinguishable jetting structures formed. The phase map of the jetting formation is established in the space defined by two dimensionless parameters which characterize the timescales of the shock compaction and the gas infiltration, respectively.



Regular Sessions – Contributed Talks

Session: Granulate-structure interaction

Modeling of a laboratory cone crusher using the discrete element method

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Keywords Discrete element method, breakage, cone crusher, polyhedral particles

Crushers are machines used in the Chilean copper mining industry in the comminution stage. In secondary and tertiary crushing, cone crushers are the most common machines that work by squeezing the rock between a rotating head and a concave [1]. Knowing the operational parameters, particularly the crushing power, is fundamental for optimizing their performance and improving control systems [2]. This work aims to investigate the operation of cone crushers through numerical models and laboratory experiments. Regarding the numerical approach, a DEM model of a laboratory cone crusher is performed in Rocky DEM 2022 R1 using a hysteretic contact model, polyhedral particles, the Tavares breakage model, and the size distribution given by the incomplete beta function [3]. A complete parameter calibration is performed, calibrating focusing on particle shape, restitution coefficients, friction coefficients, modulus of elasticity, and specific parameters of the breakage model. Experimental data were obtained from a laboratory cone crusher, measuring torque, power, angular velocity, mass flow rate, and particle size distribution. These data are directly compared and discussed with the numerical ones, and the numerical DEM model is validated. The results demonstrate a good agreement between the experiments and help to understand the operation of this machine.

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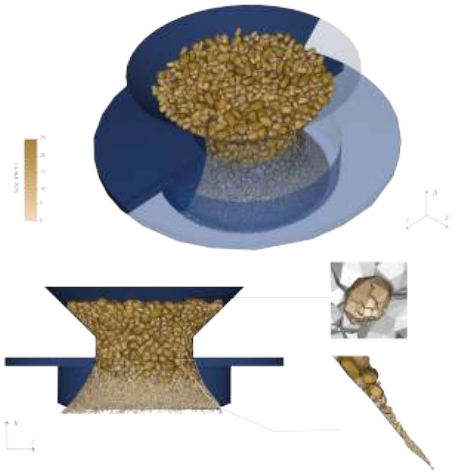

DEM modelling of object penetrating through granular media with different particle shapes

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Keywords Shape, Polyhedrons, Penetration Resistance, Rock

In light of carbon neutrality by 2050, the world's energy supply is moving from fossil-based towards clean and green energy sources, e.g., solar and wind. Due to limited space onshore, the offshore wind industry gains its popularity in the past decade and over 80% of offshore wind turbines have monopile foundations (Hageman, 2022). During the installation of these foundations, the monopiles have to penetrate through a few rock layers before they get fixed inside the seabed. However, the interactions between the monopile and rocks are poorly understood and the technical feasibility of monopile installation through scour protection layers has not been researched yet. This leads to difficulties during the driving/penetrating process, such as misalignment and rejection. Due to the discrete nature of the rock-rock and rock-monopile interactions, Discrete Element Method (DEM) appears promising to offer more insights into this complex process (Cerfontaine et al., 2021; Li et al., 2021).

DEM simulations are computationally expensive, spherical discs (2D) or particles (3D) are often preferred when selecting the shape of particles. However, using a perfectly spherical shape creates limitations in capturing the geometrical effect, such as interlocking between particles. It is thus preferable to model the particles using more realistic, non-spherical shapes, like clumps (multi-spheres) or polyhedrons (Coetzee, 2017). In addition, most previous studies are focusing on the penetration of the solid/close-ended objects through sand/soil layers formed by relatively small size particles, where the interlocking effect is less conspicuous. Therefore, in the current study, we shed light on two aspects: i) the eligibility of non-spherical DEM models capturing the particle interlocking behaviour; ii) the interaction between the open-ended pile and the large-size particles. Finally, the monopile driveability and the scour layer resistance will also be addressed.

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Numerical Simulations of the Penetration Process of Open-Ended Piles using DEM

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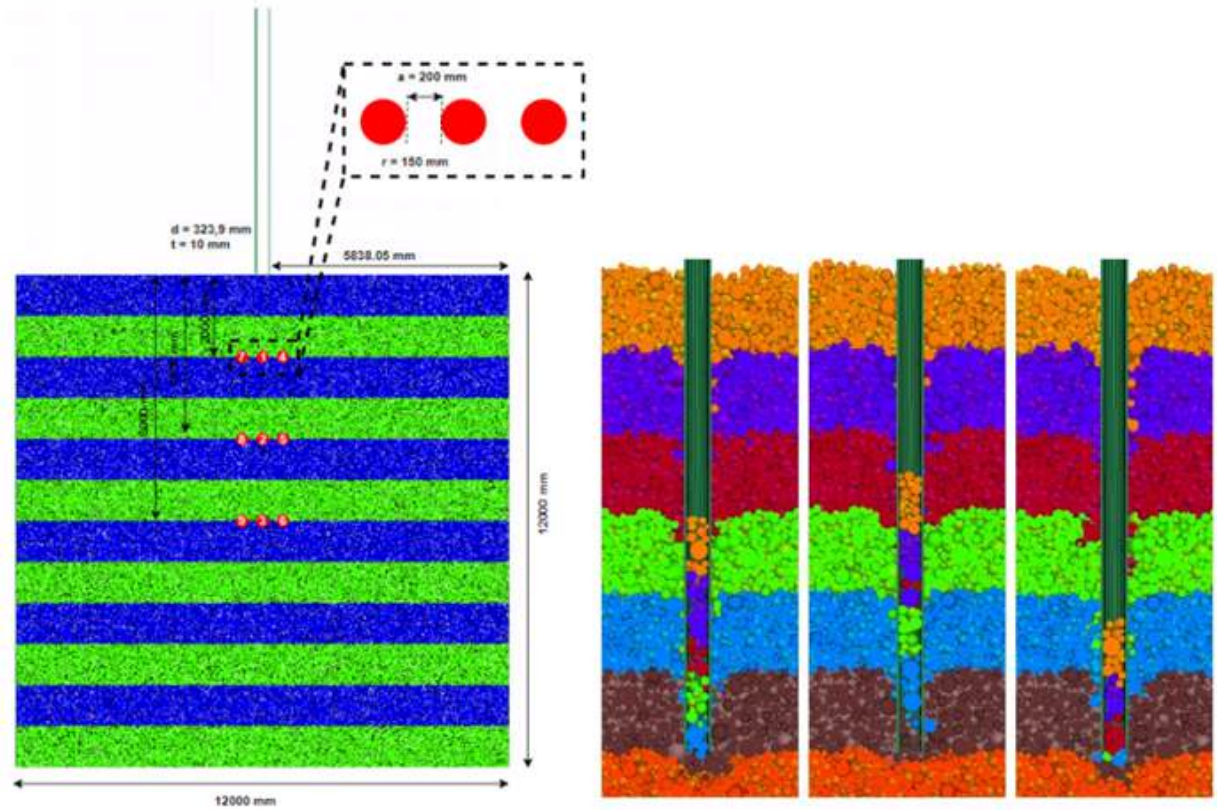
Keywords Pile plugging, Open-ended pile, DEM, Static load capacity

During the installation of open-pipe piles, soil enters the pile until an inner-soil- cylinder is formed which might develop sufficient resistance to prevent further soil intrusion and thus the pile becomes "plugged". This pile plugging phenomenon, is not yet fully understood but has a great influence on the load bearing resistance of open-ended piles. In this study pile plugging is investigated through conducting a series of pile penetration tests using 2D and 3D DEM simulations and considering different installation methods – impact driving, vibro-driving, and jacking. After the pile installation, the load bearing resistance is obtained by static load tests.. The simulation results of the pile installation depict how the stress perturbation induced into the soil relates to the plugging effect, the inner shaft resistance, and the overall pile load bearing resistance. The numerical simulations under the investigated conditions show that pile jacking induces the highest stress perturbation into the soil and thus, pile plugging is more likely to occur. However, it is also shown that pile plugging might be more likely under specific conditions for vibratory driving. Furthermore, it was observed that a soil plug can form, dissolve, and reform again during the pile installation process. Additionally, ideas for future work are presented in this paper.



Stress redistributions under varying trapdoor configurations for buried structures using DEM

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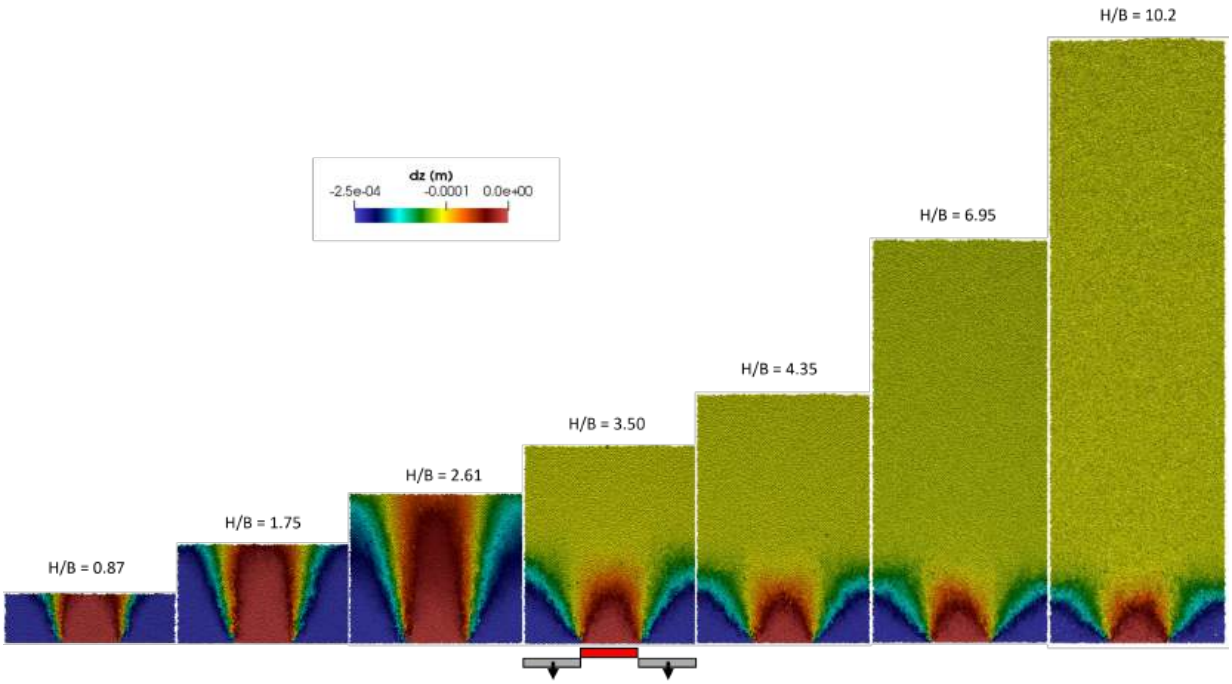
Keywords DEM, Trapdoor, Stress Redistribution, Soil Arching

Soil arching is a well-known geotechnical engineering related phenomenon where the relative movement of soil with soil/structure causes fabric and stress redistribution in the surrounding media. Soil arching causes loss of precious exchequer along with damages to the infrastructure, and is increasingly affecting the society due to increasing urbanization and utilization of sub-surface space. Trapdoor condition is considered a base for understanding soil arching and stress redistribution phenomenon under the action of relative movement of buried structures and the soil. Such stress redistribution can cause substantial differential surface settlement and can increase the stresses on the buried structures to many folds. The urgency of repair for such damages does not allow on-site detailed analysis, which necessitates the in-depth numerical investigation of the mechanism of soil arching, its propagation, and resultant stress-redistribution.

In this study, discrete element simulations are performed using spherical and clumped particle shapes using the modified granular LAMMPS software. The simulations represent the trapdoor conditions with varying configurations, especially the effect of the ratio of buried structure width to the width of settling soil in the surroundings of the structure was observed. It is observed that there exists a critical burial depth for the structures for the development of soil arching, causing increased stresses on the structure and at the same time eliminating the differential surface settlement. The width of settling soil plays a vital role and substantially controls stress redistribution. Furthermore, a significant effect of particle shape was seen on the stress redistribution.



Propulsion of a scallop-like swimmer in granular matter

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Keywords Locomotion, experiment, elastoplastic response, shear jamming

Understanding locomotion in granular matter is challenging as the body deformation of a swimmer can trigger both solid-like and liquid-like material response. We show in Discrete Element Method simulations and in lab experiments that a scallop-like swimmer with reciprocally flapping wings generates locomotion in a granular material made of polydisperse spherical and frictional particles. This disagrees with the scallop theorem that prohibits reciprocal swimming in Newtonian liquids at low Reynolds number. The locomotion is enabled by a prolonged hysteresis in the material force response that originates from a combination of jamming-induced material rigidity and plastic deformation of the free surface. Cooperative effects are observed when the two wings are in close proximity, which further breaks the symmetry between the opening and the closing strokes of the wings, resulting in propulsion.

Session: Coupled methods I

Inertial focusing of a dilute suspension in pipe flow

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Keywords Inertial microfluidic, particle transport, particle ordering, lattice Boltzmann method, discrete element method

Rigid particle suspensions in wall-bounded flows exhibit interesting behaviours like particle ordering, lateral transport, and the formation of stable locations such as the Segre-Silberberg annulus [1]. However, the emergence of multiple annuli remains puzzling [2,3]. To shed light on this phenomenon, we conducted numerical simulations using lattice Boltzmann (LBM) and discrete element methods (DEM) to simulate a dilute particle suspension in a periodic pipe flow [4]. Our simulations track particles' complete radial position history, enabling us to gauge both transient and steady states accurately. We identify a secondary, inner annulus that consistently migrates towards the Segre-Silberberg annulus in a long channel, suggesting its transient nature for Reynolds numbers (Re) up to 600. Interestingly, we observe an increase in the channel focusing length with Re, contrary to the theoretical prediction for a point-like particle.

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A Phase-Field Discrete Element Method to study chemo-mechanical coupling in granular materials

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Keywords Chemo-Mechanical Coupling, Pressure-Solution, DEM-FEM Coupling, Phase-Field

In the classical approach of Discrete Element Method (DEM), grains are modeled as disks and spheres, however, real particles can be highly irregular. These complex shapes of the grains influence greatly the macroscopic mechanical behavior of the material (Guével et al., 2022) and accurate models should aim at capturing this complexity. Different approaches have been developed like adding a rolling resistance, using grains clusters, or recently by using a level-set discrete element model (Kawamoto et al., 2018). Moreover, grain dissolution or precipitation are important phenomena for geomaterials in applications like diagenesis, geological disposals, etc. To model these phenomena, discrete elements are often considered with a homogenous evolution of the particles diameter. But in some cases, like the pressure-solution phenomenon, dissolution and precipitation are localized. For this process, dissolution occurs at the grains contact due to the high stresses that change the chemical potentials, whereas precipitation occurs in the low stress area when there is a sufficiently large solute concentration in the pore fluid. Considering the solid skeleton as a phase, the phase-field theory (PF) is a good candidate to model with physics-based laws a local addition or reduction of material. In this study, a new coupling between PF, solved using the finite element method, and DEM is developed to simulate the irregular shapes of particles in a granular material and their heterogeneous change using the phase-field variable as a particle's geometrical descriptor. This method, implemented in an open-source framework (https://github.com/AlexSacMorane/PFDEM_ACS_MultiGrains), is applied to reproduce results from previous experiments and observations done on the pressure-solution phenomena at several grains level (Guével et al., 2020). Especially, a Andrade creep law has been reproduced (Dysthe et al., 2002). It enables us to investigate the influence of the different physical phenomena controlling the rate of material compaction at the microstructural level.

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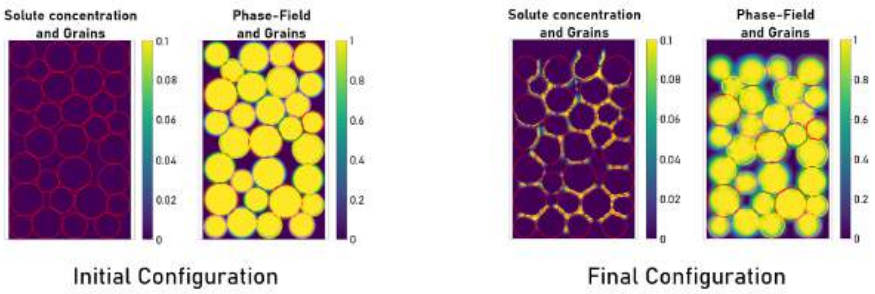

Figure 1: Pressure solution phenomena between multiple grains. For initial and final configurations, the left plot shows the position of the grains and the solute concentration and the right plot shows the phase variables. Between the initial and the final steps, solute has been generated and the shape of the grains have become less spherical. The granular material becomes denser while the pressure-solution phenomenon occurs.

Investigation of a particle location based multi-level DEM coarse graining model for bulk material flow and fluidized particle systems

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Keywords Multi-level coarse graining, DEM-CFD, Hopper, Wurster coater

Granular materials play a key role in a wide range of applications in the chemical, pharmaceutical, agricultural and process industries. A popular Lagrangian approach for modeling granular materials is the discrete element method (DEM), which is coupled to computational fluid dynamics (CFD) when a fluid-phase is involved. Currently, the computation of granular systems with more than 10e6 particles quickly saturates the computational capacity of modern computers, even with highly parallelized DEM-CFD codes. To overcome this problem, multiple original particles are bundled into large-sized particles, so-called coarse grains. The coarse grained DEM is less computationally demanding due to the reduced number of entities considered. In many industrial applications, such as hoppers, coating apparatus, circulating fluidized beds and other non-uniform systems, the physical behavior is strongly dependent on the length scale of the particles. When considering a hopper discharge, the maximum coarse grain factor l (ratio of coarse grain diameter to particle diameter) is limited by the length scale of the orifice to produce reasonable results. Simultaneously, higher coarse grain factors are acceptable far from the orifice. Therefore, a uniform coarse grain factor throughout the system often results in an inefficient computation. Multi-level coarse graining (MCG) addresses this issue by using more than one coarse grain factor in the simulation domain. In MCG the coarse grain factor represents the resolution of particles, which is adapted in critical regions of the treated system. Our goal is to apply MCG in DEM simulations of hopper discharge and at first in DEM-CFD simulations of a Wurster coater. In conclusion, MCG leads to more accurate results and an efficient computation in non-uniform granular systems because it provides a higher resolution of particles in critical regions. The careful placement of coarsening and refinement zones in MCG is important because it affects the results and computation time.

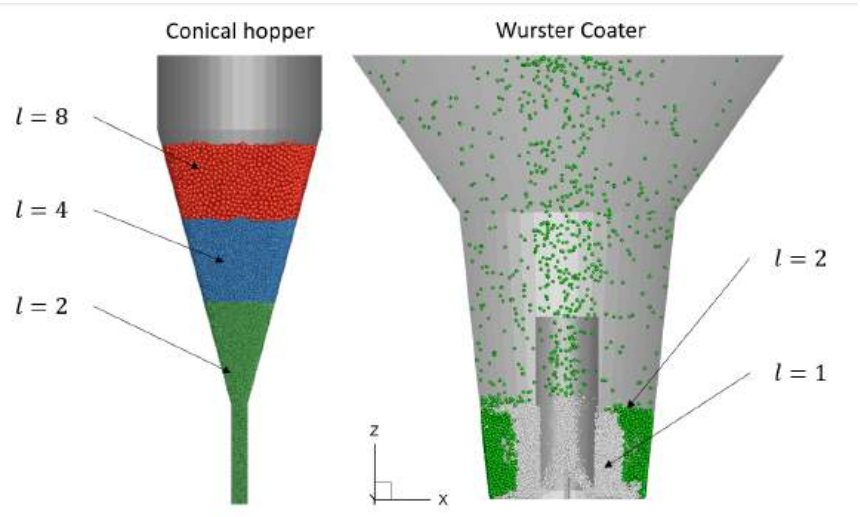

Figure 1: MCG simulation of a conical hopper (left) and a Wurster coater (right) involving multiple coarse grain levels, resulting in a higher resolution in critical regions of the treated systems

DEM and CFD-DEM: Recent progress and path into the future

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Keywords DEM

Discrete Element Method (DEM) and DEM coupled to Computational Fluid Dynamics (CFD-DEM) are established techniques for optimization and design of particle processes. Its applicability to a wide range of processes has been proven for many different industrial and environmental applications. The extension to new fields and processes has been made possible by continuous improvements of: (i) models, (ii) numerical methods and (iii) computational performance. Combining the Lagrangian nature of discretization with complex interaction models, the behaviour of viscous pastes, compressible powders, melting polymers just to name a few, has become feasible. Additionally, much attention has been given to improvement of numerical aspects, which led to improved stability and therefore applicability of the models. Last but not least, computational efficiency and possibility to make use of available computational resources has boosted DEM. More complex applications challenges often arise from a combination of large problem sizes, long process times and the fact that phenomena that arise at micro scales influence the macroscopic behaviour of the system. Advanced models are available that allow for the depiction of complex physical phenomena at very small scales, as well as coarser models for the mesoscopic scale and large-scale models for a whole reactor. The authors give their perspective on corner-stones and highlights in modelling and development that were made in the past few years, and give some concrete examples of current state of the art modelling capability. The authors will also give some insight on future opportunities for this modelling technology.

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Particle-resolved simulation of antidune migration via a coupled free-surface lattice Boltzmann and discrete element method

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Keywords Coupled simulation, particle-laden flow, sediment transport

Antidunes are a fascinating type of sedimentary bedform in the morphodynamics of streams in fluvial or coastal environments. One of their unique features is their ability to migrate upstream under certain conditions, originating from the complex interaction between a shallow, supercritical flow and the surface of the granular bed. This counterintuitive behavior has caught a strong interest in hydraulic research. However, up to date, little is known about their migration mechanism due to the inherent challenges of experimental or numerical studies. This talk presents the first attempt to simulate upstream-migrating antidunes, utilizing geometrically resolved particles and a liquid-gas interface (Schwarzmeier, Rettinger, et al., 2023). To this end, we combine the lattice Boltzmann method with the discrete element method to represent the fluid-particle and particle-particle dynamics (Rettinger & Rüde, 2022), and extend it with a volume-of-fluid scheme to track the deformable free fluid surface (Schwarzmeier, Holzer, et al., 2023). We highlight algorithmic aspects essential for massively parallel execution on supercomputers. Utilizing the efficiency of this approach allows us to carry out large-scale simulations with thousands of particles in unidirectional turbulent flows, capturing the formation and migration of antidunes. By reproducing two flow configurations of a recent experimental campaign, we demonstrate that our approach is robust and accurately predicts the antidunes' amplitude, wavelength, and celerity. The highly resolved fluid and particle motion simulation data open new perspectives for detailed studies of morphodynamics in shallow supercritical flows.

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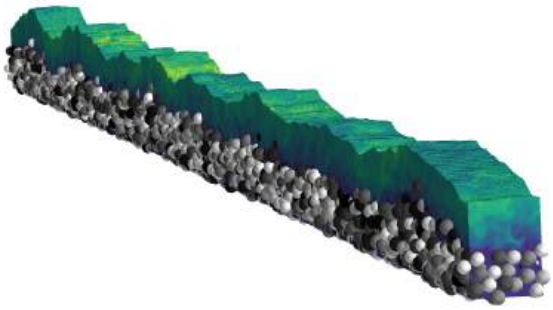

Session: Polydisperse systems

Collapse of polydisperse columns: looking for a scaling between energy and mobility

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Keywords Granular flows, polydispersity, coupled simulation

The granular column collapse is a benchmark experiment for studying granular flows [1, 2]. Granular flows are found in varying scales from handling purposes to natural debris flows and can occur in subaerial or submerged environments. Out of convenience, granular flows are commonly studied with a monodisperse distribution of grains [3, 4, 5]; however, the variety of grain sizes, known as polydispersity, is an important feature found in the previous applications. Understanding the role of polydispersity remains a challenging task and requires a series of simplifications when addressed numerically, in coupling the granular phase with a fluid phase. We study the collapse of granular columns in dry and immersed conditions with a coupled Finite Element Method (FEM) and Discrete element method (DEM) [6]. In this framework, we study the effect that polydispersity has on the collapse of granular columns. We define the polydispersity level as the ratio between the biggest and the smallest grain and study systems with a polydispersity level ranging from 1.2 to 19. We show that polydispersity has stronger effects on immersed collapses than in dry collapses. Notably, the collapse sequence and spreading velocity of immersed columns are affected by increasing the level of polydispersity [7]. Moreover, we propose a simplified model that scales the column runout with the spreading front kinetic energy, weighted by the ratio between the particles' density and the relative density between particles and fluid. We perform a series of experiments with polydisperse samples and show that this simplified model remains true in a three-dimensional configuration, validating the model with experimental results and pointing to its generality [8]. Our results are a valuable contribution to the study of granular flows, providing an understanding on the effect that polydispersity has on them and revealing that packing fraction is a characteristic to describe these systems.

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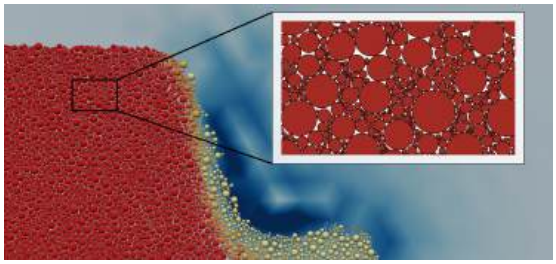

Transient size segregation of binary granular mixtures

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Keywords Granular flow, DEM simulation, Continuum model, Size segregation

Transient size segregation of a bi-disperse granular mixture flowing over a periodic chute is studied using DEM simulations and theory. A recently developed particle force-based size segregation theory has been shown to successfully predict the steady-state behaviour of binary granular mixtures (Tripathi et al., 2021). This promising theory is used to predict the time-dependent flow properties of binary mixtures starting from rest in this work. A two-way coupled continuum model is developed for the evolution of the flow. It solves the momentum balance and convection-diffusion equations by incorporating a mixture segregation model along with rheological model. The inter-coupling of segregation with rheology is accounted to predict various properties of interest such as specie concentration, inertial number, velocity, pressure and shear stress. The agreement between the theoretically-computed segregation velocity using particle force-based theory and the segregation velocity obtained from DEM data for all transient states confirms the accuracy of the segregation model. The time-varying theoretically predicted concentration profiles and flow properties are found to be in good quantitative agreement with the DEM data. Additionally, we investigate the effect of different initial configurations on the transient evolution of the flow and segregation. Three different initial configurations, namely large near base (LNB), Small near base (SNB) and mixed, are considered. The particle force-based segregation model is able to predict the evolution of the concentration profile for all three initial configurations considered in this study. The results provide insights into the complex physics of transient size segregation in granular mixtures and demonstrate the accuracy and effectiveness of the present approach in capturing this phenomenon.

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Coarse grained DEM simulation of non-spherical and poly-dispersed particles

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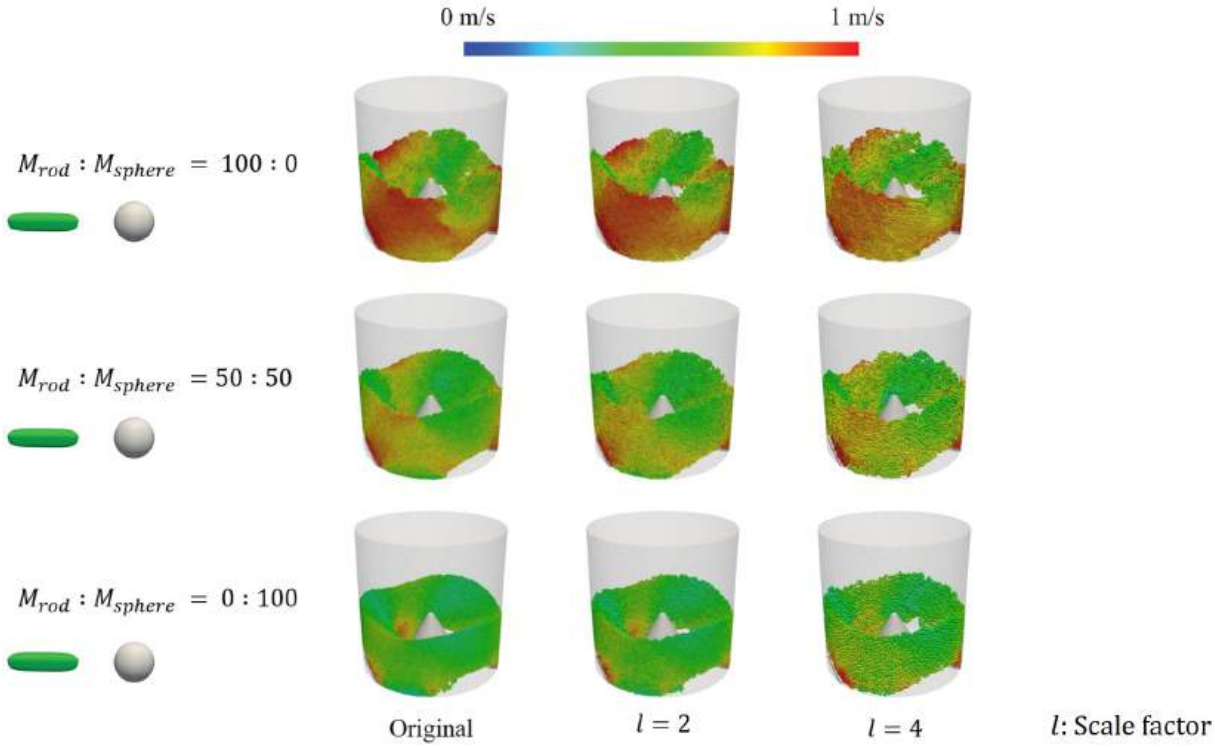
Keywords DEM, Coarse grain model, Non-sphericity, Poly-dispersity

One of the major problems of Discrete Element Method (DEM) is the extremely high computational cost to track the movement of an enormous number of particles. This makes it difficult or practically impossible to perform simulation of an industrial scale system. The coarse grain model has become increasingly popular for simulation speed-up: large particles are used in simulation to represent the original small particles. The coarse grain models in literature may be largely classified into the parameter scaling and direct force scaling approaches. The former employs scaled-up physical properties and parameters (often based on some dimensionless numbers) to achieve dynamics similarity to the original particle system. The latter first estimates the forces acting on the original particles using the original physical properties and variables, and then the resultant forces are directly scaled using certain scaling laws. In this work, a novel direct force scaling model called the Scaled-Up Particle (SUP) model is developed where the scaling laws are derived based on the continuum assumption of an arbitrary particles flow. The SUP model is highly generic and, in theory, applicable to a flow with non-spherical and poly-dispersed particles. Simulations of various systems such as heap formation and a high shear mixer are performed with the original and coarse grained particles to examine the validity of the SUP model. The multisphere and superquadric models are employed to represent the particle non-sphericity although any shape models such as the polyhedral and level set models can be used in principle. It is observed that the results obtained from the SUP model are in both qualitative and quantitative agreement with those from the original particles.



Micromechanical Effects of Sample Scale in Size Polydisperse Granular Materials under Simple Shear

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Keywords Shear strength, sample size effects, grain size distribution, discrete-element method, force networks

The shear strength properties of coarse granular materials are often challenging to characterize due to size limitations in common testing apparatus. While the standard ASTM D6528 recommends a sample scale (α=H/ dmax, being H the height of the device and dmax the maximal particle size in the sample) of 10 for simple shear tests, the influence of α on the mechanical response of the material is still not well understood, nor the standard takes into account the effect of grain size distribution. To provide an alternative perspective on this problem, we conducted a campaign of simple shear simulations in the frame of the discrete-element method called contact dynamics, in which we gradually varied the sample scale and the grain size distribution using spherical particles. We covered a large range of situations including samples with a few hundred grains to highly polydisperse assemblies with more than 130 000 grains. By means of a detailed micromechanical analysis of force distributions and stress concentrations, we discovered that the macroscopic stability of shear strength and solid fraction is closely tied to the formation of local rigid structures of grains carrying normal contact forces significantly higher than the mean force. We also determined the typical height of these structures which we identify as the precursor to larger variations of parameters at the macroscopic scale. When the height of the rigid structures is comparable to that of the sample (which occurs for α<15), the shear strength and solid fraction deviate from the values found under larger α. Although our findings still require further experimental validation or analysis of more complex particle shapes, this work suggests that the ASTM recommendations may need to be re-evaluated to achieve more representative material characterization in laboratory testing.

Granular gas mixtures: DEM simulations compared with experiments

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Keywords Granular gas, non-spherical particles, microgravity, GPU simulation

We have performed DEM simulations of granular gas mixtures consisting of two particle types in weightlessness. In particular, a mixture of two types of elongated particles (thin and thick) was considered, and the outcomes were compared with the results of ZARM Drop Tower experiments. The numerical implementation is based on a modified hybrid GPU/CPU DEM simulation code for spherocylinders previously used in a number of publications [1,2,3]. A series of simulations were run in order in order to establish the proper values of the restitution and friction coefficients, which fit to the experimental data. We have found that simulations reproduce well the most relevant features of the particle ensemble, such as homogeneous cooling with Haff's scaling of kinetic energy decay [4] as well as the energy distribution between the mixture components and among individual degrees of freedom. Moreover, simulations give access to properties which are hard to extract from the experimental data, such as accurate collision statistics and the energy associated with the rotational degree of freedom around the long cylinder axes.

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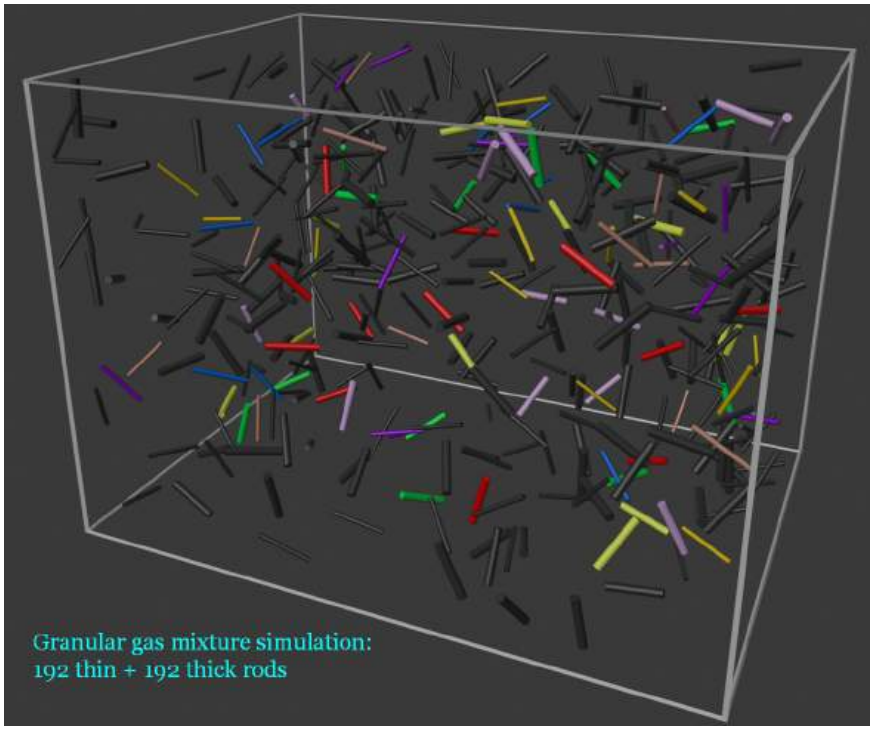

Session: Coupled methods II

Multiscale, multiphysics modelling of granular materials – Volume- & surface-coupled discrete particle simulations in MercuryDPM

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Keywords Granular Matter, Surface coupling, Volume coupling, FEM-DPM coupling

The discrete particle method (DPM) simulates the motion and interaction of discrete grains. It has been successfully used to understand and predict many granular processes. However, solving the next generation of problems will require solvers that can capture the interaction of the granular material with continuum fluids and deformable objects. Furthermore, process simulations are becoming ever more complex, pushing the limits of what is possible with DPM, as the method is computationally expensive. Hence there is a need for solvers that can capture complex multiphysics and multiscale features by coupling the method in a flexible way to a continuum solver. Here, we introduce Moomph [1], a general framework for modelling multiscale/multiphysics processes. It combines two powerful open-source packages, MercuryDPM [2] for discrete particle simulations and oomph-lib [3] for solving continuum equations, into one, easy-to-use coupled solver. Both codes are integrated into a single executable, allowing for efficient data transfer. The software utilises one of the core features of MercuryDPM, coarse-graining, to improve the coupling accuracy and flexibility. We consider three types of coupling: (1) Surface-coupling, to model the interaction of the granular material with soft geometries. (2) Volume-coupling, to model parts of the granular material with a continuum model, while other parts are resolved with the discrete particle model, allowing for efficient but accurate simulations of large amounts of granular materials. (3) Particle-fluid coupling, to model the interaction with a background fluid, or a thermal field. Both volume and surface coupling have been implemented, with particle-fluid coupling coming soon. We will demonstrate the features of the surface-coupled code via several examples, including sack filling, energy-absorbing walls and a beam deflecting under particle impact. To demonstrate volume coupling, we show wave propagation through a granular material that is modelled partially as discrete particles and partially as a continuum.

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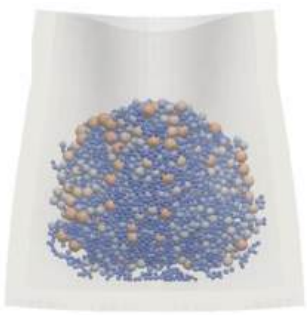

DEM simulations of wind-blown sand and dust transport

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Keywords DEM, sand, dust, wind turbulence, climate

Wind-blown sand transport is responsible for emitting dust aerosols into the atmosphere, resulting in suspended dust clouds that significantly impact Earth's weather and climate [1]. Accurate quantification of dust concentrations in the atmosphere would reduce the significant uncertainties in the current climate projections. We model this interplay between sand, dust, and wind by employing the Discrete Element Method (DEM) using LAMMPS [2], coupled with the hydrodynamics of the turbulent wind extended into the open-source library. The multi-grid neighbor search methods [3] also allow us to run massively parallel simulations for polydisperse media of sand and dust mixtures. Our numerical model accounts for the contact mechanics, lift forces, stochastic turbulent velocity fluctuations, and attractive inter-particle interactions (van der Waals) crucial in depicting the roll, flight, and splash events over the bed. Particularly for grains smaller than 100 micrometers, the initiation threshold for transport is observed to be strongly influenced by cohesion and turbulent fluctuations. Our simulations also confirm that sand bombardment is one of the major mechanisms for the emission of distinct dust grains or sand-dust aggregates that emerge from the granular impacts. We provide scaling laws validated [4] using wind-tunnel experiments for the sand and dust flux as a function of the wind shear acting over the bed surface. The universality of the model in extrapolating to extra-terrestrial environments with diverse atmospheres has been demonstrated previously [5]. The usually ignored interdependency of the turbulent fields and cohesion in the conventional models are justified in this comprehensive model, which aims to provide better empirical relations for dust estimates in future climate models.

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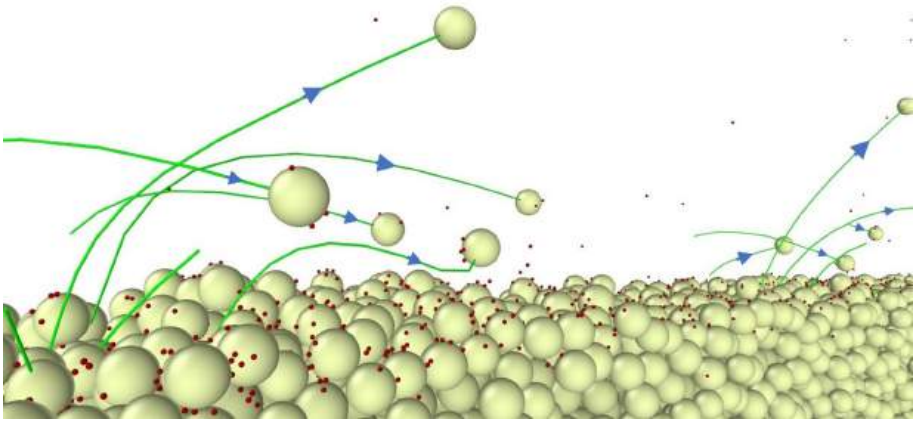

Investigation of Submerged Granular Column Collapse Using LBM-DEM Simulation

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Keywords DEM-LBM, Rheology, Submerged Granular Column Collapse

In this work, we explore the transient rheological behavior of immersed granular flows through experiments and numerical simulations. Using the lattice-Boltzmann method (LBM) coupled with the discrete element method (DEM), our simulations provide detailed data on stress and deformation conditions during submerged granular column collapses. We validate a length scale ratio G that unifies the rheology of transient granular flows across different regimes. Our findings establish a transient constitutive framework for visco-inertial granular flows, contributing to a better understanding of granular-fluid mixtures in natural and engineering contexts.

The performance of a deep-sea mining vehicle based on DEM-CFD coupling method

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Keywords DEM-CFD, nodules, deep-sea mining vehicle, the efficiency of the deep-sea mining vehicle

The deep-sea mining vehicle is designed to mine the nodules in the deep-sea seabed. The performance of the deep-sea mining vehicle is an important issue in the design and deep-sea operation. The interaction amongst the nodules, the flow and the deep-sea mining vehicle is unclear. Thus, the DEM-CFD method is established for the deep-sea mining vehicle. The effect of the shape and distribution of the nodules, and the distribution of the flow filed around the vehicle on the efficiency of the deep-sea mining vehicle will be discussed. Furthermore, the relationship between the flow and nodules will be studied. This paper may provide a comprehension of the working condition of a deep-sea mining system, which enlightens the optimization design of the deep-sea mining vehicle.

Metaball DEM for Non-Spherical Particles with realistic shapes

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Keywords DEM, Non-Spherical Particles, Metaball function, implicit function, shape descriptor

Particle shapes play a crucial role in determining the mechanical behavior of granular materials. However, accurately and efficiently modeling realistic particle shapes in DEM simulations remains a challenge. Recently, the metaball shape descriptor is introduced to DEM to handle non-spherical particles, where the shape is represented as an implicit function. Leveraging the analytical expression of metaball function, the contact between convex particles can be reformatted as an optimization problem that can be efficiently solved by Newton-Raphson method. To tackle non-convexity, a dual-shape descriptor approach has been developed. This approach represents particle shapes using both metaball functions and surface meshes, the overlapping volume is used to determine the contact force. These developments highlight that metaball DEM can be a suitable choice for simulating granular materials with realistic shapes.

Session: Cohesive & capillary interactions

JKR theory-based force-displacement relation for DEM simulations of adhesive particles

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Keywords Discrete element method (DEM), force-displacement relation, JKR's theory, adhesive particle, centroid of contact area

There is a lot of scientific and commercial interest in adhesive particles. Discrete Element Method (DEM) simulations can be used to examine their collective behavior, but they require a well-grounded force model, namely a force-displacement relation, in order to extract the contact force "F" from the relative displacement "delta". For adhesive spheres, the Johnson-Kendall-Roberts (JKR) theory (Johnson et al., 1971) gives equations for F and delta in terms of the contact radius "a", but a simple relation for "F-delta" has remained elusive. We propose an "F-delta" relation from the JKR theory as a composite function, where the effective adhesive contact radius, "lambda(delta)", is solely dictated by the relative displacement "delta". There are only two parameters, which depend on the contact curvature and material properties, in our JKR-based force model. We also present a 'smoothed JKR model by connecting two mathematically valid "a(lambda)" solutions to reduce discontinuities in the evolution of contact force and energy. In addition to the contact force magnitude, we investigated the exact contact centroid and the inaccuracies in contact geometry approximation. We discover that the exact contact area centroid of the Hertz and JKR models is determined by the stiffness quotient; failing to include this leads to incorrect torque and rotational degrees of freedom, which affects relative tangential velocity. Our investigation reveals that some nano-sized particles have substantial initial contact size ratios, at which contact geometry approximation errors become non-negligible. Overall, we derived simple JKR contact force models that are easily implementable in DEM to simulate adhesive particle dynamics.

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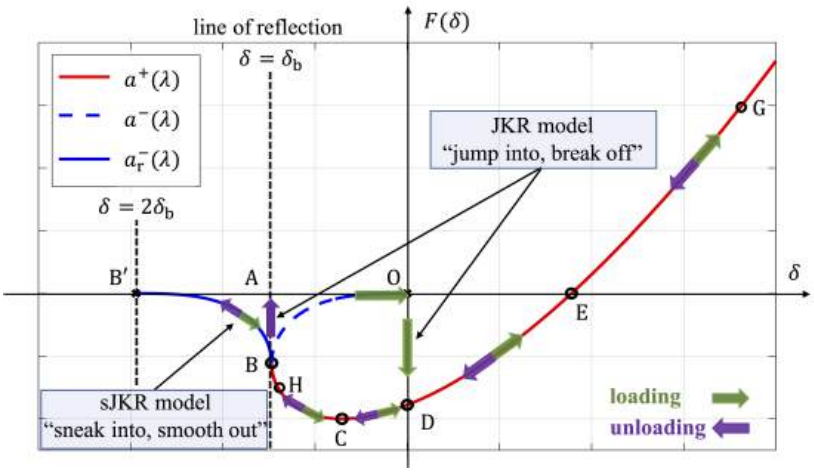

A DEM based continuum theory for fluid AND solid granular matter

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Keywords Particle simulations DEM, stochastic events, continuum models, granular solids and fluids

The simultaneous gas-, fluid- and solid-like states [1-4] of particle systems has tremendous implications in nature and engineering, where particles constitute over 75% of all raw material feedstock. Disasters/challenges involve land-slide instabilities of granular materials in nature, for sand/soil, or in particulate product- and process-engineering, where transport problems of powders are silo-clogging or -collapse. In particle systems, the co-existence of multiple states [1] and their transitions are the ultimate research challenges in mechanics and physics, due to different levels at multiple scales: micro=discrete, meso=stochastic, macro=continuum.

To bridge the gap between micro, meso and macro scales, we establish a unified, monolithic UNIVERSAL theory for particle systems that involves all the classical limits (from gas-dynamics stochastic kinetic theories via non-Newtonian rheology to elasto-plastic solid mechanics) and in addition a stochastic perspective on the meso scale mechanics [4]. Modern discrete simulations describe the particle systems in detail - as starting point - but are limited if too many particles are involved. Continuum methods are successfully applied in civil, mechanical and chemical engineering on the macro scale, but suffer from a lack of insight into micro-based mechanisms and processes. Relying on empirical constitutive laws they disregard the discrete nature of the particles, their contact mechanics, and the stochastic nature of collective mechanisms of meso-structures (like force chains).

We will review how the gap between particle- and continuum-concepts can be closed and concepts from particle simulations (DEM), stochastic/statistical physics, and continuum theory can be combined into a universal theory for granular materials [1-4], with possible applications in large-scale natural or industrial particle systems. The continuum model can be quantitatively calibrated by DEM [1] or experimental [2] data, and shows not only the fluid or solid limits, but also transient situations [3], interesting statistics [4], and transitions between the states [1,3].

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Lithium-Ion battery electrode as a cohesive granular material

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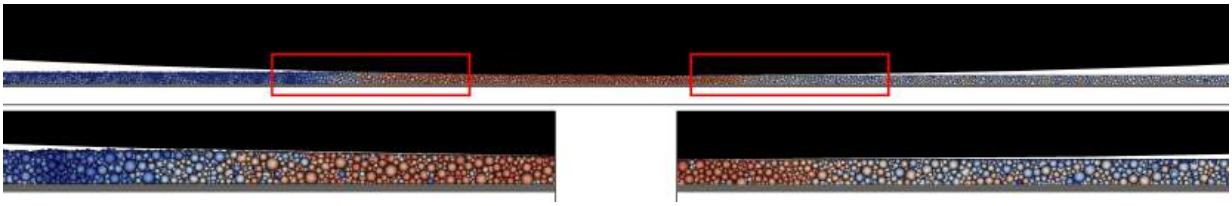
Keywords Battery, calendering, cohesion, contact law

Li-ion Batteries finds their application in a wide range of industrial and customer products. Their performances, such as charging rate and energy storage capacity, are highly influenced by the microstructure of the electrodes, and thus the manufacturing process. For modern batteries, it involves a compaction step called calendering where the thickness of the electrode is reduced between two cylinders in order to increase its density. However, this compaction step increases also the tortuosity of the electrode, which decreases the final charging rate of the battery ; thus, a compromise is necessary between energy storage and charging rate. Simulations are a useful tool to investigate this compromise and better understand the link between grains properties, operational parameters and final electrodes properties and performance. The microstructure of the electrode involves a granular media, therefore its behaviour is here simulated using the Discrete Element Method. The models usually employed in the literature lack of some physics as they tend to misrepresent the cohesive and plastic aspects of the grains and binder. We developed and tested a new contact law dedicated to Li-Ion battery which allows to implicitly take into account the presence of the binder and its mechanical contribution. Moreover the simulations performed here use a direct simulation of the calendering rolls, whereas studies from the literature use an uniaxial compression approximation. We tested and validated our contact law against experimental data and tested the influence of operational parameters such as calendering speed and loading. We observe a huge impact of the applied loading on the electrode properties, but no significant impact of the calendering speed as long as the speed is relatively low. We show that this model can be used to predict correctly the final properties of the electrode based on its composition and the calendering parameters used.



Coarse-grain Discrete Element Modelling of wet particles in a rotating drum

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Keywords Coarse-graining, DEM, liquid bridge force, rotating drum

Wet granular systems are important in different industries and geological phenomena. In these systems, the presence of liquid bridges between the particles can affect the mechanical behavior of the system. To study the behavior of such systems, Discrete Element Method (DEM) has proved to be a powerful tool. However, DEM is computationally expensive when it comes to industrial scale processes. This highlights the importance of upscaling approaches such as coarse-graining. Coarse-graining (CG) is an upscaling approach in which a group of original particles are represented by a larger particle. This can reduce the computational cost of the simulations significantly. In CG-DEM approach, scaling rules will be considered to ensure the agreement between the CG and the original particle simulations.

To our knowledge, a limited number of studies have been done on CG-DEM simulation of systems containing liquid bridges. Hence, it is important to understand how to apply the coarse-graining approach for wet particle systems and compare different scaling rules. In this study, scaling rules based on two different approaches, namely Weber number-based scaling and Bond number-based scaling have been studied for the cases of simple cohesion, wet particle system with constant liquid bridge, and wet particle system with liquid migration. The results indicate that the CG system scaled based on Weber number has a good agreement with the original system, while the CG system scaled based on Bond number does not.

The effect of particle shape, particle size, and multiple inter-particle contacts on the DEM modelling of water meniscii for coarse-grained materials

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Keywords Particle shape, liquid bridges, unsaturated contact models

Low degree of saturation in granular materials involves the formation of water menisci between particles. The physics and interactions between solid, liquid and gas phases are complex and often highly idealised. Most existing DEM contact models dealing with these phenomena assume that particles in contact via liquid bridges are spheres (and often of equal size). Furthermore, in contrast to some recent experimental evidence, often, water menisci are only considered between pairs of particles. Due to computational cost the effect of more realistic particle shapes on the formation, survival and breakage of water menisci has received little attention. Experimental approaches to study evolution of liquid bridges considering particle shape and multiple inter-particle contacts are also limited.

Nevertheless, the key aspects of DEM contact models to replicate these interactions between the solid, liquid and gas phases are the maximum separation inter-particle distance for which a liquid bridge can exist, and the capillary force. These two characteristics are normally considered in DEM simulations as a function of the volume of water in the water menisci (i.e. the volume control approach). However, the matric suction and its effect on the capillary force is often ignored in most existing DEM approaches.

The present study considers the effect of particle shape, particle size, and multiple inter-particle contacts on the formation, permanence, and breakage of water menisci at inter-particle contacts, whilst considering both water volume and suction control approaches. Numerical and analytical approaches are presented to develop an extensive database that may be used for the development of DEM contact models and/or machine learning approaches with the same purpose.

Session: Particle-fluid interactions in industrial applications I

DEM simulation of multiphase flow in solid rocket motor

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Keywords DEM, multiphase flow, solid rocket motor, particle damping, two phase flow lost

In solid rocket motor, multiple phases coexist, including the combustion gas, alumina droplet, particles and agglomerates, smoke powder and et al., in which the complex chemical reactions and thermal expansion are carried out to generate the thrust of the rocket. Discrete particle plays an important role in the influence of rocket motor performance. In particularly, the two phase flow lost in nozzle and the particle damping in combustion chamber are the most important issues, which affects the motor specific impulse and the motor combustion stability significantly. In this work, the DEM based model is newly applied to study these two issues. The particle collisions and particle-wall collision are considered to improve the accuracy of multiphase flow prediction, and subsequently to precisely calculate the two phase flow lost. Coupled with acoustic field and overload into CFD-DEM, the particle damping characteristics could be comprehensively studied to provide the fundamental understanding of damping features. The simulated results reveal that CFD-DEM could provide more precise calculation of two phase flow lost with plenty particle scale information, which indicates that the two phase flow lost may be underestimated previously. Also the particle space distribution calculated by DEM under acoustic wave and overload, indicates its evident reduce of the particle damping, which has sever influence on the motor stability. These successful trials of DEM on the study of multiphase flow in solid rocket motor show the potential applications in investigation of astronautics.

Beyond the Black Box: How DEM Gives a New Approach to Vertical Stirred Milling

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Keywords Vertical Stirred Mill, Process Optimisation, Grinding, CFD-DEM, GPU Computing

With the increased capability and speed of computing from technology such as GPU's and HPC's, industrial systems can now be studied in greater accuracy and depth than ever before. One process which has really benefited from these advances is vertical stirred milling; a complex system that requires large-scale DEM simulations, often coupled with CFD, to predict fine particle grinding. This has enabled research to go beyond the "black box" theory of only being able to demonstrate milling effectiveness from grinding output, and allowed for study on a regional and even collisional level. Almost every industry relies on particle size reduction methods, with grinding from mining alone contributing almost 2% of global energy [1]. Therefore, a better understanding of these machines could improve efficiency and reduce energy consumption. The talk demonstrates how we can develop a validated DEM mill using experimental technique. Laboratory data collected using the Positron Emission Particle Tracking (PEPT) method shows that, despite being able to collect significant data, there are limitations with current physical techniques. This is where the model gives us an ability to assess the full design space. Once built, evolutionary algorithms were used to refine the material parameters until an optimal set of conditions were found. In certain cases, it was also found that the complex and computationally expensive CFD-DEM coupling could be reduced or even removed due to the nature of the system.

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A coupled discrete element lattice Boltzmann method study of bijels as a novel type of catalyst support structure

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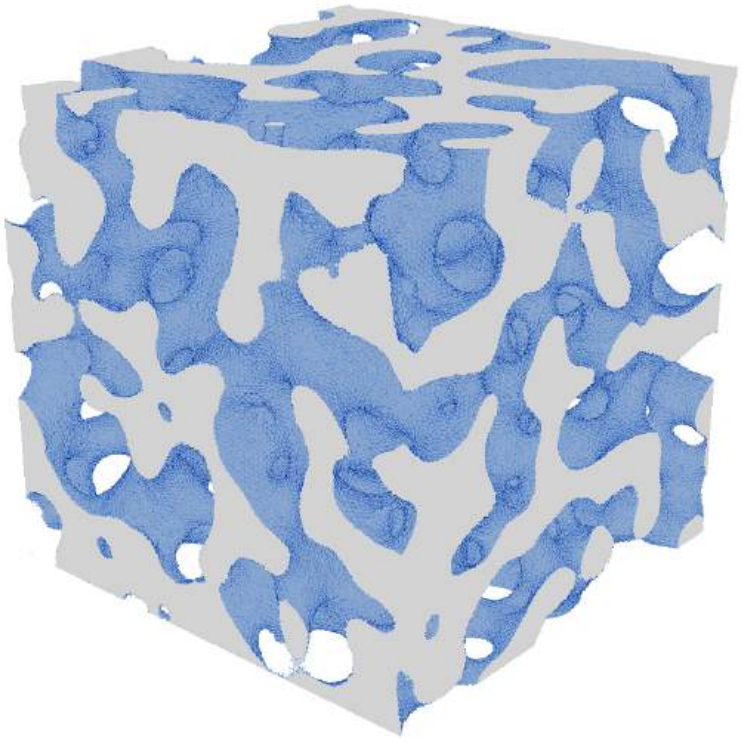
Keywords Coupled discrete element lattice Boltzmann method, colloidal suspension, spinodal structure, heterogeneous catalyst support

Porous catalyst supports are often used in industrial processes due to their high surface area to volume ratio. However, the stochastic morphology of commercially available supports generally results in poor reaction product transport and conversion inefficiencies. A recent experimental study showed that these issues can be alleviated by making use of catalyst supports acquired from spinodally derived architectures. In particular, architectures obtained from bicontinuous interfacially jammed emulsion gels (bijels) seem to be a viable route to manufacture stable catalyst supports. In this work, this type or porous support is further investigated by means of a coupled discrete element lattice Boltzmann method solver. First, bijels are generated by triggering spinodal decomposition in a bi-component fluid mixture with a large amount of dissolved particles. After the rapid initial domain coarsening and interface stabilization, the simulations are frozen and one of the fluid phases is solidified. An analysis of the properties of the resulting porous structures is presented.



Grain-scale behavior of erosion/sedimentation process studied by DEM/CFD coupling simulation

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Keywords Erosion, sedimentation, turbulent diffusion

How planetary surfaces morphology is formed and evolved is the central issue of earth & planetary sciences. On the earth, the surface water flow is a primary driving force for erosion, transportation and sedimentation of geomaterials. The models proposed in the previous research describe this phenomenon by the interplay between the turbulent diffusion and the gravitational precipitation (Rouse 1937, Lane and Kalinske 1941, Garcia and Parker 1993), but its grain scale behavior has not been fully investigated. In particular, the effect of grain properties has not been quantified yet. We tackled this problem using grain scale simulation considering the interaction with fluid flow. 3D discrete element method for grain simulation was coupled with 2D SMAC finite difference method for fluid flow simulation to reduce the computational cost. Di Felice (1994) model was adopted for the interaction between the two phases. After verifying the program with a single particle falling in a fluid and the pore fluid flow through a granular solid, a series of erosion/sedimentation simulation at a granular bed were carried out with different grain properties and flow velocity. We observed an interesting cycle of erosion and sedimentation of grains near the critical regime between the laminar and the turbulent flow. The simulation results were also compared with the experimental model by Garcia and Parker (1994).

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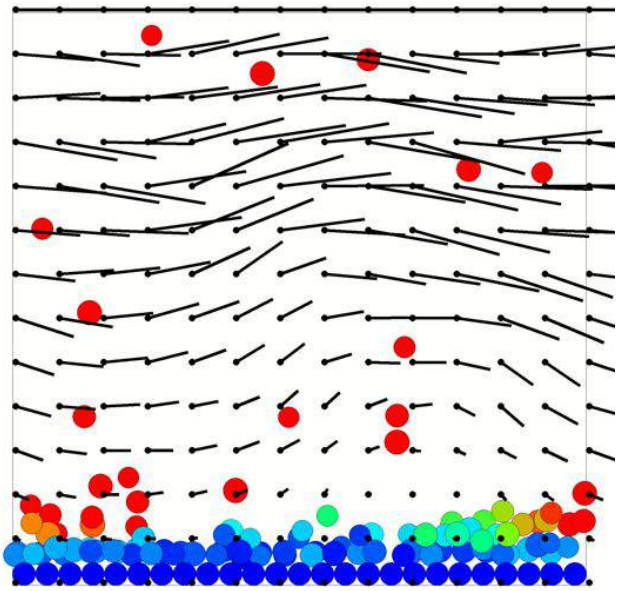

Simulation of a continuous vertical stirred mill using DEM, CFD, DPM and the UFRJ mechanistic model

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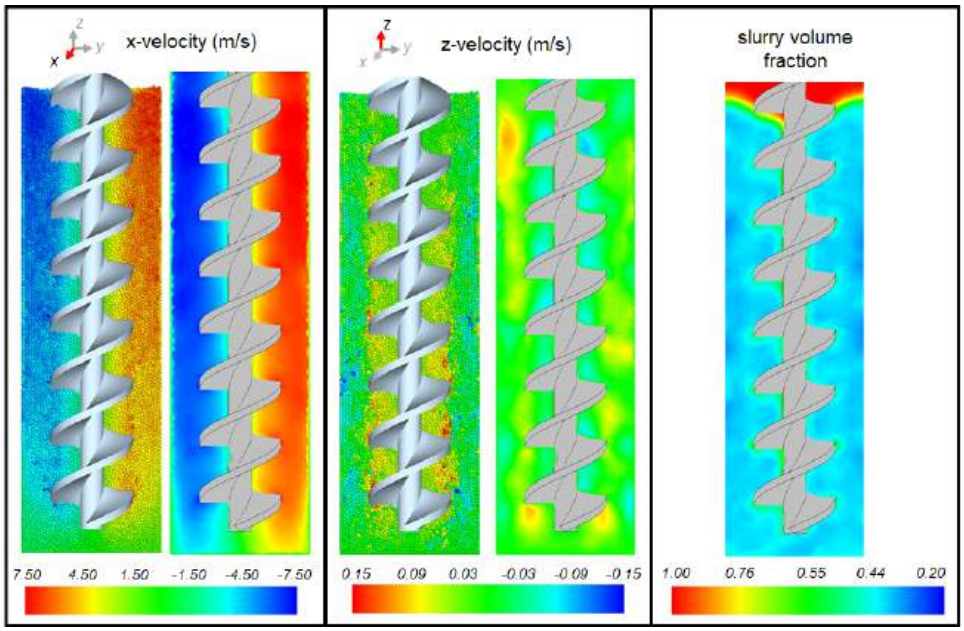
Keywords Vertical stirred mill, modeling, mechanistic, classification, CFD-DEM

Vertical stirred mills have become increasingly popular in size reduction of different materials, including minerals, chemicals and pharmaceutics. The simple design and the ability to operate at very different scales are the main advantages of stirred mills, making them versatile to be used in different industries. The modeling of the mill performance presents different layers that can be addressed. The bulk behavior of the grinding media inside the mill can be simulated with the Discrete Element Method (DEM). The slurry transport may be simulated using Computational Fluid Dynamics (CFD) or Smoothed Particle Hydrodynamic (SPH). Moreover, the breakage mechanisms that dominate the size reduction can be simulated, for instance, using the Mechanistic UFRJ model. As such, the simulation of all the mechanisms that play a part in the size reduction and transport phenomena is a complex task that presents itself as a challenge from the computational perspective. The present work describes the application of DEM and CFD-DEM coupled simulations for the description of the particle and slurry behavior inside a pilot-scale gravity-induced stirred mill. In addition, the utilization of tracer particles using the Discrete Phase Model (DPM) is explored for the estimation of the particle classification and sedimentation mechanisms that occur at the top final part of the vertical mill. Results of the simulations, such as mixing patterns and spatial distribution of collision energies are used to trigger the mechanistic UFRJ model in order to account for the size reduction inside the mill, using data from the stirred mill grinding of calcite in multiple passes for model calibration and validation. The results of the simulations demonstrate the significant effect of incorporating explicitly the fluid flow in describing the motion of the grinding media and the influence of the classification and sedimentation of particles at the top of the mill.



Session: Granular metamaterials

Stability of geometrically cohesive granular columns made of star-shaped grains

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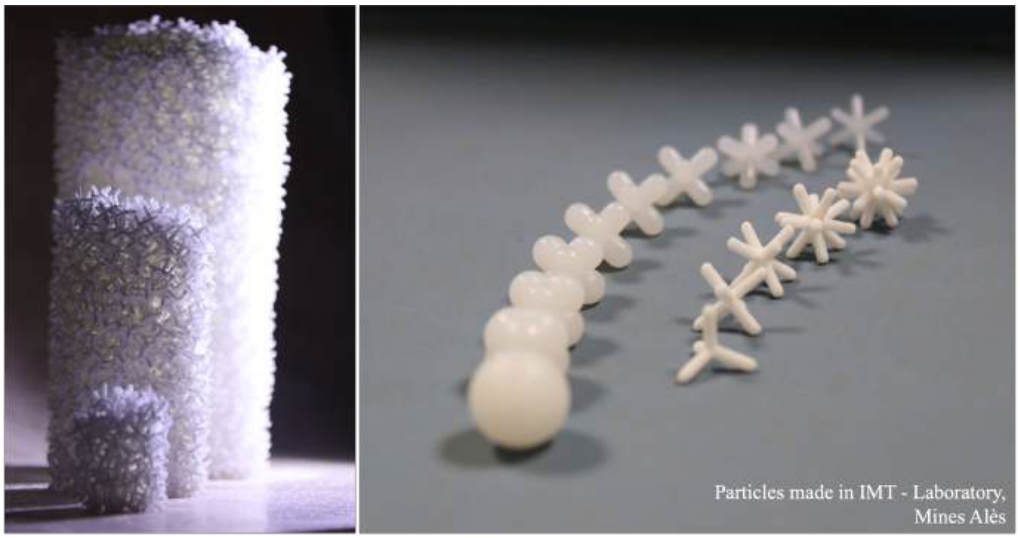
Keywords Non-convex grains, geometric cohesion, self-supported granular structures

In general, building granular columns is only possible when the grains are cemented together (as a sandcastle). In this case, adhesive forces transform the forces network into a self-stressed network of tensile and compressive forces assuring the stability of the column. But, as soon as the cohesive forces disappear, the columns collapse into a pile of grains, whose angle of repose depends mainly on the shape of the grains. Nevertheless, self-supported granular structures can also emerge without the need of any binder when considering non-convex grains. The non-convex grains can entangle inducing a cohesion of geometric origin. We designed 2D simulations to systematically explore the occurrence and magnitude (defined from the maximum height of a stable column) of geometric cohesion with star-shaped grains. Numerically, the arms of the stars are made of rectangles with rounded caps. The number of arms increases from 3 to 14. We performed a series of collapse tests on columns of increasing size. We find that the geometric cohesion increases with the number of arms up to a maximum value for 9 arms, and then declines until the behavior of the assembly remains only frictional. By studying the microstructure of the initial states, we show that the generated columns are hyperstatic (quantified via the coordination number), and that the degree of hyperstaticity is maximum for precisely 9 arms. This is explained by the entanglement of the grains and the increase in the number of multiple contacts between them as a function of the number of arms, revealing “frozen” local structures. These experimental results are confronted to 3D experiments. Many poly-pod particles derived from the platonic solids are built and shaped into columns of different diameters and height. Our preliminary experimental results confirm the existence of a maximum for the geometric cohesion with the number of arms.



Jammed granular metamaterials

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Keywords Jamming, soft robotics, micro-to-macro, DEM

Granular media near jamming exhibit interesting properties, which can be harnessed to create granular metamaterials. The characteristics of such metamaterials arise not only from the shape and properties of the particles (microscopic scale), but also from the geometric features of the granular packing, that is, the particles' arrangement.

We apply DEM simulations to investigate the bending response of a granular metamaterial beam: a granular packing enclosed in an elastic membrane, which can be jammed by pressure on-demand. We study the impact of the particles' properties and packing geometry on the metamaterial's mechanical characteristics at the macroscale, quantified by stiffness and ultimate strength. We find that the metamaterial's stiffness depends on the packing's density and hence on the preparation protocol. The ultimate strength coincides with the yield point of the internal contact network, additionally influenced by the particles' friction coefficient. Finally, we use the particles' localized non-affine motion to investigate the beam's response to deformation. In contrast to many traditional materials, we find that plastic deformation occurs through localized events homogeneously distributed throughout the beam.

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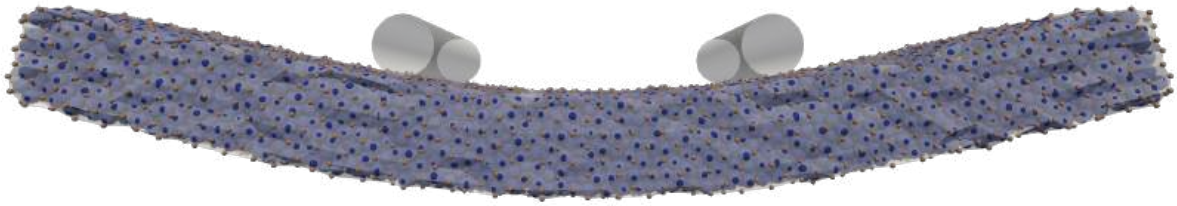

Elastic behavior of granular materials composed of polyhedral particles

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Keywords DEM, polyhedral particles, orthotropic elastic moduli

We use an in-house code based on polyhedral representation of particle shapes and a rigorous contact detection algorithm to investigate the evolution of orthotropic elastic response of regular polyhedral and spherical particle packings. Our DEM algorithm is able to distinguish different types of contact (face-face, face-edge, face-vertex, edge-edge, edge-vertex, vertex-vertex). A linear force law based on normal overlaps at the contact points between particles is implemented and face-face and face-edge contacts are represented by at least three and two contact points, respectively. Dense and isotropic packings of polyhedral particles with different numbers of faces were prepared by isostatic compaction. Then, they were sheared under tri-periodic boundary conditions for different values of interparticle friction coefficient. During shearing, 16 instances corresponding to a wide variety of contact orientation anisotropies were stored and relaxed a static state before applying two distinct strain probes to measure the five independent elastic moduli of the sample. By comparing the simulation data with effective medium theory (EMT), our results clearly show that the elastic moduli are functions of two microstructural parameters: 1) a constraint number that accounts for contact types (face-face and face-edge contacts between polyhedra), and 2) the contact orientation anisotropy. The proposed expression of elastic moduli isolates the direct effect of particle shape, related to the nonaffine particle displacement field from the indirect effect, related to the granular microstructure. The effect of particle shape appears at two levels: on the one hand, through four parameters in the proposed expression, which are independent of friction coefficient, and, on the other hand, through the microstructure reflected by the values of constraint number and fabric anisotropy, which depend on both particle shape and interparticle friction coefficient.

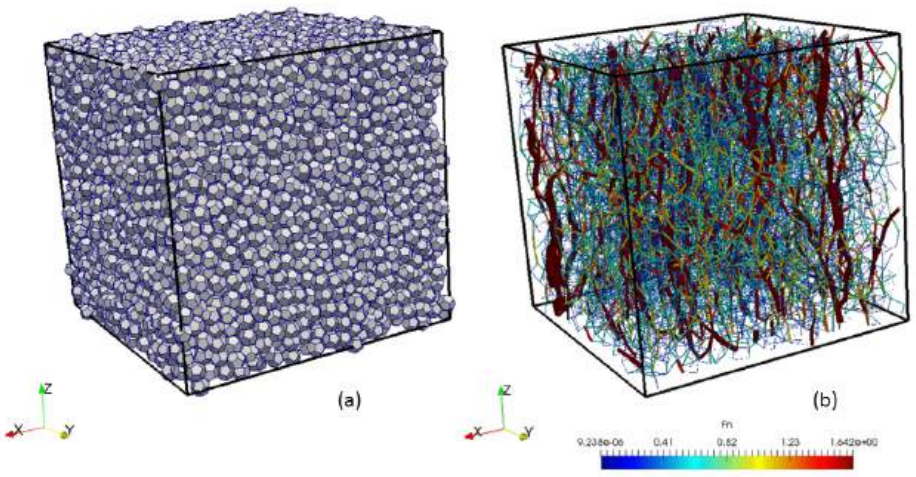

Figure : Snapshot of the dodecahedral monodisperse packing with tri-periodic boundary conditions (a) ; force chains network in the packing under tri-axial compression (b)

Soft particles reinforce robotic grippers - robotic grippers based on granular jamming of soft particles

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Keywords Granular gripper, granular jamming, soft robotics

Granular jamming has been identified as a fundamental mechanism for the operation of robotic grippers. By means of experiments, DEM simulations, and continuum mechanical theory we show, that soft particles like expanded polystyrene beads lead to significantly larger gripping forces in comparison to rigid particles [1]. In contradiction to naive expectation, the combination of jamming and elasticity gives rise to very different properties of the jammed phase, compared to the one of hard particles' systems. This may be of interest also beyond the application in robotic grippers.

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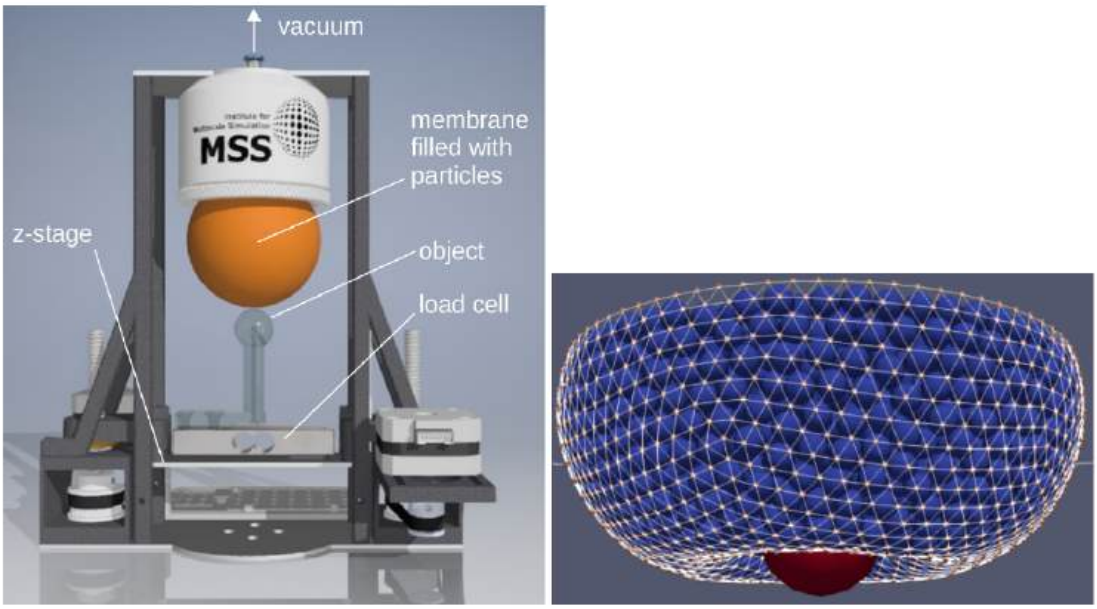

Fig. 1: (a) Experimental setup for the measurement of the holding force of a granular gripper (b) Sketch of the discrete element simulation of the granular gripping process

Mechanical characterisation of highly interlocked granular metamaterials

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Keywords Granular metamaterials, complex particles, particle shape, interlocking, shear strength

Granular materials exhibit fascinating and complex states across scales. Although the mechanical properties of materials with convex and regular particles have been extensively studied in the literature, the properties of materials with highly concave particles are still widely unexplored. Particle shape plays a key role in the packing, mechanical and rheological properties of granular systems; yet a straightforward link between particle shape and shear strength or flowability at the bulk scale has not been established. A new class of granular mechanical metamaterials exhibit extraordinary properties compared to conventional materials, such as high capacity to interlock, due to their complex particle shapes. In this work, we use the Discrete Element Method to gain micromechanical insights into the behaviour of systems made of these complex particles. Assemblies of granular metamaterials are sheared under triaxial stress conditions to establish micro-to-macro links between particle-scale features and bulk-scale behaviour. It is found that intense interlocking of these concave particles at the micromechanical level serves as the origin of apparent cohesion at the bulk scale.

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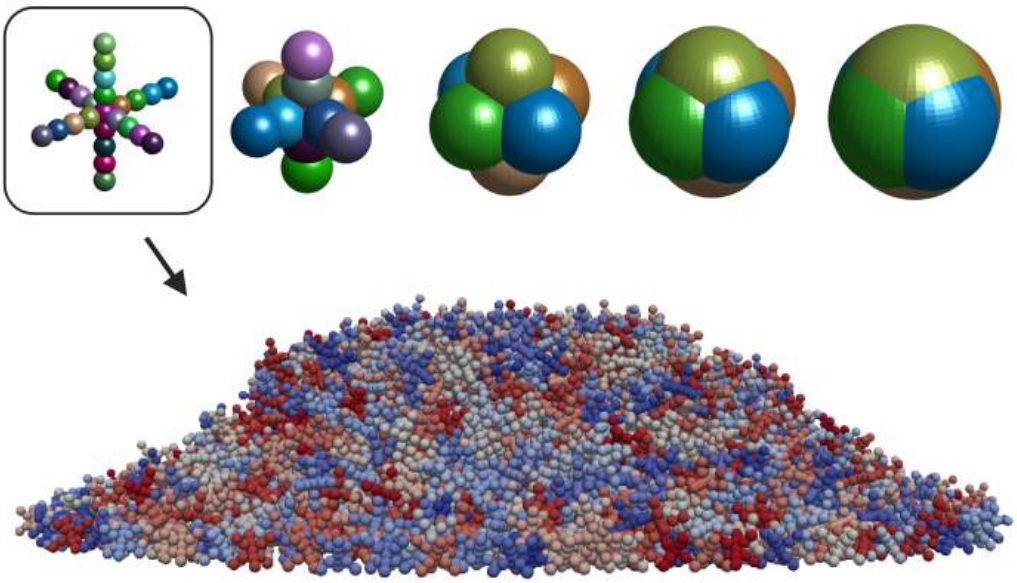

Session: Powder processes & technologies

Digital twins to improve the calibration of DEM simulation of powder processes

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Keywords Powder, calibration, DEM, characterization, digital twins

DEM simulations become largely adopted as a useful tool to study and predict the behavior of powders and granular materials inside industrial processes. However, the parameters of the model describing the interactions between the particles have to be properly determined beforehand in order to provide reliable and usable results. Conceptually, two methods can be used for the calibration of DEM simulation parameters. A first method is a bottom-up approach based on the direct measurement of the microscopic parameters at the scale of the contacts between the grains, which will then be directly used as model parameters (friction coefficient, elasticity, cohesive forces, ...). Even if this bottom-up method makes sense conceptually, it is often impossible in practice to access these properties due to the complexity of the required measurements. Also, the distribution of grain size and shape in the simulation is usually far for the real ones due to computational time limitations when dealing with fine materials.

An alternative is a top-bottom method, which consists in determining the model parameters so that the simulated behavior matches the ones of the real material. The advantage of this calibration method is that simple contact models with reduced parameters set can be used providing that the simulation is able to reproduce the real macroscopic behavior. Also, common characterization methods in simple geometries can be used to evaluate the real material behavior. Moreover, the development of digital twins of characterization methods helps to facilitate this process (Windows-Yule & Neveu, 2022). In this study, we introduce new digital twins of well-established powder characterization methods and the associated calibration procedure. The powders are first evaluated in the real characterization systems, then the model parameters are accurately determined by the digital twins.

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Numerical study of bidisperse cohesive particle blends – bulk properties and thresholds

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Keywords Discrete Elements Method, bidisperse particle blends, packing fraction, size ratio, cohesion

We present a numerical study of bulk properties of binary particle blends via Discrete Elements Method. Larger particles are modelled as free-flowing spheres, while the smaller ones possess attractive short-range attractive forces. Perfectly mixed samples are realised by varying the strength of small particle interactions (measured via the Bond number), the particle size ratio and the relative concentration of small particles in the blend. The blends are then allowed to settle under gravity, and their properties, such as the packing fraction, are computed. We show that bulk properties are independent of small particle properties below a critical value of the mass fraction. This value is connected with the particle contact network and is inversely proportional to the size ratio. Two thresholds in the Bond number are found, determining the dependence of bulk properties on relative mass fraction. For Bond numbers below unity, the effect of cohesion can be neglected. Above it, bulk properties reverse their dependency on small particles' mass fraction proportionally to the cohesion strength. Finally, bulk properties measured become independent of small particles' relative concentration when their cohesion strength is large enough to sustain a large particle.

Investigation of Bulk Material Effects on Reclaim Screw Performance: A DEM-Based Modelling Approach

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Keywords DEM, reclaim screw, auger, storage, EEPA

This study focused on assessing the feasibility of using the existing reclaim screw system of ESI Eurosilo for storing bulk materials beyond their current range. Traditionally, the screw theory, developed in the 1980s by Rademacher [1], primarily considers fine powdered bulk materials, making it challenging to accurately predict the reclaim screw's performance for other types of materials, such as iron ore with high density or lumpy materials. To address this issue, we employed Discrete Element Method (DEM) modelling to examine the impact of bulk material characteristics on the scraping process of a reclaim screw, including external factors like consolidation. The reclaim screw was simplified as a linearized flat disk, which still emulates the screw's behaviour. The DEM model was utilized to investigate the effects of various bulk parameters, comparing the results with the analytical model to validate the simulation outcomes. Additionally, a screening process was conducted to identify the most significant bulk parameters affecting the scraping process, followed by a determination of the best screw design for low- and high-density bulk materials. Through our study, we aim to provide valuable insights into the effects of bulk materials on the reclaim screw's performance. The results contributed to a better understanding of the mechanics involved and aid in the design and optimization of the screw system for a wider range of bulk materials, expanding the capabilities of ESI Eurosilo's storage solutions. We propose a modification of Rademacher's [1] theory by adding an inertia term and a weight term, which is particularly important for high density materials. Overall, this research demonstrates the application of DEM modelling in studying the scraping process of a reclaim screw, offering a promising approach for better understanding and assessing and optimizing the performance of storage systems for various bulk materials.

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Growth and Acceptance: DEM in Industry

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Keywords Industry Applications, Calibration

The discrete element method (DEM) has proven to be an effective computational approach, particularly in the bulk solids handling chute transfer community, where simulations address industrial problems in the handling of material over large distances. Chute transfers maybe its most well-known application but DEM is also used in the food & beverage industry, batteries, biomass, plastics, pharmaceuticals, and many more. From a knowledge base approach of bulk solids handling and storage, this presentation will showcase a timeline of industry projects where DEM has been successfully applied on various simulations in different industries. Let's discuss its humble beginnings, calibration, and the extensive range of projects where DEM has been utilized to gain deeper insights.

Session: Algorithmic aspects of DEM

A Level Set approach for non-spherical DEM in YADE

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Keywords Level Set, LS-DEM, Shape, YADE

For the purpose of capturing realistic particle shapes in DEM, a Level Set (LS) approach (Kawamoto et al., 2016) can be chosen whereby particle's surface is implicitly defined as the zero-level set of a discrete distance-to-surface field. The latter can be obtained for virtually any shape thanks to e.g., Fast Marching Method algorithms, conferring an interesting versatility to the approach. As a second key ingredient, a surface discretization in terms of vertices is also defined from the distance field and ray tracing methods in order to execute contact detection through a master-slave algorithm whereby surface vertices of one Discrete Element are tested against the distance field of another. After implementation in the YADE open-source code (Duriez & Galusinski, 2021), the LS method is herein discussed considering different kinds of shape. The spherical case is first revisited as it enables one to validate the implementation by comparing to a classical DEM reference and measure its computational costs (Duriez & Bonelli, 2021). The LS approach is then illustrated to require around 100 times more memory (for storing the distance field, mostly) and time (for looping over surface vertices during the contact algorithm) than classical DEM. OpenMP parallelization is nevertheless shown to be beneficial for effectively reducing time costs and memory costs could also be optimized (Duriez & Galusinski, 2020). Then, a direct application of the LS approach is proposed to convex superquadrics (superellipsoids). Describing non-convex rock aggregates from 3D scans is also discussed.

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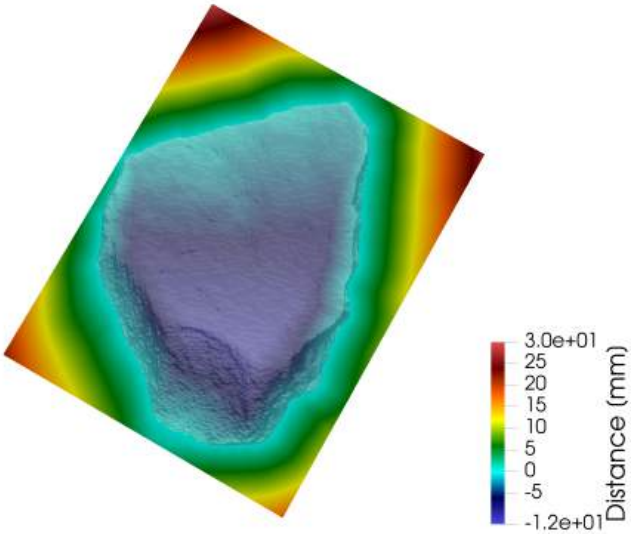

Modelling Complex Particle Shapes with the Volume-interacting Level-Set Discrete Element Method

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Keywords Non-spherical, shape, geometry, concave, level set

The description of particle shapes, particularly concave and complex shapes, remains a major challenge for the discrete element method (DEM). The geometry of particles is a key factor in determining various properties such as the angle of repose (AoR) and porosity (or packing fraction) of granular materials. While many techniques have been developed to try and capture shape effects, they are often limited by the computational cost or complexity of the particles. The level-set discrete element method (LS-DEM) shows great promise for describing non-spherical particles [1,2]. By using a discrete yet implicit description of the particle's geometry, LS-DEM can describe any particle shape at a computational cost less than that of polyhedra for similar accuracies [3]. However, the treatment of particle contacts in LS-DEM can give rise to a number of pathological cases and does not allow for concave particle geometries. We present the volume-interacting level-set discrete element method (VLS-DEM), which overcomes the limitations of LS-DEM by providing a physically consistent method that allows concave and arbitrarily complex-shaped particles [4]. VLS-DEM outperforms polyhedral methods and, at higher particle complexities, even clumped-sphere methods. We present various test cases to validate VLS-DEM and a systematic study on the porosity and AoR of the Platonic solids and their concave variants. Results show that both angularity and concavity strongly affect the porosity and AoR, with the effect being further amplified when particles are both angular and concave. Moreover, trends in the porosity and AoR are dissimilar. This suggests that even convex polyhedra with rolling friction may not be able to capture the correct behaviour of both properties simultaneously. Overall, the VLS-DEM method provides a promising approach to accurately and efficiently describe complex particle shapes using the discrete element method.

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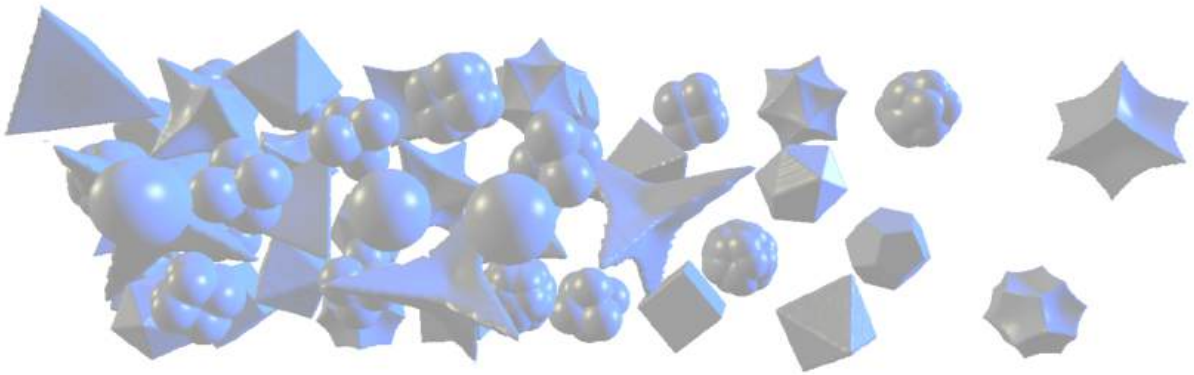

A new molecular dynamics-like approach for true polyhedra assemblies – Application to the simulation of crushing

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Keywords Modelling approach, molecular dynamics, polyhedra, crushing, Voronoï tessellation

Modelling the behaviour of granular media using discrete element methods (DEM) has received wide attention for more than four decades. Although granular media composed of non-spherical particles are very common both in nature (rock particles, blood cells) and manufactured activities (tablets in pharmaceuticals industry, aggregates in the construction sector) [Zhong_2016], most DEM simulation tools still model granular media as rounded particle assemblies, mainly spheres and super-quadrics [Lu_2015]. Yet, these spherical-DEM tools tend to suffer several limitations: first, paving a void-less granular medium such as a crushed rock aggregate with a solid fraction equal to 1, using non-overlapping spherical particles is not possible, which makes volume conservation impossible during fragmentation process simulation [Orozco_2019]; second, both experimentations and simulations show that triggering and sustaining avalanches of dense assemblies of angular particles requires significantly more energy compared to spherical particles [Azéma_2012]. The present contribution introduces a new molecular dynamics-like modelling approach aimed at simulating the mechanical behaviour of rigid true polyhedra dense assemblies [Descantes_2022]. Single or multipoint contacts between any set of two polyhedra of various size and shape are detected without prior edge rounding thanks to the combination of the multi-grids linked-cells method [Ogarko_2012] with an improved version of the Gilbert-Johnson-Keerthi algorithm [Descantes_2019]. Particles orientation and angular velocity are calculated upon integrating the torques equations using an original leap-frog Verlet algorithm [Omelyan_1999], in which no periodic renormalization of the quaternions is necessary. The potential of this new discrete element approach is then highlighted by simulating the crushing of void-less granular cylinders, each discretized into polyhedral Voronoï cells, in various loading configurations [Artoni_2019]. As illustrated by figure 1 with Brazilian test results (inset displays 3D loading configuration and red marks show broken cohesive bonds), dimensionless force-displacement curves similar to those reported by these authors are obtained.

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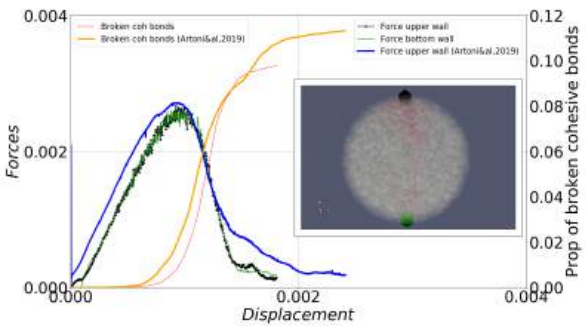

A novel superellipsoid particle collision model

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Keywords Non-spherical particles, particle collisions, superellipsoid, Newton-Raphson, OpenFOAM

Suspended particles in flows are widely present in nature and in various industries such as pharmaceutical, petrochemical, and wastewater treatment. In general, most natural and man-made particles are non-spherical, such as blood composites, dust particles, or microplastics, [1]. In most suspensions, particle interactions are present, i.e. particle-wall as well as particle-particle contact, such as the deposition of fibers in human lungs. To increase the efficiency of pharmaceutical and industrial applications, such as targeted drug delivery or particle segregation, the physics of these non-spherical particle systems must be well understood. However, the motion and interactions, i.e. collision, of arbitrarily shaped solids suspended in flows are complex, and to date, research in this area has been sparse. In general, most studies have focused on spherical particles (as they simplify the description of motion) in combination with shape factors to account for non-sphericity. However, these shape factors usually fail to accurately predict particle motion, [2], and there is no applicable correction for rotational motion. Using the superellipsoid formulation, which is an extension of the spherical or ellipsoidal shape, various non-spherical shapes can be generated, ranging from spheres, ellipsoids, cylinder-like and cubic particles to diamond-like shapes, [3]. In our work, we aim to accurately describe non-spherical particle systems by employing a novel fast, accurate, and stable non-spherical interaction model, i.e., a superellipsoid particle collision method that uses a fast, stable Newton-Raphson-based approach to predict collisions of non-spherical superellipsoidal particles. The developed model is based on the point-particle approach and is implemented in OpenFOAM. We first validate the proposed numerical scheme using analytical results, followed by more complicated collision examples including multiple contacts. We show that the use of our novel model leads to sufficient accuracy of predicting particle motion and particle interactions, which enables a further step towards modeling arbitrarily shaped particle systems.

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Stable integration of rotations for non-spherical particles in the Discrete Element Method

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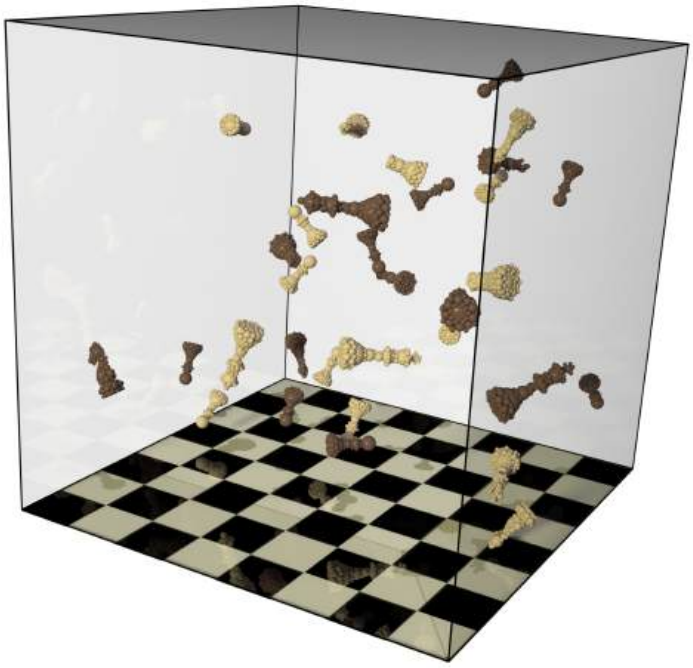
Keywords DEM, Integration Algorithms, Non-spherical particles

Efficient integration of motion is crucial for simulating a wide range of physical systems. Despite better algorithms for integrating the motion of non-spherical particles being available for over 25 years, the current State-of-the-art discrete element method (DEM) codes still rely on inaccurate rotation integration algorithms. This issue is particularly noticeable with the increasing popularity of simulations featuring non-spherical objects. We aim to address this issue, highlight the advantages and limitations of existing algorithms, and propose solutions. We have developed a new third-order algorithm that does not require quaternion normalization for each timestep and works for leapfrog and non-leapfrog schemes. The algorithm provides significant improvements over existing methods with only minor increases in computational cost. Our work includes the implementation and a comparison with those currently used in various DEM codes. Our results show that this approach improves accuracy, stability, and overall simulation performance over existing methods. We believe this algorithm can potentially become the new standard in the field. Furthermore, the outcomes of this algorithm are not limited to the discrete element method but can also be valuable for other particle-based techniques such as molecular dynamics (MD).



On the order of the leapfrog-Verlet method applied to the Kuwabara-Kono force model in Discrete Element Method simulations of granular materials

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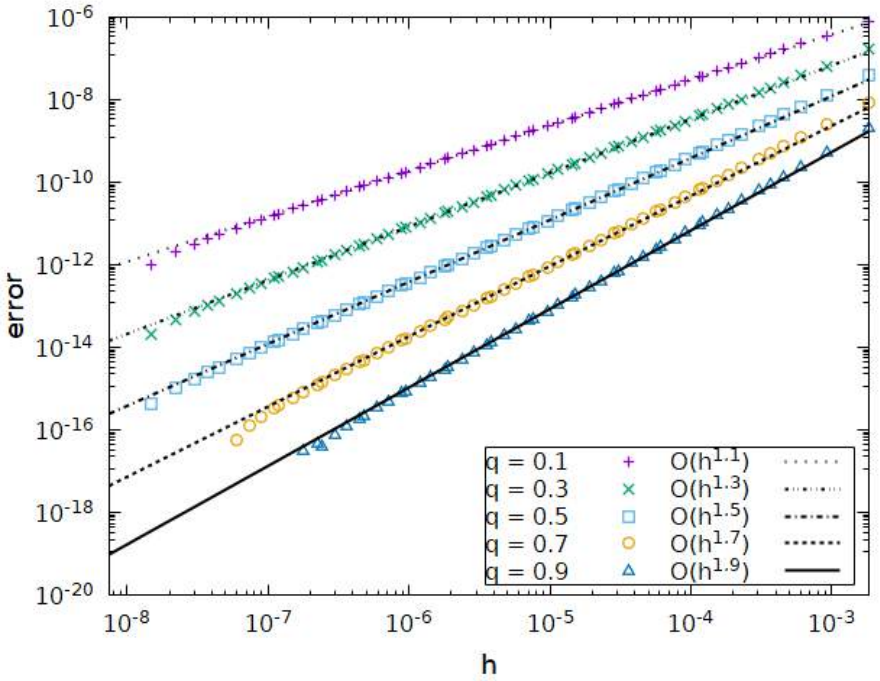
Keywords Granular materials, discrete element method, Verlet method, leapfrog method, Kuwabara-Kono model

The discrete element method (DEM) is a numerical technique widely used to simulate granular materials. The temporal evolution of these simulations is often performed using a Verlet-type algorithm, because of its second order and its desirable property of energy conservation. However, when dissipative forces are considered in the model, such as the nonlinear Kuwabara-Kono model, the Verlet method no longer behaves as a second order method, but instead its order decreases to 1.5. This is caused by the singular behavior of the damping force in the Kuwabara-Kono model at the beginning and in the end of particle collisions. In this work, we introduce a simplified problem which reproduces the singularity of the Kuwabara-Kono model and prove that the order of the method decreases from 2 to 1 + q, where 0 < q < 1 is the exponent of the nonlinear singular term. Furthermore, we propose a regularized normal force model based on the concept of mollifiers. We show numerically that the Verlet method combined with this regularized force model can integrate collisions with second order accuracy and that the coefficient of restitution of the system tends to increase as a function of the regularization parameter.



Session: Flexible shape particles

Discrete Element Modelling of Flexible and Shape Memory Fibres

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Keywords Flexible ribbon-like particle, Shape memory, Discrete Element Method

The bonded fibre model [1] was extended to simulate flexible ribbon-like particles, which can be biomass and agricultural materials, rubber chips, and textile products. In the model, a ribbon-like particle is discretized into triangular elements, and the neighbouring nodes are connected by the elastic bonds. The contact detection between two composite particles is determined by the node-node, node-band, band-band, and node-face contacts. A library of irregular shaped ribbon-like particle templates with various circularities is created for generation of a mixture of particles with various shapes. The numerical model is then utilized to investigate the effects of particle size and shape distributions on packing densities of cut biomass leaves. As a further development, constitutive relation of fibre bond bending moment and deformation is modified to account for the shape memory effect. The shape memory fibre exhibits large plastic deformation subject to large loads, and the deformed fibre can recover to its original shape under high temperatures. The model is validated by comparing with the experimental results, and several mechanical properties of such temperature-controlled shape memory fibres are explored.

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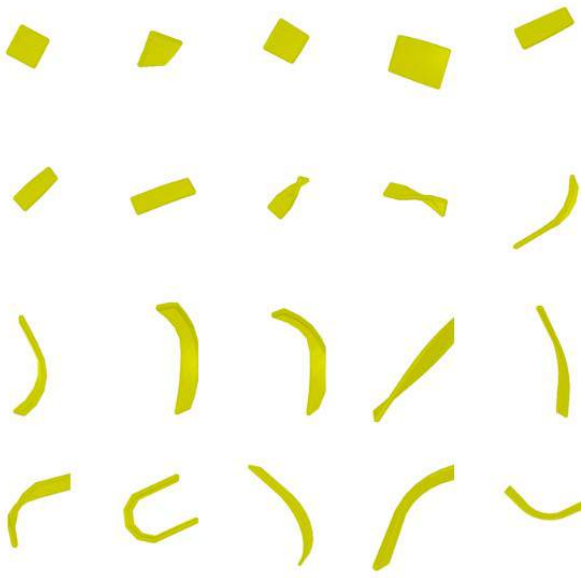

Calibration of a Discrete Element Model of Gelatine

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Keywords Biological tissue, gelatine, calibration, penetration

Remote Drug Delivery Systems (RDDS) are often used in the veterinary industry to sedate animals that cannot be safely approached for medical treatment for example. A common form of RDDS is the tranquilizer dart, often deployed using an air rifle. These rifles are set up beforehand to fire a specified payload at a target over a set distance. The challenge is to set the rifle such that the dart would penetrate the skin of a larger animal and also not injure a smaller animal. Tests on sedated animals are expensive and require ethical clearance. Thus, tissue surrogates with similar material properties are often used, and one such surrogate is Fackler gelatine. Numerical modelling could also prove to be a powerful tool for studies involving biological tissue, because it eliminates the need for ethical clearance. One such tool is the discrete element method (DEM). In this study a series of experiments were conducted on Fackler gelatine to determine the material properties. This included uniaxial compression, a penetrator and a drop-ball experiment which were then used to calibrate the model. A contact model was used to bond particles together and the standard formulation of the bond normal stiffness was modified to incorporate a viscous term and a strain-dependent term. Finally, the model was validated by firing a spherical steel projectile, with diameter ranging from 11.0 mm to 12.3 mm, into Fackler gelatine at speeds ranging from 62 m/s to 130 m/s and comparing the measured results to the simulation results.

Modeling soft particles by a coupled DEM-MPM method

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Keywords Material Point Method (MPM), Contact Dynamics Method (CDM), Soft particle, Granular materials, Compaction

Soft particles can be described by their shape degrees of freedom, i.e. particle-level deformations, contrasting therefore the general approach used in the conventional DEM based on strains whcih are assumed to be localized at the contact points between particles. Many materials such as pharmaceutical and food products are composed of soft particles that can deform elastically or plastically under low confining pressure. To model the rheology of soft-particle materials, we use the Material Point Method (MPM) to calculate the particle strains and the Contact Dynamics Method (CDM) for the treatment of unilateral contact and Coulomb friction law. MPM is adapted for large deformations and makes it possible to avoid cumbersome remeshing (in FEM) of particles close to the contact regions. We apply this approach to investigate the compaction of an assembly of elastic or plastic particles [1-4]. In particular, we are interested in the behavior beyond the jamming state as a function of material parameters including the friction coefficient between particles, the Poisson ratio, and the plastic hardening parameter.

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Discrete element method for smooth polyhedron with rigidity and large deformation based on Minkowski sum method

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Keywords Discrete element method, Minkowski sum method, Arbitrarily shaped particles, Dilated triangular elements, Large deformation

Arbitrarily shaped particles with smooth surfaces are widely found in nature, and rubber particles have large deformations in industrial processing and production. However, the traditional discrete element method (DEM) has difficulty in simulating arbitrarily shaped particles and in reflecting the large deformation of granular materials. In this study, a smooth polyhedral discrete element method based on the Minkowski sum method is developed, and a chain-link algorithm is adopted to simulate large deformations of particles and structures. An arbitrarily shaped particle with smooth surfaces is composed of several dilated triangular elements, and the contact problem between particles is transformed into contact detection between dilated triangular elements. Subsequently, the internal forces and large deformations of chains, nets, thin shells and particles under external forces are calculated by introducing a chain-link method and considering the tensile, shear, bending and torsional stiffnesses on cylindrical elements. This DEM model provides an effective numerical method for engineering applications of large deformations of particles and structures.

Session: Particle-fluid interactions in industrial applications II

CFD/DEM simulations of a pilot scale blast furnace raceways dynamics

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Keywords Blast furnace, Raceway dynamics, core-shrinking, cohesion

The raceway stability and dynamics of an experimental blast furnace pilot are studied with an unresolved CFD/DEM approach. Particles-gas simulation results show that a cohesion force is necessary to obtain a stable raceway which is initially imposed. A core-shrinking model to mimic the coke consumption has been used to study the dynamics of the raceway. The gas pressure fluctuations in the raceway and the collapse cycles found in the pilot experiment are qualitatively reproduced in the model. A sensitivity analysis on the injection flow rate showed that the CFD/DEM model can capture the time increase between two collapses as the flow rate increases, in agreement with the experimental observations. Predicted raceway size and shapes are also in a good agreement with the experimental measurements in the range of investigated flow rates. Overall present findings show that a cohesion force exists at the raceway interface which controls the stability and the dynamics of the raceway at the pilot scale. The application of the model on a larger scale is then considered.

Numerical modeling of wet ball milling process by CFD-DEM-VOF

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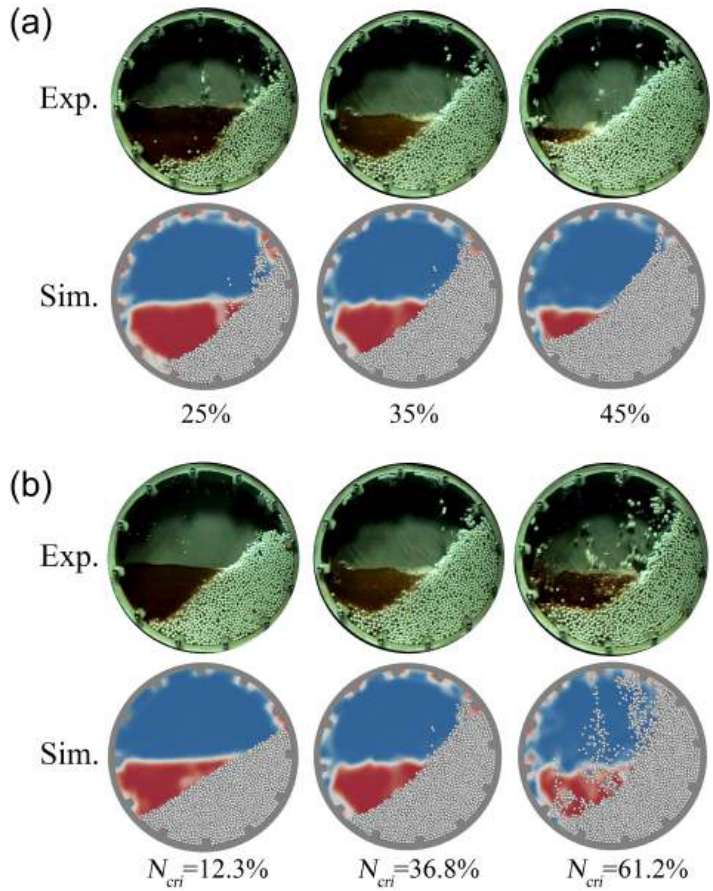
Keywords Multi-phase flow, gas-liquid-solid coupling, wet ball milling process, CFD-DEM-VOF, comparable particle and CFD cell size

Wet ball mill possesses the advantages of large production capacity, high grinding efficiency, low investment and so on. Therefore, it has been widely used in the industries involving mineral processing. However, the investigations focusing on the wet ball milling process should be relatively few up to now. Considering the wet mill is a typical gas-liquid-solid three-phase system, therefore, a numerical model by coupling CFD (Computational Fluid Dynamics), DEM (Discrete Element Method) and VOF (Volume of Fluid) that can treat the flow of particles possessing the comparable size with CFD cells in the gas-liquid systems is first developed for simulating the wet milling process. The accuracy of the established CFD-DEM-VOF coupling model is then demonstrated with the single particle sedimentation in air-liquid domain, water entry of particle assembly and three-phase flow in a lab-scale wet mill. Subsequently, the flow dynamics in an industrial-scale SAG (Semi-Automatic Grinding) mill with and without liquid are simulated by the established model. According to the simulation results, the performances of dry and wet ball milling processes, including the overall charge behaviors, power consumption and grinding media wear, are emphatically evaluated. The rather obvious differences between the dry and wet ball milling can be found.



DEM-SPH based ship-ice-water-propeller coupling simulation for ship speed analysis in sea ice regions

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Keywords Discrete element method, DEM-SPH coupling, dilated polyhedron, ship-ice-water-propeller coupling

The discrete element method is acknowledged as a valid approach in the simulation of ice-structure interactions. A dilated-polyhedron-based DEM, named DPDEM, is developed to simulate the sea ice fracture and ice load on structures. The dilated polyhedron, based on the Minkowski sum theory, is used as the irregularly shaped element in the DEM to simulate the sea ice in this study. The bond-failure model is developed to simulate the breaking process of sea ice, considering the energy release rate and stiffness softening. The seawater is simulated with an explicit incompressible smoothed hydrodynamics (SPH) method. The DEM-SPH coupling between seawater and sea ice, ship hull and propeller is also established with a direct interaction model. The ship hull and propeller are regarded as rigid bodies. To simulate the ship navigation in seawater, a buffer particle zone is used to add/delete particles to implement the speed and pressure boundary of the SPH domain. A full-domain DEM-SPH simulation is conducted to obtain the resistance of the ship hull, while the rotation of the propeller is neglected. Meanwhile, a local domain simulation around the propeller is conducted to obtain the thrust, while the rotation of the propeller is considered. Through a group of simulations under different rotational speeds of the propeller, a specific rotational speed of the propeller and ship navigation speed in sea ice can be determined. Then, the relationship between ship speed and sea ice thickness can also be obtained. The results are partly validated with that of model tests, which are in good agreement. The DEM-SPH coupling model can be further used in ship hull design and analysis in cold waters.

An application of the DEM-CFD approach to the various industrial devices

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Keywords DEM-CFD, VOF, IBM, iGRAF, Mixing

In industrial fields, there are many kinds of powder processes such as mixing, packing, storage, transportation, separation, crush, fluidization, stirring, and so on. In our research group, we have developed a comprehensive software named the Integrated Granular Flow Simulation Software, iGRAF. iGRAF can be applied not only to the powder simulation but also to the fluid flow simulation and has contributed to various kinds of industrial fields. The discrete element method is adopted for the powder simulation and the finite volume method, FVM is for the fluid flow simulation. In the DEM, the van der Waals force, the lubrication force, and the liquid bridge force up to moisture content of 15% are considered. In addition, the coarse graining approach which drastically reduces the number of particles to be solved is also implemented, and therefore the actual system with large scale can be solved within reasonable computational effort. The analytical objects with complex geometry are described with the immersed boundary method, IBM. Further, moving boundaries are also represented with the IBM, allowing to treat the various kinds of the industrial devices easily without any complex mesh. Fluid flow simulation with free surface, as is seen in the gas-liquid two-phase system, is conducted by using the volume of fluid method, VOF method. In the presentation, we will present some achievements by using the above-mentioned software, iGRAF. For example, the powder mixing in the ribbon-mixer is numerically solved, and the mixing was quantitatively evaluated by using the Mixing Index. As a result, the initial packing position of the particles strongly affected the mixing performance. Therefore, the mixing could be understood not only from animation but also from numerical value. Another application is the planetary mixer. The simulation successfully evaluated the dispersed state of particles during mixing by quantitating the spatial void fraction.

Investigation of high-throughput particle separation in DLD-DEP microsystems by resolved CFD-DEM simulations

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Keywords CFD-DEM coupling, IBM, microfluidic systems, high throughput, multiphase flow

In the industrial production of active pharmaceutical ingredients, ceramics and particle-laden printing inks, particles in the size range below 10 µm are increasingly required. Only a few currently known separation processes cover this size range – Deterministic Lateral Displacement (DLD) is one of them. The DLD describes a microfluidic channel interspersed by a large number of specially arranged posts that create a characteristic flow pattern. Particles following the flow occasionally bump against the posts, resulting in size separation. Influencing factors are the arrangement and shape of the posts as well as the Reynolds number. For additional fractionation according to material-specific properties (permittivity, zeta potential), the DLD structure will be combined with dielectrophoresis (DEP). The DEP describes a material-dependent force exerted on uncharged particles by an inhomogeneous electric field. Within the DFG priority program 2045 "MehrDimPart" we investigate multidimensional fractionation using a combined DLD-DEP microsystem. The aim is to use both methods of particle fractionation for industrial purposes. Therefore, we try to overcome the existing limitations by redesigning the microsystems for the highest possible solids content and throughput. For this reason, parameter studies were performed using four-way coupled immersed boundary CFD-DEM simulations. In a simplified DLD simulation model, the post arrangement, size, and shape were varied, as well as the throughput, solid concentration, and particle shape. The results show that increasing the Reynolds number to Re = 50 and choosing triangular posts improves the separation. The particle volume concentration should not exceed 3.6 %, because beyond that the separation efficiency decreases significantly. To study the DEP process, the resolved CFD-DEM solver was extended to calculate the inhomogeneous electric field on the FV mesh. This allows to apply electric and dielectrophoretic forces to the particles.

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Session: Vibrated systems and charged particles

Discrete-element modeling and experimental validation of the charging kinetics of a vibrated layer of particles

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Keywords Electrostatic, DEM simulations, tribocharging, model material

Electrostatic separation processes rely on the triboelectric properties of particles to sort them in an electrical field. This process has received increasing interest in many applications such as recycling of plastics particles, removal of unburned carbon from fly ash or separation of the components of interest from low-value agricultural resources such as extraction of lignin from wheat straw residues [1]. To better understand the triboelectric separation, we developed a numerical model based on the Discrete Element Method (DEM) to simulate the charging kinetics of a thin layer of particles subjected to vertical vibrations and performed experiments for validation. This model is based combines the equation of Laurentie et al [2] for charge transfer at the particle scale and the conceptual approach of Matsuyama and Yamamoto [3] for charge relaxation. The experiments were used to calibrate and validate the model using a vibrated cell containing glass beads. The charging kinetics was monitored by means of a Faraday cage for several values of the total mass of the particle bed. In all cases, we find that the global charge increases rapidly before leveling off at a constant value. Furthermore, the global specific charge (per unit of mass) decreases as the thickness of the particle bed increases due to charge relaxation during collisions between particles. We show that the charging process is governed by a characteristic time which allows us to scale the charging kinetics whatever the mass of particles. This scaling reveals the dynamic origin of the charging process of a granular material.

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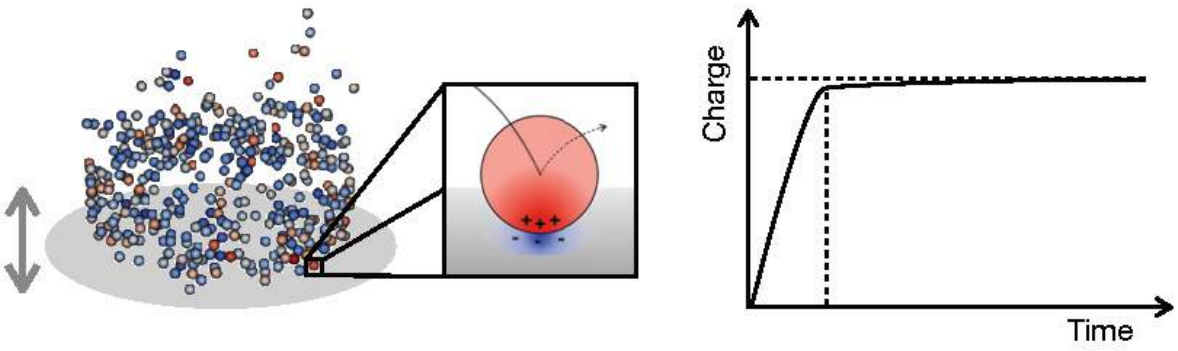

Tribocharging of patchy particles

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Keywords Tribo-eletricity, charging, granular flow, cohesion

During granular flow, particles may charge significantly resulting in a strong alteration of the material's cohesiveness. This tribo-electric charging arises from charge transfers during contacts between grains. It depends on many parameters such as ambient humidity or particle size making this effect complex to understand. A popular model reproducing same-materials tribocharging relies on the existence of patches at the surface of the particles. When in contact, such patches may transfer charges from on to another, leading to a global redistribution of charges. We performed DEM numerical simulations of patchy particles and obtained charge transfers which are consistent with experimental results. Moreover, our model correctly reproduces the characteristic charging of bi-disperse granular materials where small particles charge negatively while large particles charge positively. Finally, we studied the flowing properties of patchy particles and recovered many cohesion related phenomena, such as plug-flow, once tribocharging occurred.

About phase transition in vibrated granular material

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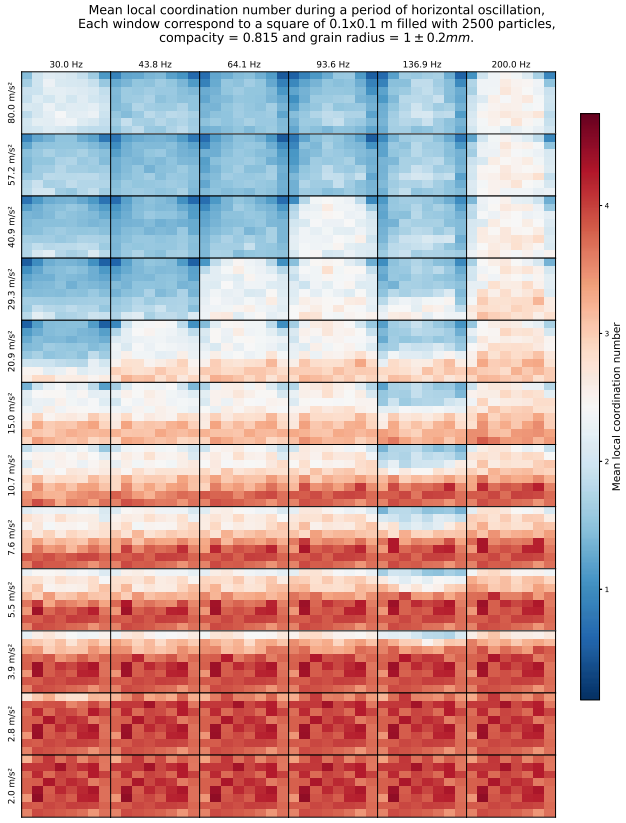
Keywords Phase DEM contact dynamics granular vibration

The behaviour of vibrated granular media is widespread in the literature. Therefore, the influence of frequency, amplitude and direction of loading are among the most studied parameters. However, it remains very difficult to characterise the transitions in the behaviour of the medium (solid/liquid/gaseous) because the different studies do not overlap and when they do, the filling rates are often different. Moreover, there is no real indicator to unify the different behaviours. In this study, we investigate the behaviour of a vibrated granular material confined in a hollow structure under different vibration amplitudes and frequencies. The study is performed using the 2D contact dynamics approach. The reference simulation considers 2500 circles of radius 1 mm, with a variation of 20%, subjected to horizontal excitation from 10 Hz to 1000Hz and 0.1m/s² to 10 g. The granular material is contained in a quadrangular box. After the system has reached a steady state, we investigate the effects of frequency and acceleration as well as the effects of compactness and the value of the Coulomb friction and coefficient of restitution. Our results reveal that the acceleration amplitude of 1g commonly used as a limit for the solid regime is a rough approximation of reality. The transition between solid and liquid behaviour is mainly influenced by the height and width of the structure. We demonstrate the complexity of the boundary between the collective solid and liquid behaviour of grains by using relevant indicators, such as the periodic local coordination number or the average affinity path. Furthermore, we propose a phase transition law that incorporates the contribution of static stress and the characteristic times of flight of the grains.



A discrete element model for investigating the electromechanical characteristics of particulate systems

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Keywords Discrete element method, Electromechanical coupling behaviour, Resistance measurement, Electrical conductivity

The electrical transfer during mechanical actions in particle-to-particle contact is a crucial aspect across many fields [1]. The complexity of particle characteristics leads to challenges in quantitatively assessing the electromechanical behaviour in the experimental studies. In this work, a 3D discrete element model has been developed based on previous work [1–3] to investigate the conductive behaviour during particle-to-surface contact under combined mechanical motions of loading and torsion. The Hertz-Mindlin model has been employed to detect mechanical reactions at each contact point, while Ohm's law and Kirchhoff's law define the electrical characteristics of local contacts and global network. The model has been run through the EDEMTM software package and then validated by comparing it against data from high pressure torsion (HPT) test. The results show a good agreement between the simulation and experimental results. In addition, the results indicate a strong correlation linking particle size, contact area, resistance, and electrical tension. This study has implications for the development and optimisation of materials and electromechanical systems.

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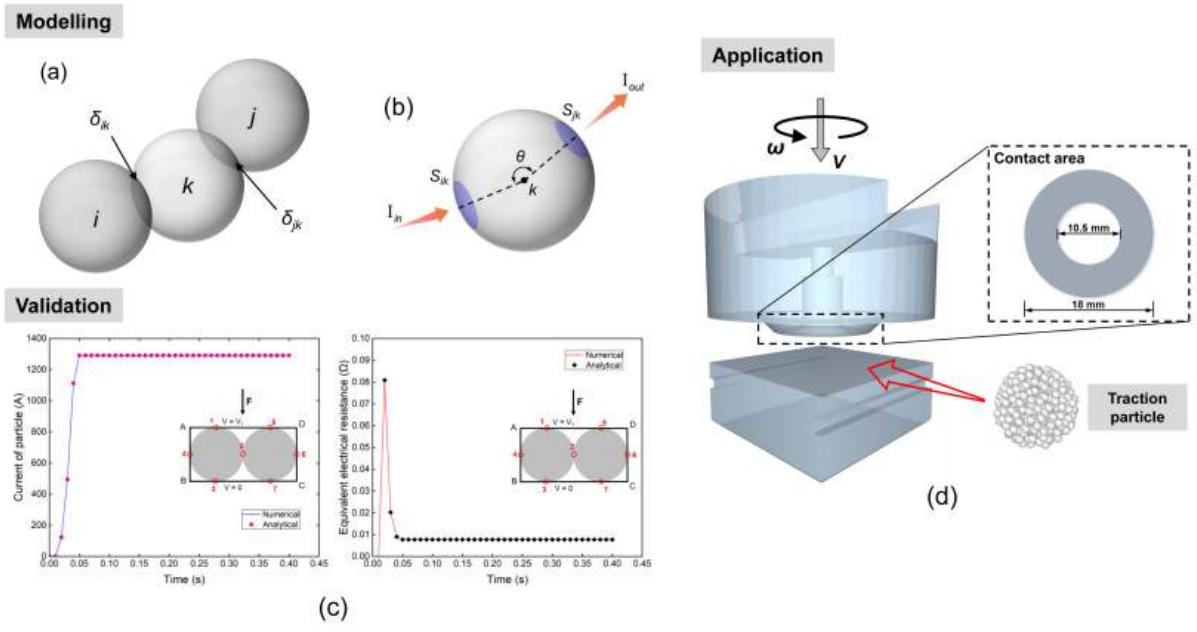

Granular Convection in Micro-Gravity

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Keywords Granular convection, micro-gravity

When a cylindrical container partly filled with granular material is shaken vertically, in the presence of gravity, a pronounced convection pattern is observed, where the material moves upwards in the center part and downwards in the region close to the vertical wall. In the absence of gravity, we find a new convection pattern characterized by a symmetry break due to tiny imperfections of the apparatus. The experimental data can be well understood by means of DEM simulations. While in gravity, the convection is driven by an interplay of shear dilatancy and freezing through a shock wave, the mechanism that drives the convection in the absence of gravity is yet unknown.

Session: Powder processes technology: Additive Manufacturing

Microstructure evolution during sintering: Discrete Element Method approach

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Keywords Sintering, grain growth, microstructure, polycrystal

We present a new numerical model for the sintering of a powder of crystalline particles into a dense, polycrystalline solid. Although our method can be categorized as a Discrete Element Method, it over-comes some of the typical limitations of these methods: 1) The method derives shrinkage and grain coarsening from the minimization of the free energy. 2) By representing each grain as a truncated sphere, it takes the complex and changing shape of the grains into account to determine the thermo-dynamic driving forces and associated kinetic coefficients. We avoid the calculation of diffusion fields at the sub-grain scale, but validate the model by comparing the temporal evolution of a system of 4 particles with results from such a continuum model. Taking advantage of the computational efficiency of Discrete Element Methods, we simulated the sintering of polydisperse agglomerates of up to 16000 particles on a standard desktop workstation. Using material and process parameters from the literature, the model accurately reproduces experimental data on the evolution of the grain size distribution for alumina [1].

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Wall effects in granular column: Revisiting Janssen's equation

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Keywords Reverse Janssen effect, wall stress, Frictional contact, silo, DEM simulations

Granular materials in vertical containers have numerous industrial applications. The forces exerted by the granular materials on the walls of the containers stand as an important indicator for the collapse of storage systems such as silos. In this work, we systematically study the filling of the granular container computationally, to analyze the evolution of the wall forces as the filling progresses. Janssen was the first to study experimentally the filling of the granular columns and found that the force on the base saturates after a filling height is reached. Part of the weight of the filled mass is transferred to the wall of the container. Recently, the reverse Janssen effect was studied both experimentally and computationally, which demonstrated the force carried by the base within certain range of smaller filling heights overcomes the actual weight of the particles in the container. A qualitative trend was found between experiments and simulations. In this work, we revisit the filling phenomena to study computationally the essential features present in Janssen's model. The reverse Janssen effect is also observed in our simulations by means of discrete element method (DEM). Our work also considers the role of particle size, column diameter and friction parameters.

Powder spreading of irregular particles with thermal properties

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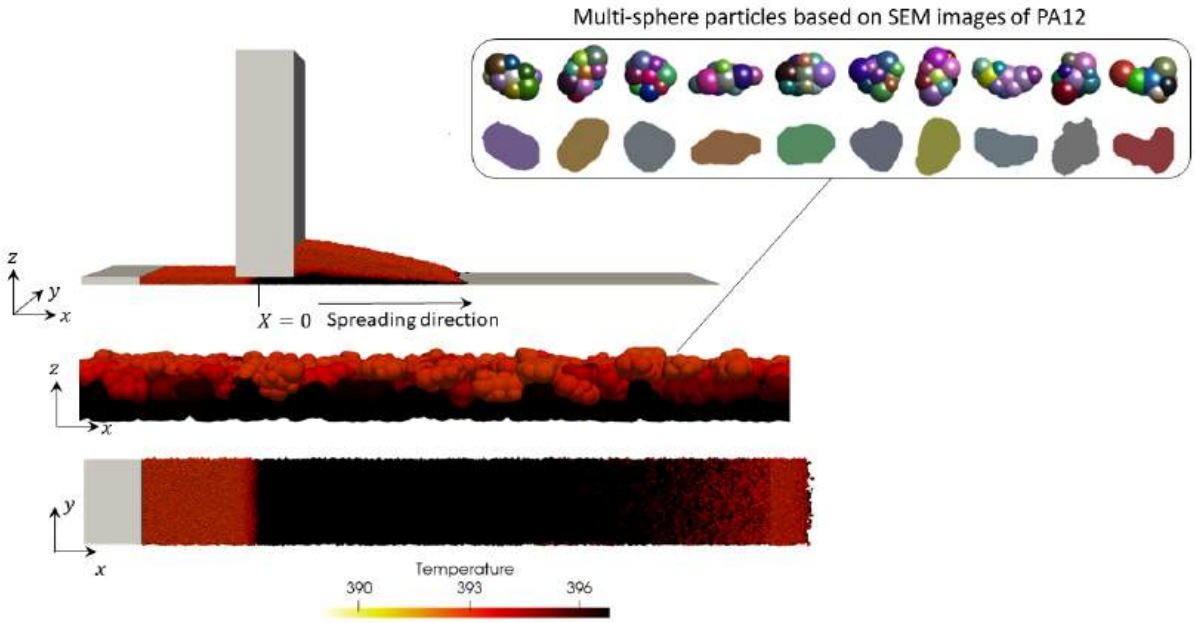
Keywords Multiparticle, Discrete Element Method, powder spreading, thermal

Understanding the thermal and mechanical behavior of the powders used in additive manufacturing is important for improving the quality and reliability of the finished part. The heat transfer in the powder bed is influenced by particle shape, the dependence of interaction properties on temperature as well as the blade speed. The heat transfer in the powder bed strongly influences the quality of the finished powder layer, such as the packing density and the surface profile. In this context, the role of particle shape coupled with its thermal properties is hardly ever explored in the literature and thus is a subject of great potential. In this study, we introduce an extension of the Discrete Element Method (DEM), to simulate non-spherical particles with heat transfer enabled by merging a multisphere algorithm with a thermal discrete particle model. The application of this model is demonstrated with simulations of a powder spreading process using Polyamide 12 (PA12) powder particles of irregular shapes. We characterize the packing density and the surface profile of the powder layer subjected to varying blade speed and the dependence of the particle stiffness on temperature. We observe that the packing density decreases and its standard deviation increases with increasing blade speed. Further, the packing density is more sensitive to small values of dependence of the particle stiffness on temperature. The mean surface roughness is observed to increase with increasing blade velocity. These results demonstrate the potential of our model in exploring the spreading process for real powder particles featuring variety of irregular shapes by considering their thermal and mechanical aspects.



Sintering of particles: grain-growth and non-sphericity treated with DEM

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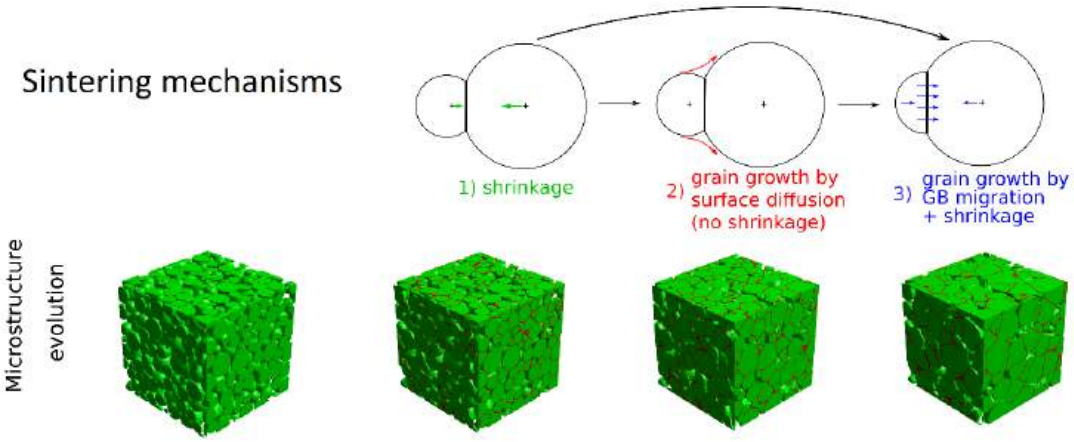
Keywords Non-spherical particles, grain growth, sintering, LS-DEM

Sintering of ceramic powders is a high-temperature process that aims to densify an initially particulate material. The driving force is the reduction of the interfacial energy of the system. The same driving force leads to grain growth, which is generally considered detrimental. Here we explore the coupling between densification and grain growth at the particle scale. Simultaneously occurring shrinkage, surface diffusion, grain boundary migration and particle coalescence are implemented in a DEM framework. The adopted model treats the main fluxes of matter through physics-based interaction laws. Small particles are gradually eaten away by larger ones, leading to coalescence and grain growth. The results of these simulations are compared to experimental data with good accordance of key features of microstructure evolution (densification kinetics, grain size-density trajectory, average grain size evolution). By taking advantage of the possibility to simulate initially a large number of particles (which gradually disappear with coalescence), the model elucidates the influence of the initial particle size distribution on the grain growth kinetics. Because ceramic particles are seldom spherical, we also implemented non-spherical particles using the Level-Set method. This is particularly important for sintering, as it is a curvature driven process. Contact detection, which is the critical step, is treated as an optimization problem, to reduce computational costs. The proposed implementation of LS-DEM is a proof of concept of its potential effectiveness for sintering. For illustration, simulations of packings of ellipsoidal particles with elastic and sintering interactions are described. The sintering simulations are used to analyze the influence of the particle aspect ratio, in particular on the shrinkage rate.



Computational studies of the effect of moisture on powder bed quality in metal additive manufacturing

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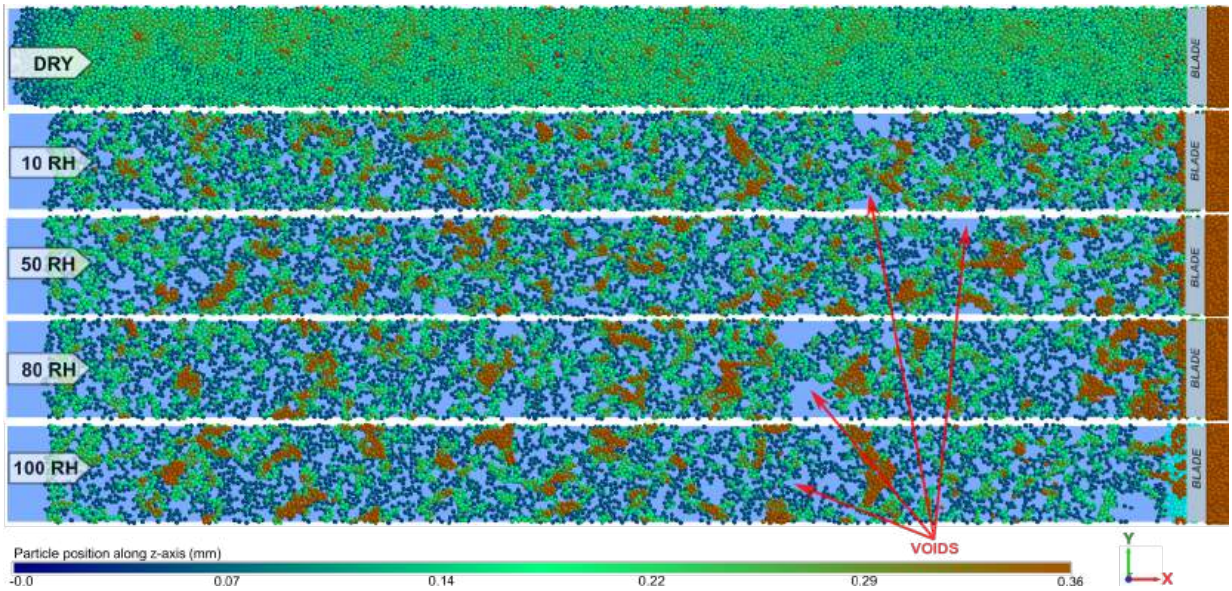
Keywords Metal Additive Manufacturing, Powder Bed Laser Fusion, Mikami Liquid-Bridge Contact Model, CFD, DEM

Metal additive manufacturing techniques based on the powder-bed laser fusion (PBLF) process rely on a high-quality powder bed to minimize the formation of defects in the manufactured parts. Various parameters such as the blade velocity, the thickness of the powder layer, shape and size of particles, angle of repose, coefficient of friction, moisture, and restitution are known to influence the bed quality. There is limited information available on the effect of moisture on powder bed quality while the effect of other parameters have been studied to varying degrees of thoroughness.

The purpose of this study is to simulate the powder spreading process considering the interactions between individual particles in the presence of moisture using a 3D discrete element method (DEM) model and to evaluate the effect of particle moisture on powder bed quality. The commercial DEM software package EDEM along with the Mikami liquid-bridge contact model and the Hertz-Mindlin contact model are used for the simulations. In addition, the combined effects of the gas-particle interaction forces on the spreading process of moisturized particles generated due to shield gas flow are simulated using a four-way CFD-DEM coupling. EDEM-OpenFOAM coupling is utilized for this purpose. The quality of the powder bed is measured in terms of void fraction, mass flow rate, surface roughness, and particle agglomeration. The results obtained show an increase in void fraction and surface roughness of the powder bed, indicating a degradation of the powder bed quality. The shield gas flow helps in reducing the void fraction of the moisturized powder bed. The average mass flow rate, agglomeration, and stress distribution results demonstrate that particles form aggregates due to moisture which may lead to jamming.



Session: Fracture & fragmentation

DEM study on ice block breakage

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Keywords Particle breakage, ice rubble, shear failure

Ice rubble, a collection of broken ice pieces, forms when intact ice fragments into a pile of discrete ice blocks. Ice rubble is a granular material, thus, discrete element (DEM) simulations can be effectively used to study its mechanical behavior. Continuous fragmentation of the ice blocks within deforming ice rubble is often ignored in DE simulations due to the lack of understanding of the underlying mechanics of ice block breakage as well as the scarcity of simple particle breakage models. Therefore, in this study, we investigated the mechanics of ice block breakage by using a bonded particle model (BPM) HiDEM. In the BPM study, we modeled a series of ice block breakage experiments by Prasanna et al. (2021). Stress distributions from the BPM simulations revealed that Mohr-Coulomb failure criterion can be used to model the failure of ice blocks under compressive ice-to-ice contacts. Following that, a simplified particle breakage model was developed and integrated in to an existing DEM simulation tool, and mechanical behavior of ice rubble was studied. In the breakage model, failure was determined by checking if the the quasi-static force equilibrium of contact forces acting on a particle meets the Mohr-Coulomb failure criterion. Simulations of direct shear box experiments on ice rubble with the particle breakage model revealed that ice block breakage is an important mode of failure for the load carrying force chains within deforming ice rubble.

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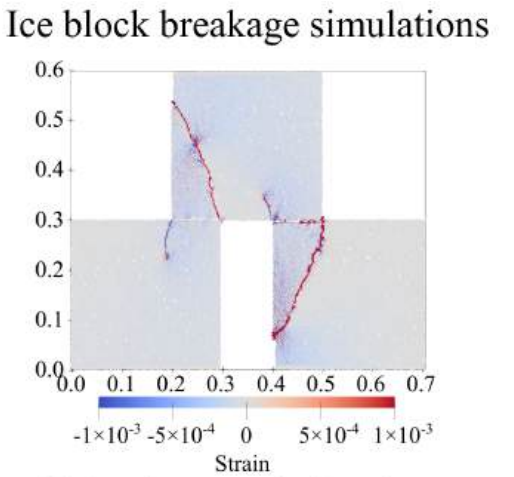
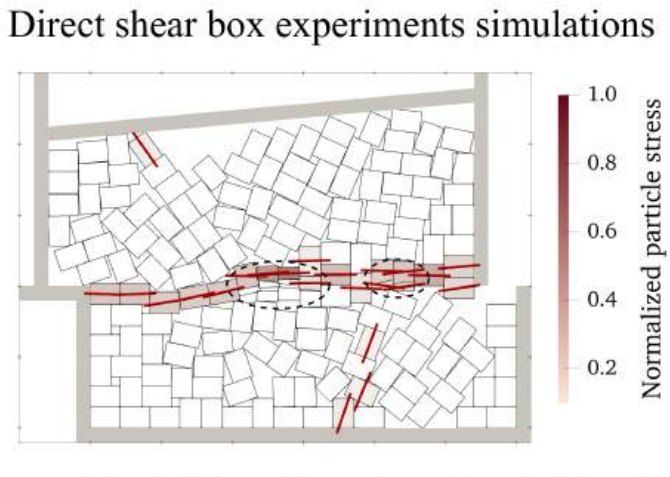


Ice blocks under compressive ice-to-ice contacts fail due to shear.



Force chains within ice rubble can collapse due to the failure of ice blocks. This deceases force transmission within the material.

DEM simulation of the fracture behavior of a composite with aerogel particles characterized by X-ray tomography

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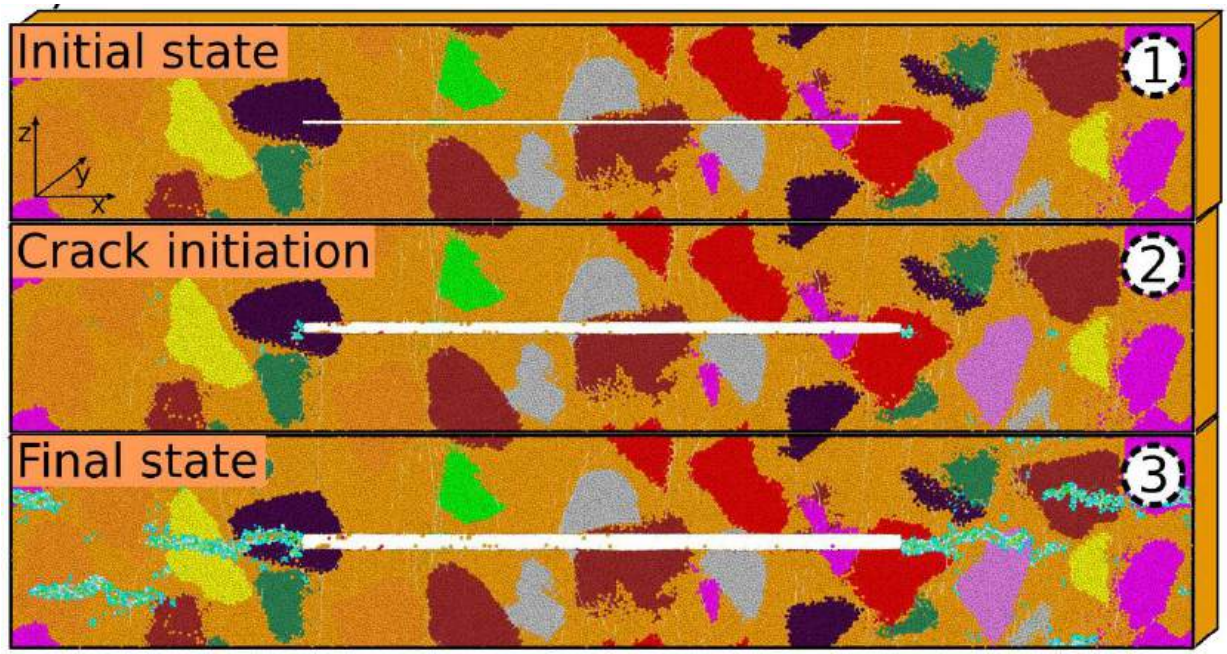
Keywords Fracture toughness composite bonds

Silica aerogel particles are an innovative solution for the development of a new class of products, the super-insulating materials. Their high nanoporosity (95%) is responsible for their unprecedented low thermal conductivities but also for their very low mechanical properties. Their use (for example in the building sector) therefore requires a better understanding of the link between the discrete microstructure of the material and the mechanical properties. DEM simulations are a powerful tool for this task and the aim of this presentation is to describe the procedure to model the fracture behavior of these complex materials. The materials studied here are composite panels produced using a bimodal distribution of silica aerogel grains, latex as binder and optionally some polypropylene fibers. Each of these components is represented in our DEM model using elastic bonds with an integrated shear and tensile failure criterion. Mechanical characterization (crushing) of individual silica aerogel particles is used to calibrate the material parameters of the digital particles, whose morphology is extracted from X-ray tomography. The simulated failure of individual digital particles is accurate enough to reproduce the crack patterns similar to those observed by X-ray tomography in real silica aerogel particles. Once this first validation is obtained, large numerical particulate composites are generated using the calibrated numerical silica aerogel particles. The elastic behavior of the composite is properly recovered from DEM simulations using the mechanical response of each of its individual components. The fracture behavior of composite samples is simulated by reproducing a pre-notched sample to assess their toughness. In particular, the crack growth behavior is investigated. The effect of the size distribution of silica particles is studied to propose some avenues for optimization. Similarly, the benefit of introducing of a small amount of fibers is demonstrated.



ANM-based fragmentation model of granular materials

Yohann Trivino[1,2], Farhang Radjai[2], Komlanvi Lampoh[1], Xavier Frank[1], Jean-Yves Delenne[1]

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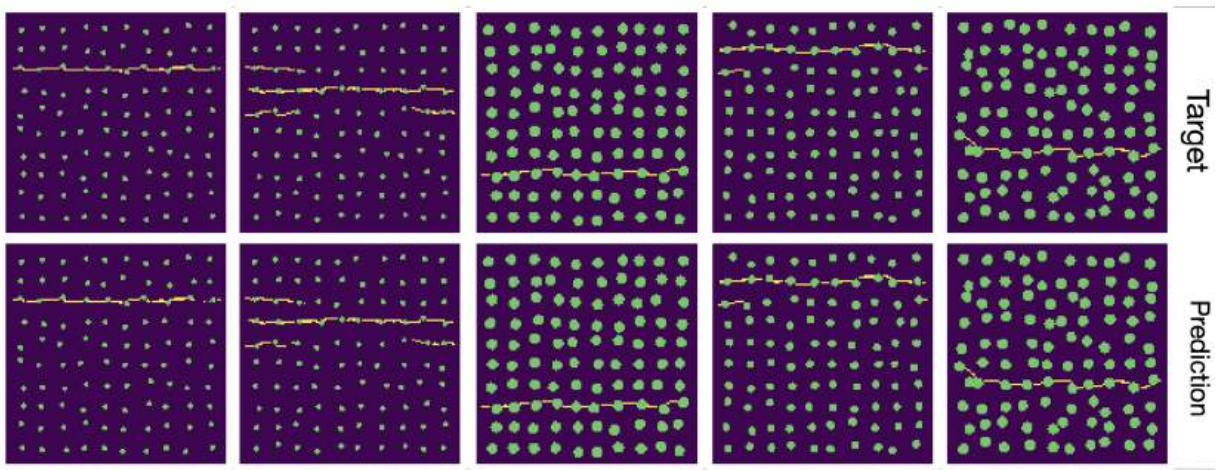
Keywords Fragmentation, Deep Learning, Neural Networks, Peridynamics

We present a new model for the fragmentation behavior of granular materials based on Artificial Neural Maps (ANMs), a deep learning architecture. To generate learning datasets, we consider the fragmentation of a unit square including a controlled level of disorder subjected to diametral traction and simulated by the Peridynamic method. More than 900 samples were simulated and the output data recorded up to failure. We used a specific 3-layer autoencoder for each pixel described by its fracture state (failed or unfailed). The loss function is based on the correlation between the dataset and the prediction. When a notch is introduced, the cracks are initiated from the notch and the crack is predicted with an accuracy of 100% independently of disorder. The speedup is at least 10000-fold between the peridynamic and ANM-based simulations. Our results show that ANMs can accurately capture the complex crack paths in the presence of disorder; see Figure. ANMs can be easily implemented in a DEM software to simulate an assembly of breakable particles with built-in texture.



Examples of the crack paths predicted by our ANM-based model (bottom line) and calculated by the peridynamic method (top line) with a resolution of 128×128 pixels. The pores are shown in green.

Image-informed Fracture Model for Complex-Shaped Particles in Discrete Element Simulations

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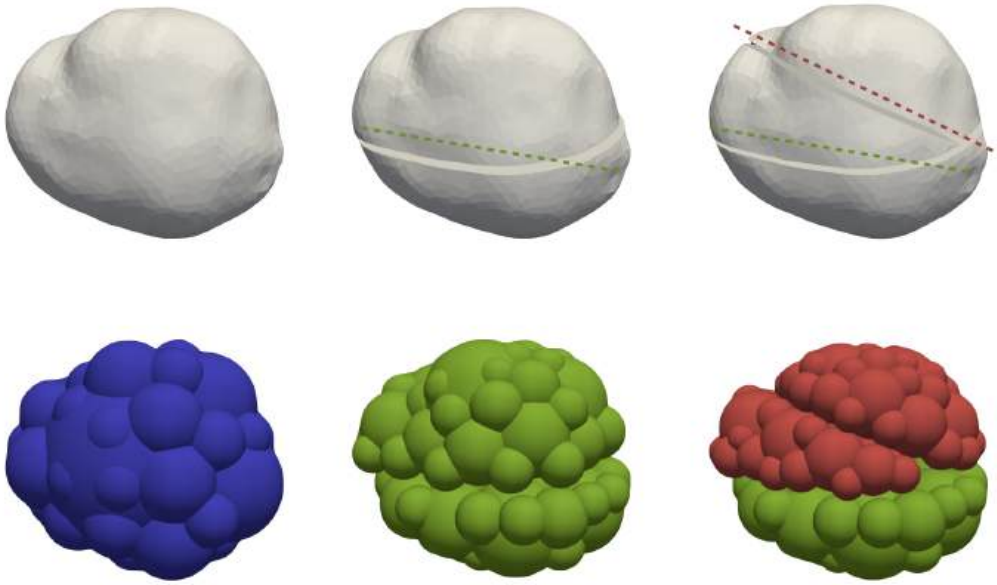
Keywords Fracture, fragmentation, complex-shaped, clump, image-informed

Particle breakage is a complex physical process that immensely affects the behavior of granular systems. Achieving accurate simulations of real crushable materials is challenging since modeling irregular particles is computationally intensive and hinders scaling up to large granular assemblies while predicting the evolution of particle morphology after each breakage event. The factors affecting it still need to be explored. We propose a novel particle breakage algorithm for irregular particles in the Discrete Element Method (DEM). Unlike standard practices in the literature, the proposed algorithm intrinsically preserves material bulk properties during the fragmentation of complex-shaped particles. This is achieved via the concurrent consideration of imaging data in the form of surface meshes and multi-sphere particle representations. The particle meshes are used to provide morphological information and to generate multi-spheres for each new generation of fragments, while the multi-spheres are used to determine the contact forces acting on the particles in the DEM simulations. We employ a combined Mohr-Coulomb-Weibull failure criterion to determine when a fracture occurs. The validity of the proposed algorithm is demonstrated via comparison with available experimental tests, where the model is found to result in statistically reliable results.



Session: Performance analysis & Machine Learning

A graph neural network based surrogate model for granular flows with complex boundary geometries

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Keywords Granular flow, Surrogate model, Graph neural network, Signed distance function

Numerical simulations of industrial-scale granular flows are quite challenging due to high computational costs. To address this issue, various surrogate models developed in recent years are rather promising technologies. In this study, we present a novel graph neural network (GNN)-based surrogate model, coupled with a signed distance function (SDF), to simulate granular flows with complex boundary geometries. Our proposed model adopts an encoder-decoder architecture within a graph-based framework, leveraging a message passing module to model particle collisions. Arbitrary-shaped wall boundaries are modeled through the SDF field. Validation tests are carried out in various powder mixing systems. Our results demonstrate that this model can accurately predict particles' dynamics and macroscopic mixing behavior in the long term. Furthermore, this model is shown to significantly reduce computational time by several orders of magnitude as compared with the original DEM simulation. This work would significantly contribute to the progress of modeling for industrial granular flows.

Acknowledgement
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Discrete Element Method with Machine Learning model of Liquid Bridge Force

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Keywords Discrete element method, Liquid bridge, Machine learning, Catboost algorithm, Geometric approximation energetic approach

Developing an accurate and efficient contact model for discrete element method (DEM) simulations that can describe the microscopic dynamics of low moisture content wet granular systems continues to be a major challenge. In this study, we introduce a geometric approximation energetic approach based on the traditional linear unit discretization method to solve liquid bridge problems. This simplified approach significantly improves the efficiency of constructing the dataset while ensuring high data accuracy. Using the proposed optimization method, we generate datasets consisting of 163,440,000 and 2,043,000 data points for the sphere-sphere and sphere-wall systems, respectively. Machine learning capillary force models (ML-CSP and ML-CW) are trained using the Catboost algorithm. These models demonstrate excellent performance in predicting capillary forces between particles as well as between particles and walls, considering different particle sizes, moisture levels, and contact angles, while neglecting the influence of gravity. The corresponding average absolute percentage errors are below 1% and 2%, respectively, which are lower than existing analytical models. We incorporate the obtained models into the discrete element method and calculate capillary force between particle pair and simulate wet granular column collapse tests using the discrete element method. The simulation results show good agreement with experimental results in terms of parameters such as inter-particle capillary forces and particle collapse run-off length. This study will provide an accurate and efficient numerical model for simulating low saturation wet granular systems using the discrete element method.

Data-driven multiscale modelling of granular materials via transfer learning

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Keywords Granular materials, DEM, Transfer learning, Data-driven material modelling, FEM×DEM Multi-scale modelling

The potential of data-driven approaches to revolutionize the constitutive modelling of granular materials has recently been the subject of intensive exploration [1-2]. However, despite the excellent ability of machine learning to capture stress-strain relations of granular materials, data scarcity poses a significant challenge to the development of this emerging constitutive modelling paradigm [3-4]. In this study, we propose two transfer learning-based strategies to leverage all available constitutive knowledge to assist material modelling. One approach utilizes phenomenological constitutive models to artificially generate massive stress-strain and volumetric strain data to train a base model, which is then repurposed to the data from numerical simulations via transfer learning. The other approach involves using available data on similar materials to train a base model, which is then applied to other targeted materials with limited data. The proposed transfer learning methods are tested on both DEM simulations of representative volume elements (RVEs) and FEM×DEM hierarchical multiscale modelling of boundary value problems (BVPs) of granular materials. The trained data-driven material model is embedded in implicit FEM simulations to validate its accuracy, efficiency, and stability. The results demonstrate that transfer learning can be an effective strategy to achieve high-quality machine learning predictions with limited data. The unique advantages, potential applications and limitations of transfer learning are also discussed in detail.

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Optimizing Particle Simulations: Performance Analysis and Code Generation with MD-Bench and P4IRS

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Keywords Particle simulations, code optimization, performance analysis, parallel architectures

Particle simulations are widely used in materials science, engineering, and physics to model the behavior of a large number of particles interacting with each other. A few examples of applications that rely on such simulations are Molecular Dynamics and the Discrete Element Method. Optimizing the code for modern parallel architectures such as multi-core CPUs and GPUs is crucial for running such simulations efficiently. In this talk, we will discuss performance analysis and code generation techniques for particle simulations using MD-Bench, a proxy-app for performance analysis and benchmarking of short-range MD kernels, and P4IRS, a python-based code generator tool that targets modern parallel architectures. We evaluate how we can leverage the knowledge obtained by MD-Bench for generating efficient codes beyond MD simulations such as DEM, where particles represent rigid bodies or spheres instead of point masses. MD-Bench aims at providing clean and direct implementations of state-of-the-art algorithms available in MD packages such as Verlet Lists and Cluster Pair, and then use the implemented kernels for performance engineering purposes. Further, we focus on our P4IRS code generator to demonstrate how we can generate flexible and fast particle simulation implementations upon a high-level intermediate representation, also using the knowledge obtained with MD-Bench. We also discuss the challenges of designing efficient data structures and algorithms for particle simulations, such as neighbor search and collision detection, and how P4IRS can be used to abstract them, allowing experimentation to achieve better performance. A few case studies are also displayed to show how P4IRS can be used to generate code for distributed-memory parallel clusters with MPI targeting both CPU and GPU nodes. We will discuss the benefits and limitations of these approaches, and how they can help researchers optimize the performance of their own simulations.

Investigation of the shape effect of granular material by Bayesian calibration

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Keywords Discrete Element Method (DEM), Triaxial compression, Machine learning, Bayesian calibration, Multi-objective optimisation

This research undertakes an in-depth investigation of contact parameters calibration within the Discrete Element Method (DEM) framework, leveraging the capabilities of the calibration toolbox GrainLearning (GL). Conventionally, GL is employed to calibrate contact parameters within predefined particle assemblies. This research extends its use, introducing an innovative approach where GL is also employed to calibrate the content of each grain shape class. A synthetic data set is meticulously constructed, including different classes of grain shapes in varying proportions. The aim of this study is to assess the effectiveness of GL in accurately identifying these undisclosed proportions alongside the simultaneous calibration of contact parameters. GL generates several samples at each iteration, each resulting in a diverse particle assembly. To evaluate these assemblies, the DEM framework is employed to simulate two different loading scenarios, namely the oedometric and triaxial compression tests. GL utilises the difference between the outcomes of the simulations and the synthetic data set to produce new samples in the following iteration to reduce this discrepancy. Consequently, the study paves the way for significant advancements in better understanding the importance of the grain shape of granular material.

Session: Geomaterials

Particle Discrete Element Modeling of Transversely Anisotropic Rock with Discontinuous Fabric

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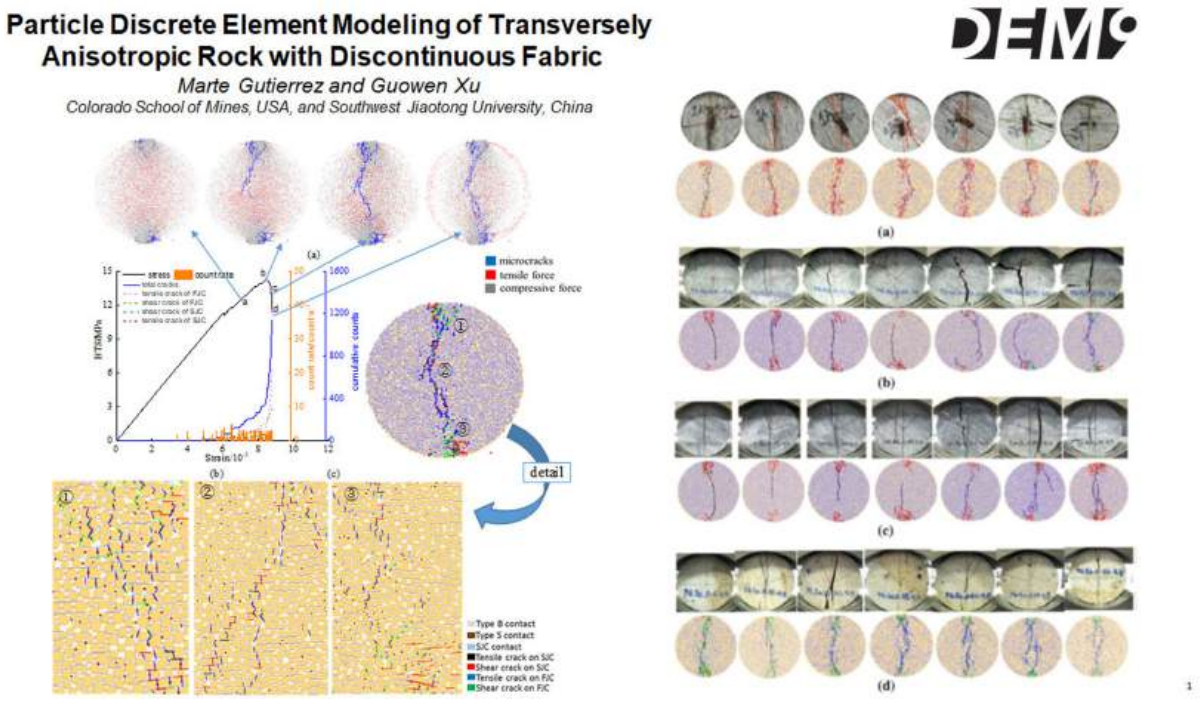
Keywords Brazilian test, transverse isotropy, non-continuous planar fabrics, particle discrete element method, fracture pattern

A new numerical approach based on the particle discrete element method (PDEM) is put forward to investigate the mechanical behavior of transversely isotropic rocks with non-continuous planar fabrics. This numerical model represents the rock matrix and fabric as flat-joint contacts and smooth-joint contacts, respectively. The numerical model is deployed to study the effects of the rock microstructure and the fabric micro-parameters on the shear strength and the fracture patterns of rocks under the Brazilian Test (BT). The PDEM showed BT test results with 20 different types of transversely isotropic rocks with non-continuous planar fabrics and six patterns regarding the relationship between the Normalized Failure Strength (NFS) and fabric-loading angles. The patterns of NFS curves are slightly affected by the coordination numbers of the particles in the rock matrix but strongly affected by the amount of pre-existing micro-cracks in the rock matrix and the stiffness, strength, and distributed region of the fabrics. The calibrated results of six typical rocks with different patterns agreed well with the experimental results regarding failure strength and fracture patterns.



Tomography-Based Additive Reconstruction of Sand Particles and its Application in DEM Simulation

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Keywords Discreate-element modelling, Fabric/structure of soils, Numerical methods, Particle-scale behaviour, Shear

Particle morphology is multi-scale in nature. To investigate the effects of particle morphology at a specific length scale on the macro-micro mechanical behaviours of granular soils, morphological gene decay and mutation were incorporated into the discrete element method (DEM) simulations through spherical harmonic-based principal component analysis. All DEM samples were subjected to axial compression and constant confining stress. The macro-scale and grain-scale behaviours of the granular assembly were investigated. It is found that particle morphology shows significant effects on macro-scale behaviours including initial stiffness, peak stress ratio, volumetric contraction and dilation, and shear band formation, as well as grain-scale behaviours including coordination number, particle rotation, and granular skeleton sustaining the major contact force chains. Among different length scales, local roundness contributes the most to stress ratio, volumetric strain and particle coordination number, while general form contributes the most to shear strain, particle rotation and fabric structure. Another interesting finding is that the particle morphological effects are well reflected in the granular skeleton sustaining the major contact force chains, which is featured with a strong variation of the degree of particle shape irregularity among different kinds of gene-mutated samples.

Numerical granular rock-box DEM simulation to investigate the thrusting motion at geologically relevant scales

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Keywords DEM, Geodynamic modelling, Thrust formation, Accretionary wedge, HPC

The thrusting in the accretionary prisms, which control material flux within subduction zones and generate large earthquakes, and tsunami events remain poorly constrained. Here, the numerical granular rock-box simulation based on the Discrete Element Method (DEM) is presented to study the role of granularity in geological structures with thrusting. The numerical rock box experiment is an extension to a sandbox simulation using adhesive interparticle forces. Most earlier DEM studies of geological processes were conducted mainly for two dimensional problems due to the high computational cost. Recently, with progress in parallel computing and algorithms, it has become possible to perform DEM simulations in 3D using more than one billion particles [Furuichi et.al. 2018]. Thus, our study could deal with more than five million elements (12.5 m) on geologically relevant scales (100 km × 2 km × 250 m). In addition, the interparticle interaction model employed imitates failure behavior (i.e., realistic failure envelope and Young's modulus) of rocks through the triaxial compression test.

The shortening test of numerical the rock box generated in-sequence forward propagation of thrusts similar to those of the sandbox experiments. The sequential thrust formation formed characteristic structures of accretionary prisms. The simulation results show that adhesion forces, which mimic rock properties, can lead to the development of steeper surface angles, near-surface vertical faults, and enhanced bifurcation of shear bands. Furthermore, the geometric network of fault planes was observed to be influenced by the healing of adhesion forces. We also found that thrust thickness depended on the number of frictional elements rather than physical length. We discuss the consistency between the observational data and the simulation result.

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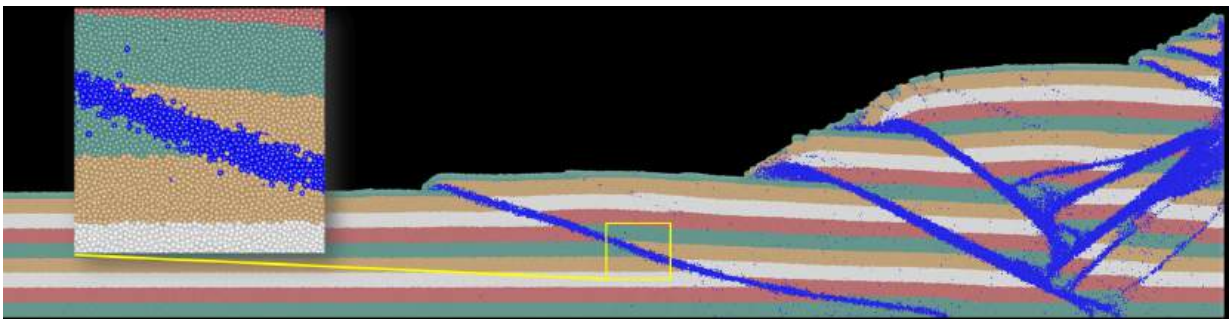

Geogrid-Stabilised soils under a cyclic load

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Keywords Soil, Discrete Element Method, Cyclic Loading, Geogrid, Stabilisation

Geogrid has been increasingly used to stabilise foundation subbases and ballasted trackbed in construction. Whilst there have been numerous previous studies of geogrid reinforcement, there is still a significant lack of understanding of the soil-geogrid interaction and the mechanisms involved. The current design methods with geogrids also appear to be largely empirical and do not consider the actual soil-geogrid interaction at the particle level which has the potential to provide important insights to support geogrid technological development. In this paper, the DEM simulations of a cyclic wheel loading on a granular bed with and without geogrid are presented. The simulations are also compared with experiments to assess the performance of the model. In this study the geogrid is modelled using a bonded assembly of particles to capture the flexural and tensile stiffness of the geogrid. The geogrid model is calibrated from ISO standard tensile tests for geogrid that have been carried out by Tensar International. Wheel loadings are applied to the granular bed via multi-body dynamics coupling to ensure an accurate representation of the experimental setup. A coarse-graining analysis is performed on the DEM simulation results to study the evolution of the internal stress field in the sample during loading both with and without the geogrid. The computed internal stress field reveals significant stress non-homogeneity which provides useful insights of the evolving state of stress in the granular solid under cyclic loading both with and without geogrid. The presence of geogrid has been found to increase the surrounding confining stress in response to the vertical wheel load, enhancing the strength and stability of the bed.

From Microscopic Clues to Macroscopic Insights: Exploring Potential Quantifiers and Predictors of Crack Onset in Drying Suspensions

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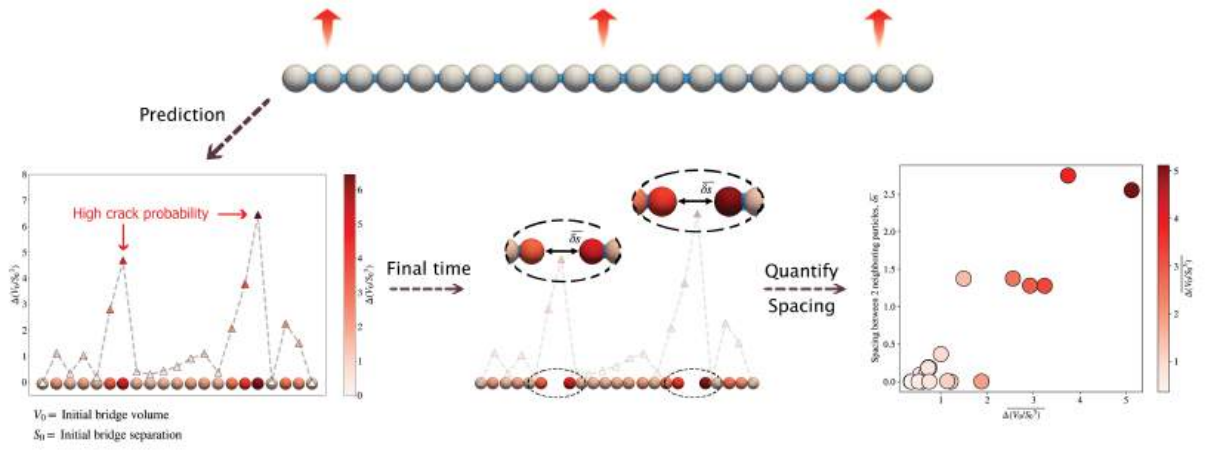
Keywords Capillary bridges, suspensions, drying, crack prediction

The drying of colloidal suspensions leads to the creation of fascinating crack patterns resulting from the complex interactions between particles. As the fluid evaporates, the particles are concentrated into a close packed array. Further drying results in a network of particles interconnected by liquid menisci, i.e. capillary bridges. The capillary bridges are known to be responsible for the emergence of cracks, which occur when they evaporate or are squeezed out.

The attractive force between two particles connected by a capillary bridge is determined by the volume of the liquid and the distance between particles. During the drying process, the capillary force magnitude changes due to the evaporation of the liquid volume, leading to the movement and rearrangement of the particles. Consequently, the separation distance between the particles alters, causing further changes in the capillary force. In this investigation, we utilize computational analysis to examine changes in capillary force during the drying process under various conditions. Our objective is to demonstrate how capillary force plays a crucial role in the resultant microstructure. To accomplish this, we introduce a new dimensionless number, the evolution ratio, which is defined as the ratio of evaporation to the separation velocity. The evolution ratio enables us to identify areas where capillary force may increase, decrease, or remain constant, providing valuable insights into the mechanisms underlying crack formation in colloidal suspensions.

Furthermore, by studying a simple system of linked particles by capillary bridges with various configurations but equal capillary forces (analogous to a system in a state of equilibrium, before the evaporation), we demonstrate how we can locally predict the probability of crack formation solely by analyzing the initial state of capillary bridges. This inquiry can also be employed to estimate the spacing that will arise between adjacent elements in the system, here represented by particles.



Session: Flow of non-spherical particles

Non-spherical particle flows in silos and hoppers

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Keywords DEM, Non-spherical particles, silo, GPU

In our contribution, we will discuss the obtained macroscopic response of granular materials made of non-spherical grains in experiments and with DEM implemented on GPUs. In particular, the silo/hopper discharge is investigated for different particle shapes. We also will present a theoretical analysis of these systems in terms of Eulerian continuum fields. Using the DEM trajectories of the simulated particles and contact network, we employ a coarse-graining methodology, computing several continuous fields required for theoretical analysis. The stress decomposition into contact and kinetic parts provides a suitable theoretical framework to distinguish between the role played by the force chains and velocity fluctuations. In general, in the range of study apertures, the outcomes indicate that the exit size is the relevant scale quantifying the volumetric flow rate. However, the particle shape and the container size also play a significant role. For instance, in the case of a narrow silo, we find a peculiar flow rate increase for larger orifices before the end of the discharge process. While the flow field is practically homogeneous for spherical grains, it has strong gradients for elongated particles, with a fast-flowing region in the middle of the silo surrounded by a stagnant zone. For large enough orifice sizes, the flow rate increase is connected with a suppression of the stagnant zone, increasing both the packing fraction and flow velocity near the silo outlet. In all cases, the contact pressure typically results in several orders of magnitude higher than the kinetic pressure, which monotonically decreases as one approaches the exit. This picture contrasts with the traditional view of a free-fall arch, where assuming a stress discontinuity is a crucial factor when explaining the characteristic velocity at the outlet.

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Effect of different categories of nonsphericity on mixing in a rotating drum using the Discrete Element Method (DEM)

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Keywords Mixing, Segregation, Superquadric, Non-spherical particles, DEM

Particle shape affects the segregation behavior of binary mixtures in a rotating drum [1]. This study uses the Discrete Element Method (DEM) to investigate radial segregation and its dependence on particle shape by varying the particle's aspect ratio. Eighteen binary mixtures are generated by altering particle shape and aspect ratio. The simulation results are validated with the corresponding experimental result for the base case to validate the DEM model. Two scenarios are examined: one where the shape of the fine particle is held constant, and the shape of the coarse particle is varied and another where the shape of the coarse particle is held constant, and the shape of the fine particle is varied. These scenarios help quantify the overall mixing observed in the system for the fine and coarse particle shapes. The figure shows the absolute segregation index values for different coarse particle shapes when the shape of the fine particle is spherical. The results indicate that in the case of coarse particles, the spherical shape exhibits the highest segregation compared to other shapes. Furthermore, for fine particles, particles with aspect ratio 5 exhibit the highest degree of segregation, followed by particles with aspect ratios of 1 and 2.5. Coarse particles with higher monodisperse random packing density exhibit lesser segregation, while fine particles with greater interlocking enhance mixing. Overall, this study highlights the importance of particle shape in segregation behavior and provides insight into how different particle shapes compare with each other on different levels of segregation.

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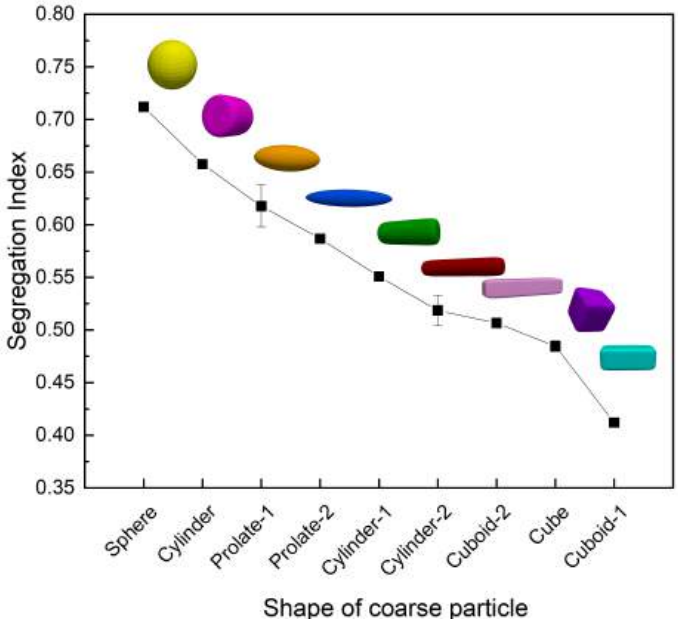

Influence of Mechanical Interlocking on the Flow Behavior of Granular Particles

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Keywords Mechanical Interlocking, Particle Stress

In order to obtain reliable predictions for the flow behavior of highly angular particles, such as Lunar and Martian soils, mechanical interlocking associated with sustained particle-particle interactions needs to be described. Mechanical interlocking gives rise to large particle-phase stress in granular soils and a significant resistance to deformation. In this study, the effect of particle interlocking in dilute and dense-phase granular flows is investigated via discrete element method (DEM) simulation of a 3D system of hook-shaped particles in simple shear flow using Lees-Edwards periodic boundary conditions. The effect of particle shape is assessed by progressively varying the degree of curvature of the hook-shaped particles. The particle shape varied from a straight, elongated particle to one in which the straight particle is folded in half. For each particle shape, a total normalized interlocking time and distribution of particle interlocks are determined over a range of solid concentrations. At low solid volume fractions, the normal and shear stresses are proportional to the inverse of the projected area of the particle in the plane perpendicular to the flow, consistent with the stress behavior of elongated particles [Guo et al., 2012]. For larger solid volume fractions, normal and shear stresses increases with increasing interlocking, showing a direct dependence between stress and degree of mechanical interlocking.

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Rigid Clumps in MercuryDPM Particle Dynamics Code

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Keywords Rigid Clumps, MercuryDPM, CLUMP tool

Discrete element method (DEM) simulations usually rely on the concept of interacting spherical particles. However, the correct representation of the particle's aspherical shape is crucial for many applications. A widely used approach to this problem is the introduction of clumps - rigid assemblies of multiple spherical particles. In this work we describe the novel implementation of clumps within the MercuryDPM particle dynamics code. MercuryDPM is highly efficient in treating polydisperse systems, which makes it well-suited for simulations of large multiresolution clump systems, representing irregular particle shapes. We employ the recently released CLUMP library to generate clump particles. The talk details the pre-processing tools providing necessary input to DEM engine, adjustments of the MercuryDPM algorithms of contact detection, collision/migration and numerical time integration. The capabilities of our implementation, as well as some derived modeling techniques, are illustrated with a number of examples.

Flow of strongly concave particles in a rotating drum: stress profile predictions

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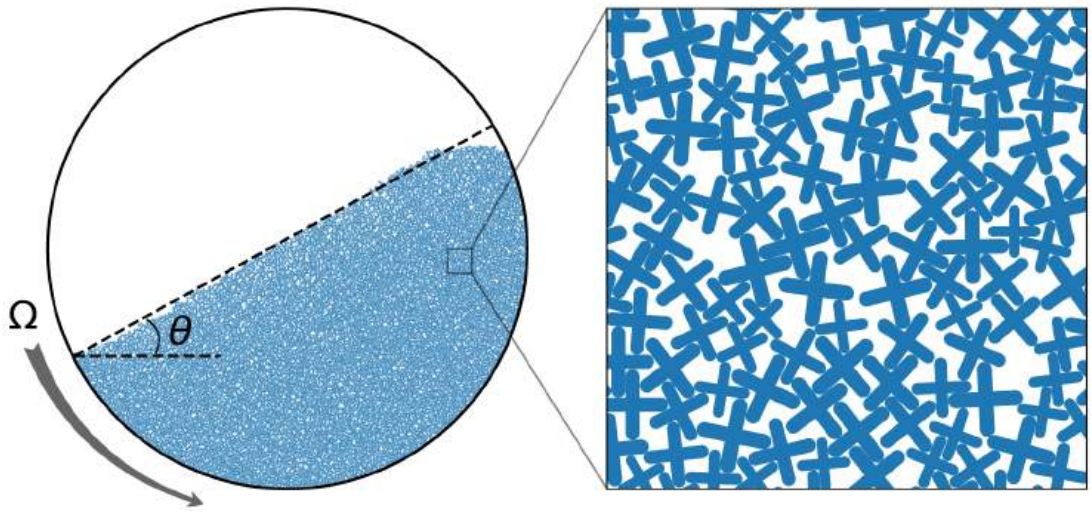
Keywords Granular media, Strongly concave, Rotating drum, Discrete element methods (DEM), Granular flows

The flow of granular matter is highly influenced by the shape among the properties of the constitutive grains. This is even more critical when the grain-shape is getting highly concave since the packing properties exhibit non-trivial features like high porosity level and sharp jamming/unjamming transition. Despite the richness and ubiquitousness of these systems, very few is known about their flow behavior and the local mechanisms involved. By means of 2D Contact Dynamics simulations, we investigate the flow properties of strongly concave grains within a rotating drum. The system has the advantage of presenting, in a single test, almost all the flow characteristics that have been observed in granular systems: a solid to quasi-static and inertial flow phases. The shape of the grains is systematically varied from disks to crosses. Rotation speeds are also varied, while making sure to remain in a dense and continuous flow regime with a well-defined free surface for all shapes. In general terms we find that, for a given rotation speed, the slope of the free surface increases with the concavity and then saturates at a certain grain concavity value. The stress profiles vary significantly with grain shape, but still exhibit common generic trends. For example, the shear stress profile is characterized by an initial linear increase as the depth increases, then becomes independent of the depth close the drum walls. On the contrary, the normal stresses decrease linearly with depth. Momentum balance equations allows to correctly predict the normal stress profile for all shapes and drum velocities but fails in predicting the shear stress profiles. By postulating that in the drum geometry annular regions of small thicknesses exist, we develop a new model that perfectly predict the shear stress profiles in a drum, whatever the shape of the grains and the rotational speeds.



Performance of sand granulated rubber mixture for soil stabilization using DEM method

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Keywords DEM modelling, sand, granulated rubber, PFC2D, sheet pile

This paper studies a detailed analysis of the capability of the Discrete Element Method (DEM) to replicate a physical model of a sheet pile rubber-sand mixture backfill material under static loading conditions. Particle Flow Code 2-D (PFC2D) is used to model experimental tests in the DEM environment which can investigate the mechanical behavior of materials at both micro and macro levels. First, the numerical model of the direct shear test on clean sand and sand mixed with 10% granulated rubber (2.5-5mm diameter) has been done to calibrate the micromechanical parameters of the sand and rubber. The micro-mechanical properties which correspond to macro-mechanical strength parameters have been obtained for further DEM simulations. A total of four DEM models of the sheet pile foundation with different sand-rubber mixture backfill areas were tested and analyzed. During the calibration process, we observed that the loading process speed, contact stiffnesses, and porosity of the system had a significant impact on the deformation parameters of the sheet pile and lateral pressure distribution of the granulated rubber-sand mixture backfill. Finally, the ability of the PFC2D code as a DEM approach in modeling of cohesionless granular material at sheet pile backfill foundation is shown.

Development of a Rapid Particle Replacement Method for Comminution Circuit Modelling of Particle Breakage

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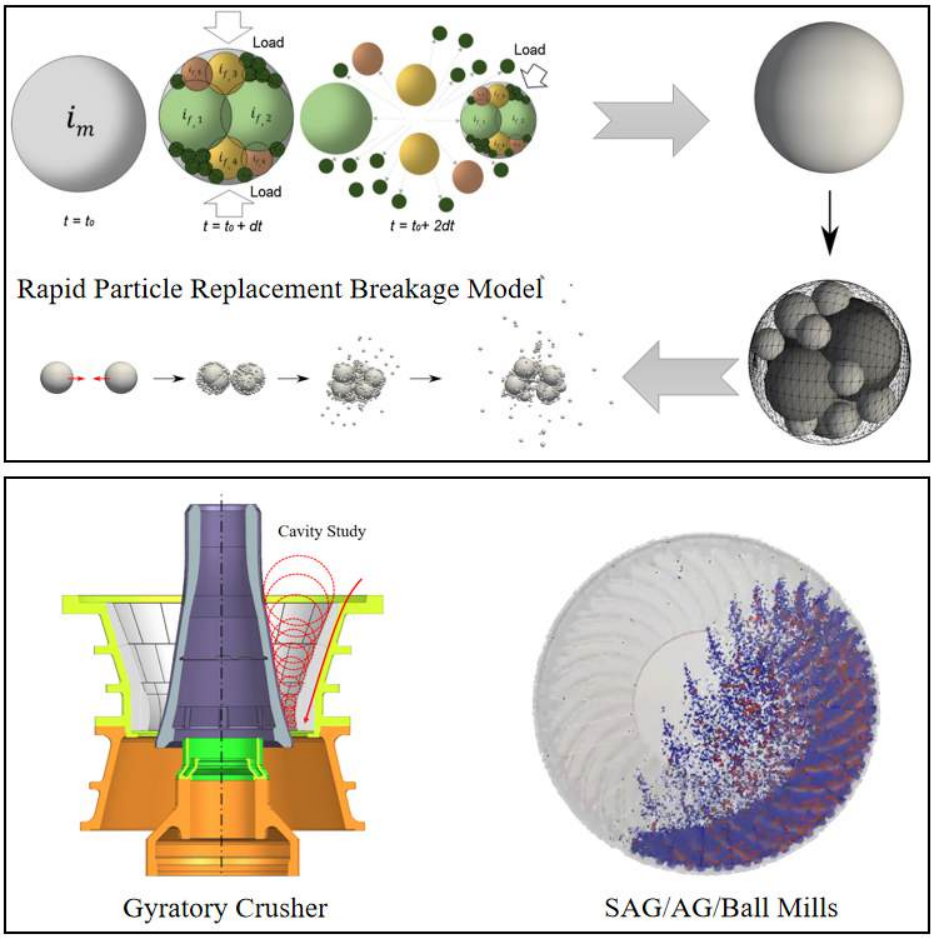
Keywords DEM, Particle Replacement Method, GPU, SAG, AG, Crushers

Primary grinding circuit is one of the most important stages in the overall comminution circuit in mineral processing. Modelling of the continuous rock size reduction process is of critical important when assessing the effectiveness of a liner design in the processing equipment. The conventional collisional energy method merely indirectly compares the rock breakage in isolated states of crushing and grinding, which draws partial comparison between liner mechanical designs. This study aims to develop a rapid particle replacement-based breakage model to investigate the continuous size reduction process in crushing and grinding. The integration with ore hardness-based parameters is also performed to reflect the ore properties during modelling. Results of the developed method led to a direct comparative framework when assess liner performance in crushing and grinding process. Consequently, the outcome of this research can be directly applied to holistically evaluate the rock breakage and discharge process of crusher and mill liners.



Optimization of an Asphalt Mixer using Machine Learning and HPC

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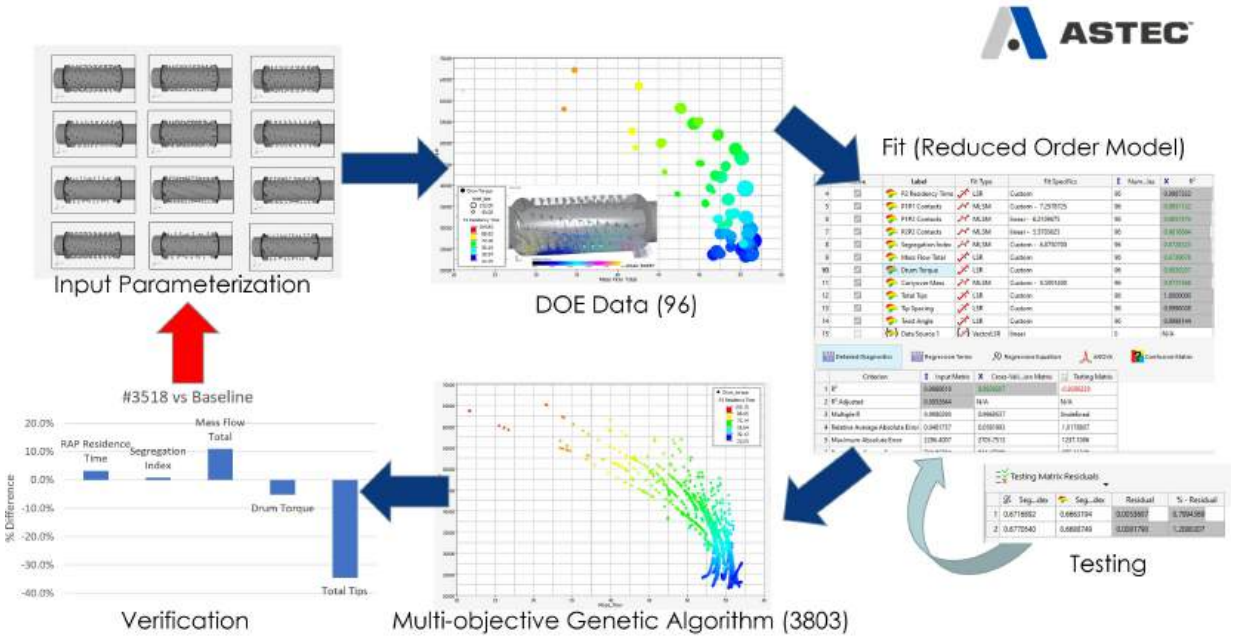
Keywords Optimization, Mixing, Machine Learning, DEM

Efficient mixing of reclaimed asphalt product (RAP) is a crucial part of the process of making hot mix asphalt more sustainable but the traditional optimization approach, which is heavily reliant on physical trial-and-error, is prohibitively time consuming and expensive. Virtual design optimization has significant utility in this context. This work demonstrates an efficient methodology for virtual design optimization that combines high-fidelity physics-based simulation, High Performance Computing (HPC), machine learning and optimization to rapidly identify the globally optimal equipment design. The methodology consists of parametrizing the equipment geometry, automatically generating and running Discrete Element Method (DEM) simulations for a well distributed quasi-random sample of the geometric parameter space on the cloud and fitting a response surface to the results using machine learning. A Multi-Objective Genetic Algorithm (MOGA) is then utilized to rapidly estimate the globally optimal parameter set from the fitted response surface. The complete workflow is shown in Figure 1. Optima from the MOGA were verified and a new mixer configuration was identified which provides similar mixing with fewer paddles, lower torque, and greater mass flow representing a superior design.



Implementation of Van-der Waals forces for arbitrary oriented, finite sized platy nanoparticles in discrete element simulations

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Keywords Van der Waals forces, physio-chemical forces, particle shape effects, clays

Clays are important in geological fields as well as geotechnical and medical applications, from the stability of soils to the delivery of drugs. They consist of fine-grained adhesive nanoscale platy particles that interact via long-ranged Van-der-Waals forces which strongly depend on the relative particle orientation. Textbook definitions of the Van-der-Waals force are limited to forces between spheres, or between spheres and infinitely long walls, where the relative orientation of the particle is irrelevant. Anandarajah and Chen (Anandarajah & Chen, 1997) derived an interaction law for tilted cuboids with infinitely long walls, but without a clear explanation how their solution for an infinite wall could be applied in discrete element simulations with finite sized particles. In this work, we present the necessary changes in Anandarajahs model to compute the force between two finite sized particles in arbitrary relative orientation and location as well as the implementation for a discrete element framework. As the non-spherical, elongated nature of the clay platelets leads to non-central forces, we also present a simple geometrical model for the force point on both platelets which is required to compute the torque induced by the Van-der-Waals forces. We further discuss the effect of the necessary simplifications made in our model, as well as the normalizations which are necessary to avoid the divergence of the forces. Finally, we demonstrate the use of the Van-der-Waals force for rectangular particles in a small test implementation.

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Sensitivity analysis of DEM parameters for multi-component segregation during heap formation, hopper discharge and chute flow

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Keywords Granular materials, Segregation, Discrete element method, Sensitivity analysis

Granular segregation is a critical phenomenon in various industries, such as food processing, pharmaceuticals, and mining. The Discrete Element Method (DEM) is an effective tool for gaining insight into granular segregation since it provides particle-level information that is often difficult or impossible to obtain through experiments. To ensure realistic material behaviour and correct representation of segregation, it is essential to systematically calibrate the model against experimental results. However, in the context of multi-component segregation, it is extremely challenging and computationally expensive to consider all parameters in the calibration procedure since interaction parameters between components must also be taken into account. This work aims to identify the most influential DEM parameters for modelling multi-component segregation during heap formation, hopper discharge, and chute flow. Our findings will aid researchers in calibrating DEM models for multi-component segregation more efficiently.

Correlation between measured acoustic emission in uplift pipeline-soil interaction and energy dissipation in DEM

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Keywords Pipeline soil interaction, acoustic emission, energy dissipation, DEM

Pipeline networks cover vast geographical areas to transport water, oil and gas, and hence are critical infrastructure underpinning society. The buried pipelines are often exposed to potential damage from ground movement. This paper presents a 2D DEM study of pipeline-soil interaction. The experimental results (Smith et al. 2019), i.e., the net uplift force, displacement of pipeline and the displacement contour, were used to calibrate the DEM model. After the model parameters were calibrated, the dissipated energy obtained from DEM and acoustic emission (AE) behaviour measured in a large-scale physical test were compared. It was found that the both the plastic dissipated energy rate, namely the friction energy due to particle-particle friction, and the damping energy showed a strong correlation with the measured AE in the experiment. The dissipated energy and the measured AE were affected by burial depth (stress level) and applied uplifting velocity in the same way. The new findings in this study enables improved interpretation of AE and underpin the development of theoretical and numerical approaches to model and predict AE behaviour in soil-structure interactions.

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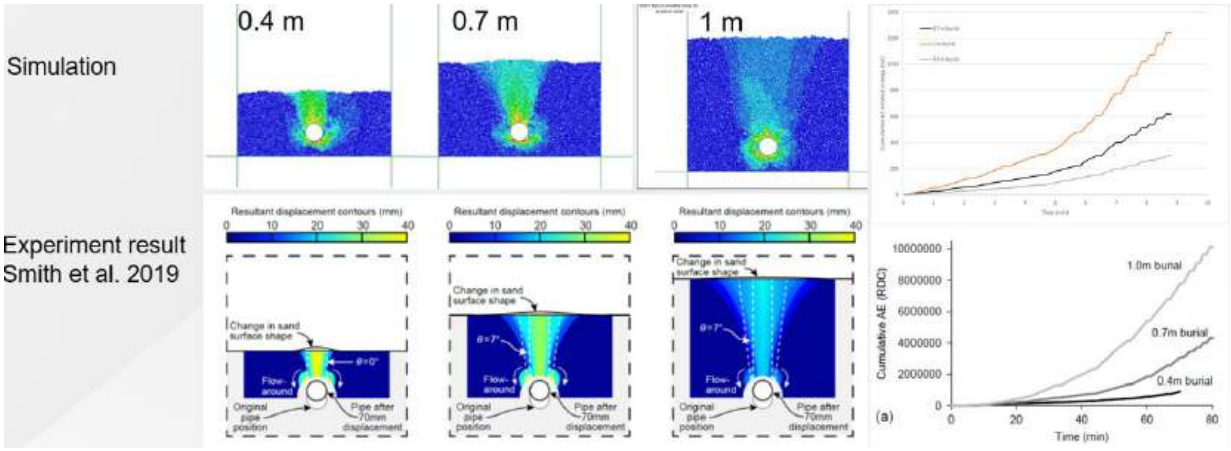

Simulation of granular materials by using combined discrete element models

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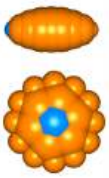
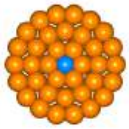
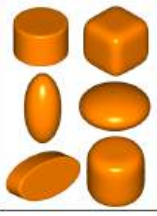
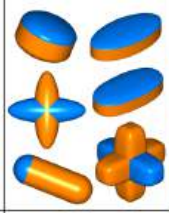
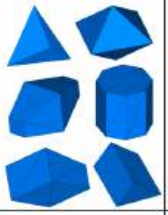
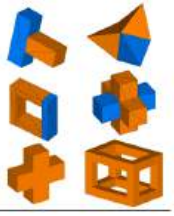
Keywords Non-spherical particle, Super-ellipsoid model, Polyhedron model, Discrete element method, Granular Material

Granular materials can be found in many industrial processes from chemical to energy, agriculture, mining, pharmacy and many other fields. They are almost always opaque, making the acquisition of experimental data below the surface difficult. DEM (Discrete Element Method) simulations are an effective way to study the physics of granular materials because they can simulate the micro-dynamic behavior of granular material on an individual particle scale and the motion of every particle can be traced. Since DEM was first considered, many modified discrete element models have been developed. However, most existing DEM simulation are for spherical particles or a specific type of non-spherical particles. In this work, a combination of several types of discrete element models including sphere-based model, super-ellipsoid-based model, and polyhedron-based model were used to simulate the flow of granular materials with many different shapes. Several simulation cases including the flow of particles in tumblers, blenders, and other devices were performed to validate the modeling approaches. The simulation results show that it is practical and efficient to combine different discrete element models together for simulating both spherical and non-spherical granular materials.

Category	Sphere-based model				Super-ellipsoid-based model		Polyhedron-based model	
	Sphere	Multi-sphere	Bonded-sphere	Droplet	Super-ellipsoid	Multi-super-ellipsoid	Convex polyhedron	Concave polyhedron
Type								
Shapes	Spherical shape	Any shapes	Any deformable and breakable shapes	Spherical shape	Spherical, ellipsoidal, cylindrical, cubic, and so on.	Any shapes (Especially tablets)	Any convex shapes	Any concave shapes
Accuracy	High	Low	Low	High	High	High	High	High
Speed	Fast	Depend on N spheres	Depend on N spheres	Fast	Medium	Depend on N super-ellipsoids	Depend on N faces	Depend on N polyhedron

Simulation of polyhedral particle breakage in DEM using a fast-cutting method

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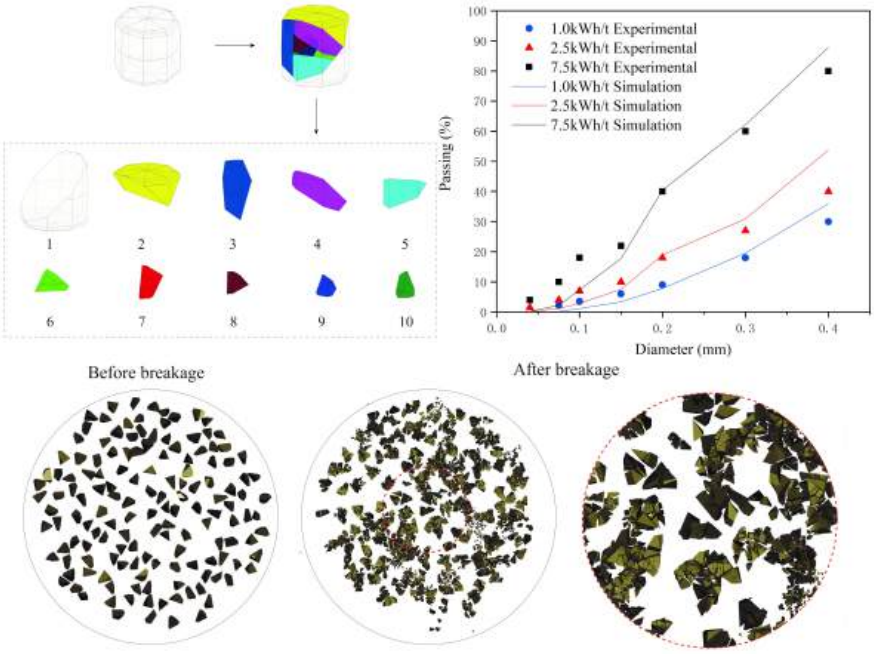
Keywords Particle fragmentation, polyhedron, fast-cutting algorithm, breakage model

Several types of approaches have been established to describe breakage using DEM. In order to accurately describe the breakage of a group of particles while ensuring computational efficiency, the current work proposes a particle breakage model, which uses a particle replacement scheme. It describes the break probability of each particle and the size distribution of progeny particles, to accurately reproduce the size distribution described by the model in simulation, a fast-cutting algorithm for polyhedron is proposed. The accuracy, efficiency, and stability of the cutting algorithm were verified by cutting particles of different shapes. Comparing the results of bed breakage experiments and the simulation, the breakage model well describes the fragmentation of a group of particles under impact. The main research content and results are as follows:

(1) A fast-cutting algorithm that a polyhedron particle can be cut into several parts is proposed. The effects of the number of polyhedral faces and progeny particles on algorithm runtime and volume error of each progeny particle have been studied. For the progeny particles broken from a parental particle, the average relative volume error is less than 3%, maximum relative volume error is less than 7%.
(2) A breakage model based on energy accumulation is established. The size distribution of progeny particles is based on the "t10 theory" proposed by Tavares. The breakage model controls the probability of particle fragmentation by generating virtual energy after each time step during simulation.
(3) Bed breakage experiments were simulated, and all the particles in the simulation were polyhedrons. The results well described the size distribution of the particle bed after being impacted by a falling hammer. Therefore, the breakage model and the fast-cutting algorithm were verified.



Analysis of effect of packing structure on grain breakage with DEM

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Keywords Discrete Element Method, Grain crushing, Structural characteristics, Weibull statistics, Disordered packing structure

The self-organization of granular systems with different grain parameters is largely responsible for the formation of grain contact network, which is the main frame for withstanding the loads. In the present study, the effect of disordered contact network of bonded granular materials on crushing characteristics is investigated by means of 2D Discrete Element Method (DEM). The packing structure of 2D polydisperse disc is depicted by virtue of quadron-based structural description (closed loop of contacts around a void), in addition, the standard deviation of areas of loops is deemed as the quantification of structural characteristics. The Weibull statistics is adopted to reflect the variation in grain crushing strength. The simulation results demonstrate that the Weibull modulus decreases from 9.395 to 6.671 with increasing structural disorder, indicating a higher degree of crushing strength variation. In accordance with this result, the stress concentration inside the grain becomes more prominent with a more disordered structure. Last but not least, the relationship between fracture pattern and structural disorder is revealed in order to explore the fracture mechanism. All these findings provide insight into the influence of structural disorder over mechanical properties of granular matters.

DEM modelling of dry mixing in industrial blenders

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Keywords DEM, industrial mixing, ribbon blender, in-bin blender, mixing index

In-Bin (IB) and ribbon blenders are widely employed to blend multi-components mixtures in various industries. The resultant mixing quality depends on operating conditions, grain morphology and physical properties such as cohesion. Typical industrial analysis on mixing quality is centred around experimental trial and error by measuring select spatial locations with a thief probe. Simulation using the Discrete Element Method (DEM) allows for a fundamental approach to mixing by providing a grain scale analysis of the material distribution over the entire mixer. However, simulating the equipment and material at industrial scale presents challenges due to the particle shape and count which results in a high computational time. In this study, the GPU based code Blaze-DEM was employed to simulate the mixing of a multiple powders in a 5L IBB (Fig. 1a). The mixing quality was assessed by employing a novel mixing index (Govender et al., 2023). Particles were considered spherical, and the shape effect was accounted by increasing the cohesion through calibration with polyhedral particles and experiment. The DEM model was successfully validated with experiments on a 5L IBB by comparing the components concentration in different spatial locations. The validated model was then employed to compare the mixing quality in IBB and ribbon blenders as a function of operating conditions (RPM and fill level). Fig. 1b shows that using a Ribbon blender rather than an IBB results in a higher mixing quality (MI) in a shorter time at the same RPM. However, the simulations showed also that the average shear damage at which particles are subjected during blending is higher using a ribbon blender, which could cause unwanted breakage of the granular media. Future research aims to investigate the process scale up and the coarse graining technique to simulate larger systems.

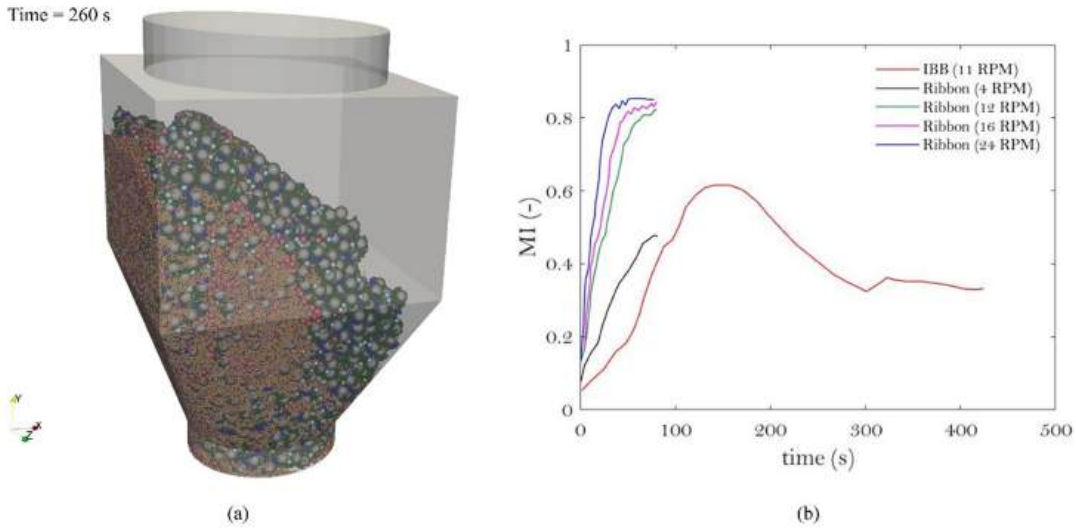

Fig. 1 (a) DEM simulation of a multi-component mixture processed in a 5L IBB (b) mixing index (MI) as affected by blender type, i.e. ribbon blender and IBB, and operating conditions (RPM)

A grid-size unlimited CFD-DEM method for gas-solid flows

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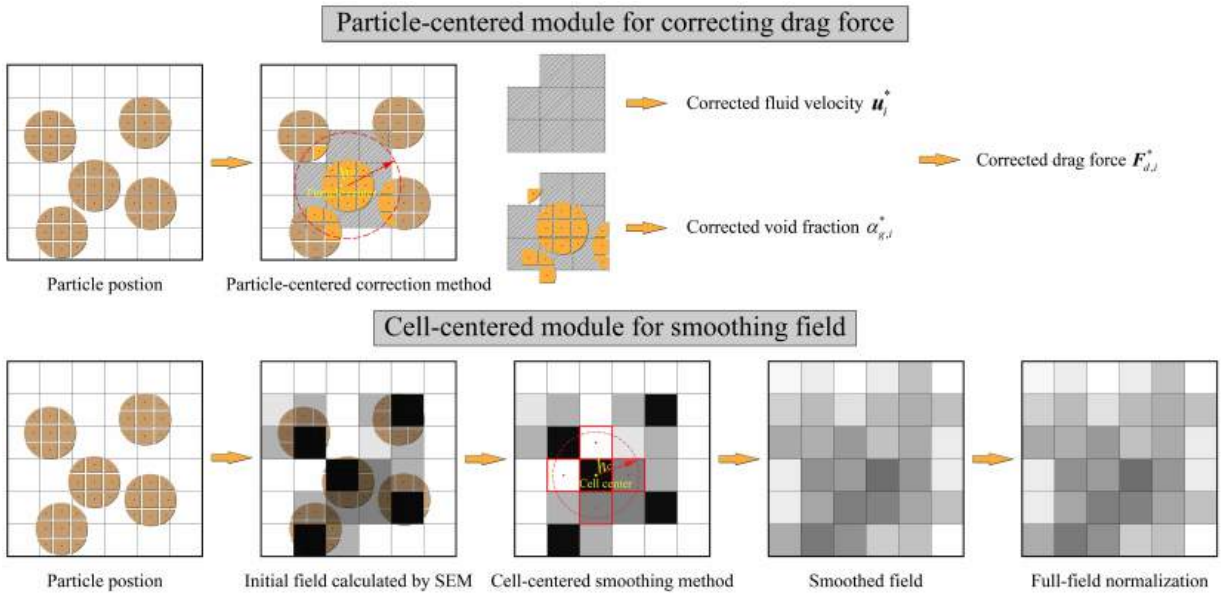
Keywords Gas-solid flows, CFD-DEM, Grid particle size ratio, Unstructured grids, Model validation

To relieve the deficiency that the unresolved CFD-DEM method can only be applied to cases where the fluid grid size is larger than the particle size, many studies have proposed new CFD-DEM methods suitable for cases where the fluid grid size is comparable with the particle size. However, few studies focus on developing a unified CFD-DEM method that can accurately handle both small grid cases and large grid cases without changing the calculation method, i.e., the simulation of small and large grid cases is performed under the same framework. In this study, a grid-size unlimited CFD-DEM method (GSU CFD-DEM) that can handle not only small grid cases but also large grid cases under the same framework is developed. GSU CFD-DEM includes the particle-centered module and the cell-centered module, aiming to realize interphase force correction and field smoothing, respectively. Mass conservation is strictly guaranteed to enhance the robustness of GSU CFD-DEM. The effectiveness and accuracy of GSU CFD-DEM are validated by comparing the simulation results with experimental data in a spouted bed and draft tube-type feeder. The main features of flow patterns, pressure drops and particle velocities are well predicted by GSU CFD-DEM, which confirms the capability of GSU CFD-DEM to simulate gas-solid flows with different grid sizes and its applicability to unstructured grids. Even under the condition of violent gas-solid interactions, GSU CFD-DEM still shows high stability and accuracy. In the future, GSU CFD-DEM has the potential to serve as a unified method to simulate gas-solid flows with different grid sizes.



Characteristics of the force chains network in a DEM model of a flat punch indentation

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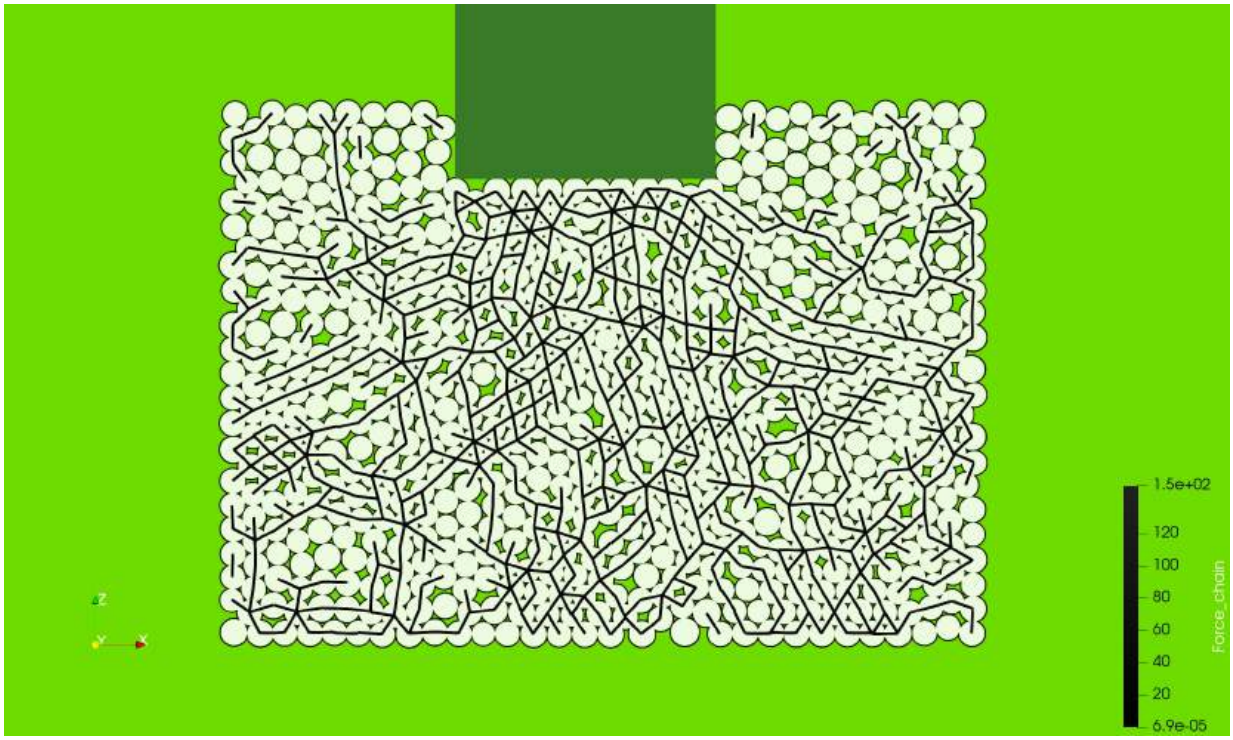
Keywords Force chains, force transmission, flat punch, photoelasticity

The transmission of load by particles forming a granular assembly has been widely studied experimentally, especially through the application of the photoelastic technique. More recently, numerical methods such as Discrete Element Methods (DEM) have also been used to study this phenomenon. The photoelastic technique enables the visualization of forces in a sample consisting of transparent grains under polarized light. The structure of bright lines that connect the most loaded grains is commonly referred to as the force chains. However, it has been revealed that in some interesting features of the force chain network and grain assembly can be easily captured in the DEM model, whereas they would be impossible or difficult to obtain from the experiment alone. Our objective is to demonstrate how the results of a simple photoelastic experiment can be partially reproduced using a properly calibrated DEM model. This knowledge can be further applied in more advanced simulations and in the design of future experimental setups. In the experiment, the photoelastic method is used to observe the development and transformation of force chains induced by the constant indentation of a piston into the granular sample. The numerical model can help us understand the structure of the force chain network and its evolution, the behaviour of the load-transmitting grains, and the development and transformation of large pores. Regarding the fact that the criteria for the separation of the strong and weak contact force networks are not clearly defined in the available literature, we will attempt to refine them and determine the threshold conditions for their identification.



Particle and domain size scaling in terramechanical simulations

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Keywords Terramechanics, plate shear test, scaling, particle size, domain size

DEM is a versatile but computationally intensive method for granular dynamics simulation. The computational intensity is largely tied to the number of particles and time-step, which itself is influenced by both particle size and simulation domain [1]. While the effect of particle size has been investigated in DEM, little work has been done to explore the impact of varying the particle size distribution spatially throughout the simulation domain or altering the domain size itself. In order to characterize the errors introduced by the domain truncation and variations in particle size distribution, we conducted numerous simulated plate traction tests. Specifically, we perform pressure-sinkage and shear-displacement tests using a plate with grousers on a soil bed confined in a rectangular bin. Throughout the tests, we measure the distribution of inter-particle forces and displacements, which we then analyze and coarse-grain into fields of stress and strain. In the domain scaling analysis, we use spatially uniform and spatially varying particle size distribution. We study how the error depends on the depth and width of the domain, including the smooth transition from 3D to quasi-2D, and the plate's proximity to the confining bin's walls. When studying the spatially varying particle size distribution, we have implemented a method that changes the particle size in a gradient going from a fine particle resolution close to the plate to a coarser resolution further away. A surprisingly aggressive gradient can be used, where the fine particles are only a fraction of the grouser size, and the large particles are up five times as large. This approach has a small effect on the pressure-sinkage and shear-displacement relations, and enables a reduction in computational effort by nearly an order of magnitude.

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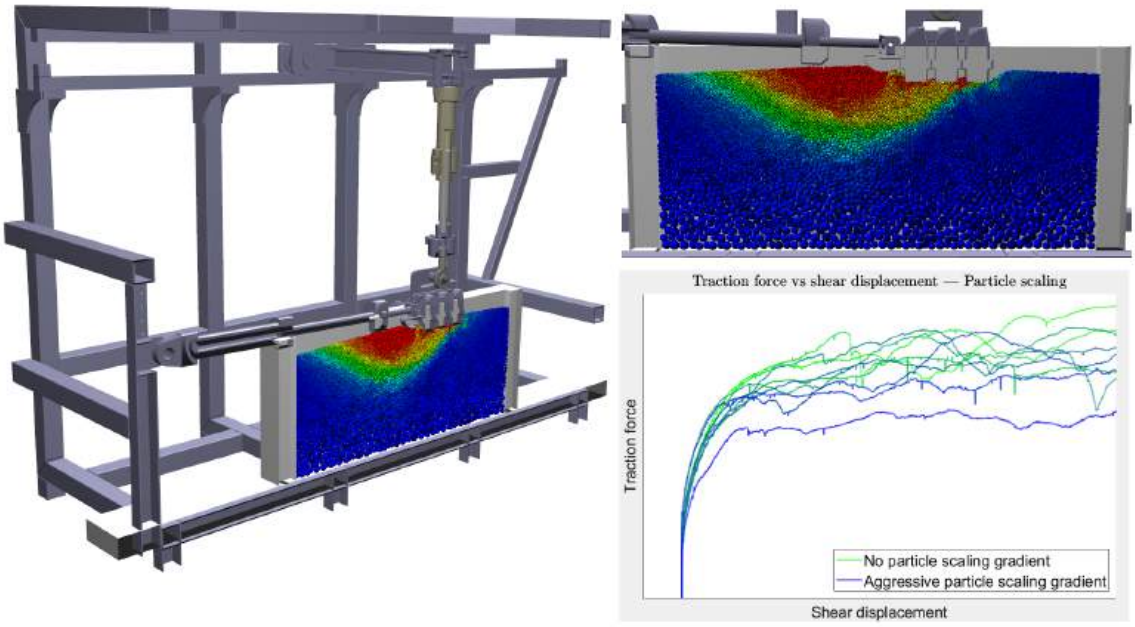

The Curious Case of Elongated Grains: 2D Simulations of Granular Material Flow in Silos with Varying Orifice Sizes

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Keywords Granular flow, DEM

By means of 2D Contact Dynamics simulations, we investigate the flow properties of granular materials composed of elongated grains within a silo of varying orifice size. The grains have a rounded-cap rectangular shape described by their aspect ratio parameter varying from 1 for a disk to 7 for a thin or long grain. In order to isolate the effects of grain shape, both the mass and surface of the grains are kept constant as well as the total mass of the system and the condition of the discharge. By simulating a large number of avalanches, the flow rates "Q", the velocity profiles and the packing fraction profiles close to the orifice are studied for increasing grain aspect ratio and for various characteristic dimensionless numbers such the orifice size normalized by the grain size, or the system size normalized either by the orifice size or by the grain size. A counterintuitive finding of this work is that the effect of grain elongation depends on the size of the orifice. Indeed, we find that Q is independent of grain elongation for small (normalized) orifice size. In contrast, Q increases with grain elongation for intermediate (normalized) orifice size, and it may saturate or continue to increase at larger grain aspect ratio. Based on the methodology proposed by Janda et al. (2012) to deduce the flow rate from the packing fraction and velocity profiles close to the orifice, we show that the nonlinear variation of Q with grain elongation results from compensation mechanisms between the velocity and the packing fraction measured at the center of the orifice.

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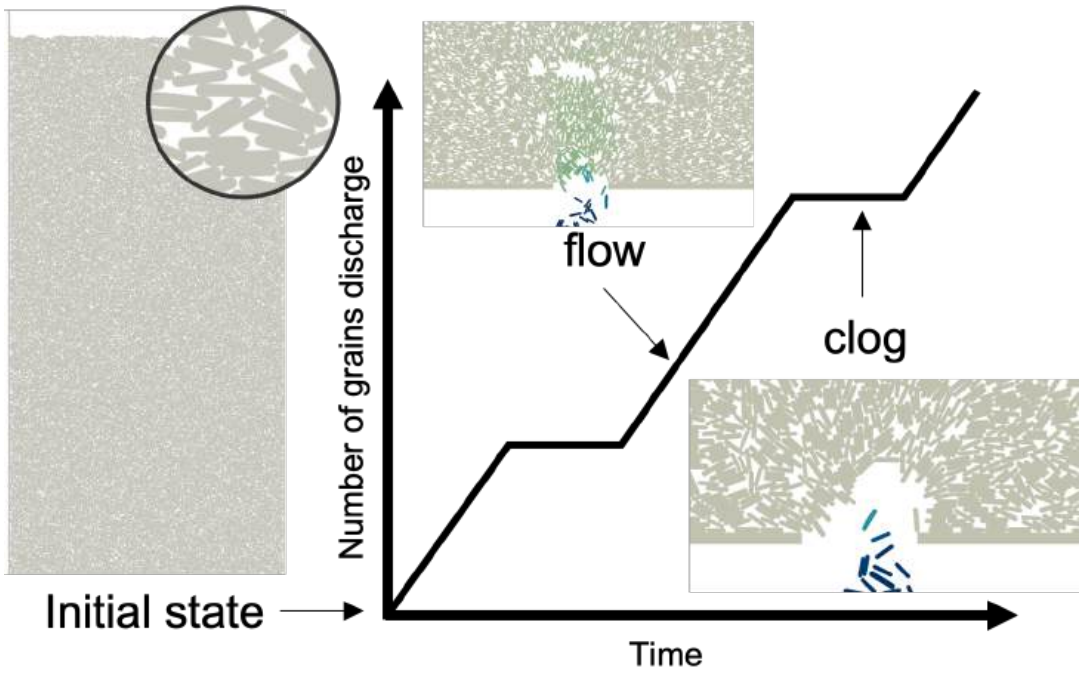

Dynamics and scaling laws of granular collapse

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Keywords Granular material, collapse, dynamics, deposit morphology, DEM

The collapse and flow of discrete material are ubiquitous in various natural disasters and environmental problems, exhibiting rich instantaneous dynamics under different scales. In this talk, we first focus on the collapse of a granular column and its spreading flow on an erodible surface based on the experiment and corresponding DEM simulations. Three different erosion-deposition regimes are observed, which primarily depend on the difference in material properties between the column and erodible bed but vary little with the initial aspect ratio of the column. In addition to reproducing various deposit morphologies observed in experiments, our DEM simulations also confirm the existence of critical particle density ratios that correspond to regime transitions and are almost independent of the initial aspect ratio of the column. Furthermore, we also investigate the collapse of wet granular columns in the pendular state experimentally and numerically and find that different collapse regimes are primarily dependent on the particle size as well as the initial aspect ratio of the column, while the water content has a quantitative effect on final deposit morphology. A dimensionless number containing the particle size and the water content is proposed to quantitatively characterize the macroscopic cohesion induced by the presence of water. On this basis, a phase diagram is put forward for describing different collapse regimes of wet granular materials. Generalized scaling laws have also been developed to characterize the dependency of deposit morphology on initial aspect ratio and dimensionless cohesion parameter. The morphological quantities in the wet case may be determined by respectively adding the variations caused by the cohesion effect to the results of dry granular material. This implies that these generalized scaling laws can be applicable to the collapse of granular material in a wider range of situations.

Coupled CFD-DEM simulations of particle and fluid behaviours during early stage of filtration

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Keywords Coupled CFD-DEM, filtration, granular media

Filtration is the phenomenon where the migration of finer particles (termed base particles) driven by seepage flow is prevented by a granular medium comprising coarser particles, termed the filter. It is widely observed in nature, industrial processes and man-made structures, such as in natural riverbeds, water treatment and embankment dams. The micro-scale mechanisms of filtration are important in assessing and improving the effectiveness of filters, which are investigated in this study using coupled Computational Fluid Dynamics and Discrete Element Method (CFD-DEM) to consider the interaction between particles and fluid. A coarse-grained CFD-DEM approach was employed for computational efficiency, which solves the averaged flow field for each CFD cell. The early stage of filtration was simulated at the micro scale with a simplified system where assemblies of finer base particles underlying coarser filter particles are subjected to upward seepage flow perpendicular to the base-filter interface. A wide range of base-filter size ratios along with different flow conditions were considered to investigate the combined influence of geometric characteristics and hydraulic loading on the effectiveness of filters. The wide range of particle sizes in filtration simulations, along with the variation in void fraction between the base and filter layer required careful consideration to ensure numerical stability. This highlights the importance of employing a robust algorithm to attain smooth transitions in the void fraction between the coarse-grained CFD cells, and thereby maintaining numerical stability. The simulation results of the fluid behaviours were validated by comparing the numerical results of hydraulic conductivity of the filter layer with empirical solutions and relevant experimental results in previous studies, where the influence of the coarse-grained CFD mesh resolution on the simulation results was also rigorously tested.

An energy-based discrete elements method

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Keywords DEM, Energy-based, optimisation, GPU acceleration

In this paper, we present a method to obtain the equilibrium state of a particle system by minimising energy, which is referred to as the energy-based discrete unit method (EDEM). For partial differential equations, the solving problem can be transformed into finding the minimal value of the functional, for example in the work of E Weinan et al [1]. In static analysis, the principle of minimum potential energy is equivalent to the weak form of the equilibrium and the Neumann boundary conditions [2]. We introduce this energy-based approach to the DEM. The system energy consists of the elastic contact energy, the potential and boundary penalty terms. The energy, subsequently, can be optimised to obtain the final equilibrium state. Particles moving in the system do not satisfy Newton's second law. First, we apply the method to a dense particle ensemble and the simulation results are good. Then we perform free-fall simulations using an ensemble of particles in different initial stacking states, with the possibility of the model falling into a locally unstable optimal solution. When small perturbations were added, the model was able to regain the global optimum solution. Then, we performed free fall simulations of polydisperse particle aggregates, servo consolidation simulations, and simple shear simulations. The EDEM can be very easily distributed to GPUs for acceleration. The process of energy optimisation is perfectly combined with the optimisation of loss functions in machine learning. This approach has the potential to be used in the initial packing generation.

Granular stresses and stress ratios in 3D obstructed granular flows

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Keywords 3D granular flows, obstacles, DEM, granular stress, stress ratio

The continuum approaches exhibit great promise to model granular flows, but the assumption of the isotropic stress state in a constitutive law should be carefully examined, especially for obstructed granular flows. This study aims to examine the effect of obstacles on granular stresses and stress ratios in granular flows by using the discrete element method (DEM). Two loading scenarios were considered: (1) a rapid avalanche of glass beads in an inclined chute with a small fixed semi-cylindrical obstacle; and (2) flows of Fe2O3 beads in silos with various inserts.

Results reveal that the blocking effect from the obstacles significantly increased normal and shear stresses. The normal stresses exhibited a stress ratio of approximately 1.0 in steady and uniform granular flows, indicating an approximately isotropic stress state. Unlike the normal stresses, the shear stresses however demonstrated strong anisotropy even in the steady and uniform regime. In both scenarios, the obstructed granular flows showed strong anisotropy not only in normal stresses but also in shear stresses. The stress ratio in the obstructed granular silo flows can vary between 0.27 and 2.24. The stress ratio in a rapid granular avalanche in an inclined chute with a small fixed semi-cylindrical obstacle can be much higher than unity and increase to a maximum value of approximately 5.0.

2D DEM study of force transmission during in-plane cutting of flexible granular chains

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Keywords Flexible granular chains, Entanglement, Interlocking, constraint, shear band

Flexible granular chains are linear chains composed of hollow spherical beads connected together by I-shaped links (Fig. 1). Because of their flexible nature, these chains interlock and entangle, thereby providing the dry and cohesionless granular materials similar mechanical rigidity as of their cohesive counterparts. This property called “geometric cohesion" has also been observed in a variety of other interlocking particle morphologies such as U-shape, Z-shape, and rod-shaped particles etc. (Gravish & Goldman, 2016). Flexible granular chains of length or number of monomers(M) greater than a certain critical chain length exhibit an array of intriguing properties such as jamming at low densities, strain stiffening and higher stiffness at smaller coordination numbers etc. (Dumont et al., 2018). Although experimental measurements have provided an insight into the kinematics of these chains at large deformation and deformation rates, the micromechanics of chain response under large deformation and deformation rates is yet to be explored. In this study we develop and calibrate a discrete element method contact model to simulate the mechanics of the macroscopic flexible granular chains, wherein the links connecting the beads in the chains are implemented as superimposed kinematic constraints on the chain motion, with a link contact consisting of a linear normal and angular stiffness (Fig. 1). The orthogonal cutting simulations are carried out with varying chain length(M), cutting depth (D0), rake angle (β) and cutting speeds (vc). We evaluate various micro-mechanical, topological and macroscopic parameters to elucidate the macro and micro-mechanical response of these chain ensembles at large deformation rates. The ability of the chains to form tensile force chains effects the formation and suppression of localized shear bands during cutting. And the flexible geometry of the chains results in dispersion of the velocity field away from the cutting tool leading to retardation of motion in the ensemble.

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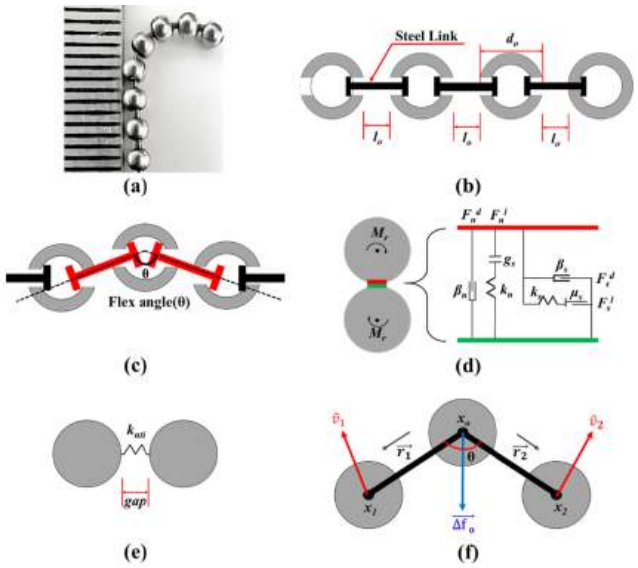

Modeling of sea ice dynamics in geological scale based on discrete element method

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Keywords Sea ice dynamics, Discrete element method, Polyhedron element, Geophysics

Significantly discrete distributions can be observed in sea ice at different spatial scales. The thermally generated geological-scale ice sheets in the Antarctic and Arctic can be observed to have obvious collisions, fractures, and ridges under the driving of the atmosphere and ocean, which are considered to have a huge impact on climate changes. The most popular sea ice dynamics simulation methods are mainly continuum methods such as finite difference method, although those methods can model sea ice phenomena in a floe size about 500m, however, the continuity and uniformity assumptions are difficult to satisfy at that resolution. In recent years, with the rapid growth of computing power and more accurate sea ice observation, it is possible to apply the discontinuous medium method to the polar sea ice dynamics simulation to obtain the ice phenomena in floe size scale. In this paper, we simulated the dynamic of polar ice based on the discrete element method(DEM), and constructed the process of level ice fracture with the bonding-fracture model between elements. With the discrete element method based on polyhedral elements, we simulate the natural phenomena of sea ice fracture and ice ridge formation in a small region. In order to model the evolution of sea ice at the geological scale, the DEM model is combined with the thermodynamic calculation in CICE sea ice model, the generation and disappearance of sea ice elements with thermal changes are considered, which proves the feasibility of the discrete element method in the simulation of climatological sea ice.

Improvement of Quantitative Accuracy of DEM simulation for Estimating Residual Settlements of Railway Ballasted Layers

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Keywords DEM, Ballasted track, OpenMP, V&V, Angularity

DEM has been used in the field of railway track research recently. However, it has been mainly used for qualitative evaluation since its quantitative accuracy was not so high. On the other hand, a railway company consider increasing of vehicle running speeds on a day following ballast renewal works. Then it is necessary to estimate residual settlements of ballasted layers immediately after ballast renewal works by using numerical methods to evaluate influences of running speeds on residual settlements. For this objective, DEMCS-track, a DEM simulation code developed by RTRI and university of Tsukuba is need to improve the quantitative accuracy to estimate residual settlement precisely. At first, DEMCS-track was parallelized by using Open MP to decrease computing time. Secondly, the author modified angularities of ballast grains models in discrete ballasted track models by using “asperity” elements. Next, the author made four types of ballasted track models of different compactness, with the densities of ballasted layers is 1.50g/cm3, 1.57g/cm3, 1.60g/cm3, and1.67g/cm3, respectively. Finally, initial settlement simulation in the process of 70 trains passing is carried out by using DEMCS-track to validate the DEM codes. The initial settlement derived from the DEM simulation was compared with data of initial settlement measured in real railway line. Findings from above mentioned process are following: 1.The computing time is reduced to one tenth at the case with 32 threads of supercomputer. 2.The shapes of ballast grains models are improved by increasing angularity with 100 – 150, by using “asperity” elements. 3.The residual settlement calculated by DEMCS-trac fit into the range of mean value plus-minus one standard deviation of measured data from real railway line.

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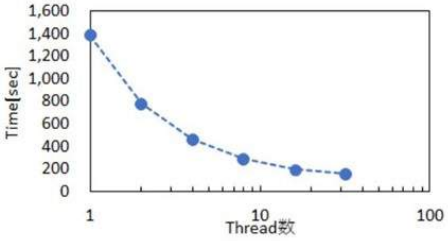

Figure.1 Increasing of computing time by OpenMP

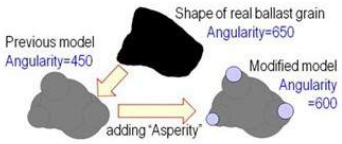

Figure.2 An example of increasing of angularity by using “asperity” elements

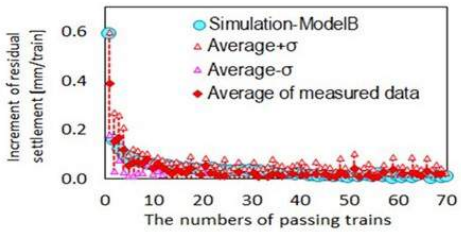

Figure.3 Comparing initial settlement of ballasted layer from DEM simulation with measured data

Assessment of drag models for CFD-DEM simulations of gas-solid flow in a pseudo-2D bubbling fluidized bed

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Keywords Multiphase flow, Fluidized bed, CFD-DEM, Simulations, Drag model

Gas-solid multiphase flows are found in various industrial processes such as in fluidized beds. In such flows, the dominating factor which governs the dynamics of multiphase flows is the gas-solid drag force that acts to suspend the particles in the air against the gravity. In order to obtain reliable flow predictions using the Computational Fluid Dynamics (CFD) - Discrete Element Method (DEM) approach, the use of appropriate interphase drag model is very crucial. Numerical simulations are performed for gas-solid flows in a pseudo-2D bubbling fluidized bed for which the experimental measurements [1] are available. Simulations using the same system have been presented in the literature [2] that lacked the comparison with full set of experimental data available. In this work, simulations are performed for three fluidization velocities using three different drag models. Our simulation results were compared to experimental data considering the important parameters such as the mesh size, root mean square of bed height and the bed expansion frequency. The results reveal that all drag models yield different flow predictions under different fluidization velocities and none of the drag model is found to match with experimental data for all cases. This type of systematic study is important to determine the appropriate drag model under different fluidizing conditions.

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Micromechanical origins of heap formation in sheared granular materials with elongated particles

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Keywords Elongated particles, Weissenberg effect, split bottom shear cell, secondary flow, normal stress differences

Granular materials with elongated particles exhibit complex flow patterns under shear deformation. Unlike spherical particles, when assemblies with shape-anisotropic particles are sheared, there is accumulation of material due to secondary convection flows (Fischer et al., 2016). This effect resembles the Weissenberg effect of non-Newtonian fluids, where secondary flows lead to phenomena such as rod climbing. Although a direct comparison between liquid and granular flow is not prudent, due to the discrete particulate nature of the latter, comparisons of the causes behind each phenomenon can be drawn. The split-bottom shear cell geometry, and linear shear cell geometry with a middle split, are employed in discrete element simulations to study the micromechanical origins of the effect. Systems of spherical and anisotropic particles are simulated in both shear cell setups, to facilitate comparisons between materials that do not exhibit heaping and systems that do. The mechanical response is characterized in terms of stress measurements, such as shear stress, normal stress and the differences between the normal components of the stress tensor. Our results reveal that a granular Weissenberg effect occurs, which is attributed to the components of the normal stress differences; this is also the driving factor for the classical Weissenberg effect. Consequently, this work brings an analogy between the Weissenberg effect observed in non-Newtonian fluids and heap formation in granular fluids composed of discrete particles.

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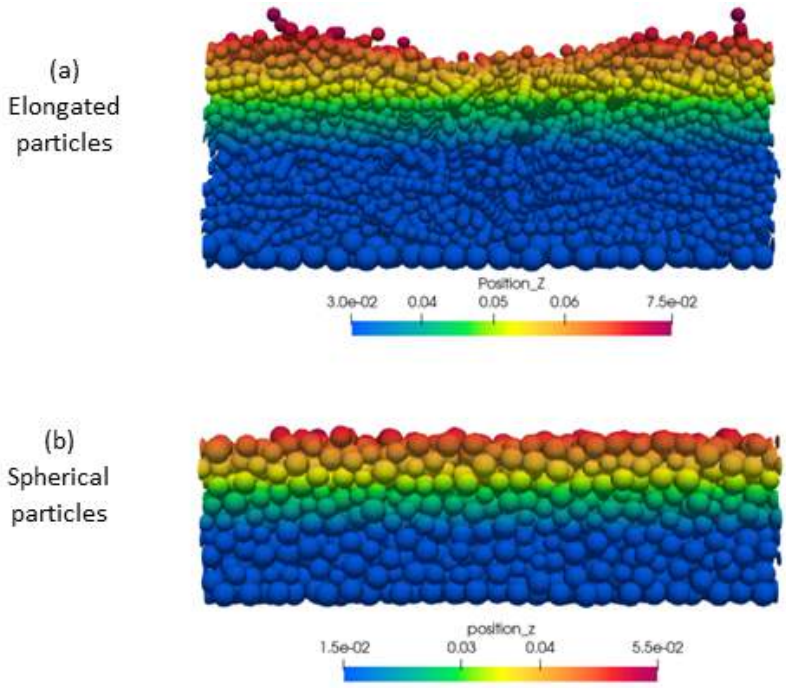

Erosion rate and mixing of dry-wet granular systems

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Keywords DEM, capillary bond, erosion, scaling

By means of particle dynamics simulations, we study the erosion of a granular system composed of wet monodisperse spherical particles interacting via elastic, frictional and capillary forces, subjected to a flow of dry grains inclined above its angle of repose. We are interested in the effect of inclination angle and surface tension on the time evolution of the erosion rate and diffusion of the cohesive particles into the dry grains. We consider two different scenarios, one in which the liquid surrounding a wet particle is evaporated after bond rupture, and another scenario in which the liquid is still available for creation of new cohesive bonds between initially wet particles. In the first case, the flowing dry particles gradually erodes the underlying wet layer and a homogeneous mixture is achieved in finite time whereas in the second case, the eroded wet particles agglomerate at the free surface as shown in Fig. 1. We analyze the short-time evolution of erosion in terms of the rate of erosion and the long-time behavior in terms of mixing for different values of surface tension and inclination angle. We find that the data can be scaled by dimensionless parameters combining system parameters.

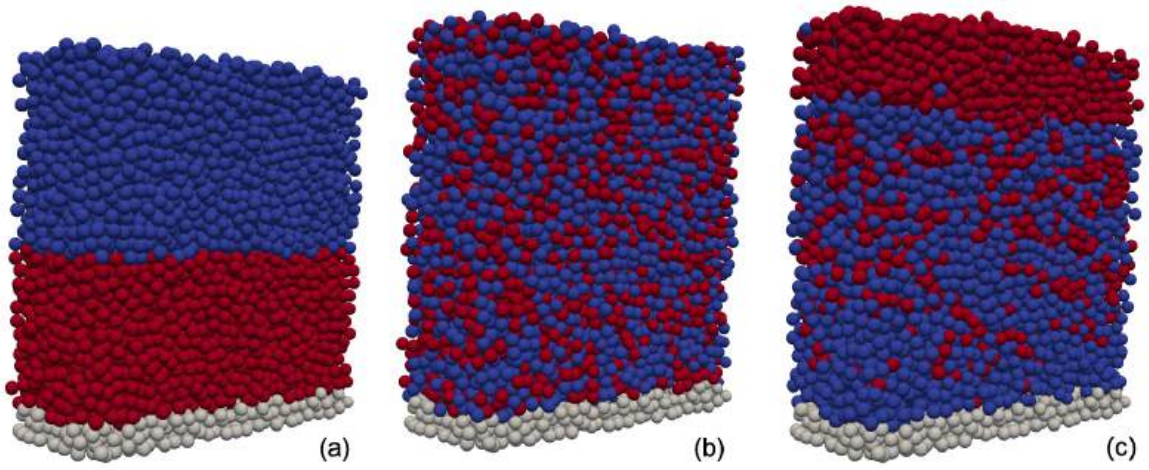

Figure 1 : Snapshots of the dry-wet system inclined at 28° and simulated by means of an in-house code based on the Discrete Element Method: (a) initial state with a layer of dry particles on top of a layer of wet particles; (b) long-time state with the scenario of liquid evaporating after debonding; (c) long-time state with the scenario of conserved liquid after debonding.

DEM investigation of the microscopic mechanism of scale effect of sandy gravel material

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Keywords Rockfill materials, Scale effect, Discrete element method, Particle breakage, Particle size distribution

It has been generally accepted that the underestimation of the high rockfill dam deformation is primarily due to the scale effect of rockfill materials, i.e., there are differences between the mechanical properties of prototype materials and scaled-down samples. Recent experimental studies again demonstrate that the scale effect of rockfill materials consisting of sandy gravels and blasting rocks is different, and the underlying mechanism is still unclear. This study uses the discrete element method (DEM) to investigate the microscopic mechanism of the scale effect of sandy gravel material collected from the Dashixia rockfill dam in China. The sandy gravel material composed of rounded gravel and pebbles is modeled as an assembly of spheres, and the rolling resistance at particle contacts considers the slight particle non-sphericity. The DEM input parameters are calibrated and verified by a series of single-particle crushing tests, angle of repose tests, and triaxial compression tests. The DEM simulations of triaxial compression tests are performed on samples with different particle crushing strengths and particle size distributions (PSD). Particle breakage weakens the shear strength and considerably lowers the deformation modulus of sandy gravel material. On the contrary, the widening of PSD has a significant effect on the force transmission structure, which is manifested as the increase of contact force and higher mobilization of frictional force at contacts, thus promoting bulk resistance to deformation. The scale effect of sandy gravel material results from the competition between these two factors. As to the rounded gravel and pebbles studied here, the scale effect is dominated by the widening of PSD, which is confirmed by the increase in the deformation modulus and shear strength with increasing maximum particle size and size span.

Investigation of flow characteristics of landslide materials through pore space topology and complex network analysis

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Keywords Seepage failure, granular packings, complex network, permeability

Unlike embankments, earth dams, and other man-made structures, most landslide dams are formed by rapid accumulation of rock or debris rather than mechanical compaction; thus, they are loose and pose a great risk of seepage failure. Landslide materials usually have complex pore structures with randomly distributed pores of various sizes, making the flow and transport processes very complex. Aiming at these challenges, we systematically investigated the influences of pore structure on the micro-and macro-scale flow characteristics of landslide materials. First, landslide materials are simplified as spherical granular packings with wide grain size distributions. Then, we use the Finite-difference method Stokes solver (FDMSS) to simulate the fluid flow through granular packings and calculate their permeability. We characterize the pore structure using different topological measures, including those borrowed from complex network theory. Among these measures, tortuosity and global efficiency show clear relations with permeability. The pore network modeling indicates that pore size heterogeneity and pore connectivity significantly influence flow characteristics. The correlation between pore-scale velocity and throat diameters follows a power-law scaling with an exponent close to 2, suggesting that the Hagen–Poiseuille law would still be valid in complex porous media. The permeability and porosity, throat radius, and tortuosity of pore structure can be related by the equation proposed by Nishiyama & Yokoyama (2017). The complex network analysis reveals that the assortative network is more permeable than the disassortative network. Furthermore, pores with larger closeness centrality have higher flow efficiency, resulting in higher macroscopic permeability.

DEM investigation on Undrained Cyclic Behavior of Granular Soils under True Triaxial Conditions

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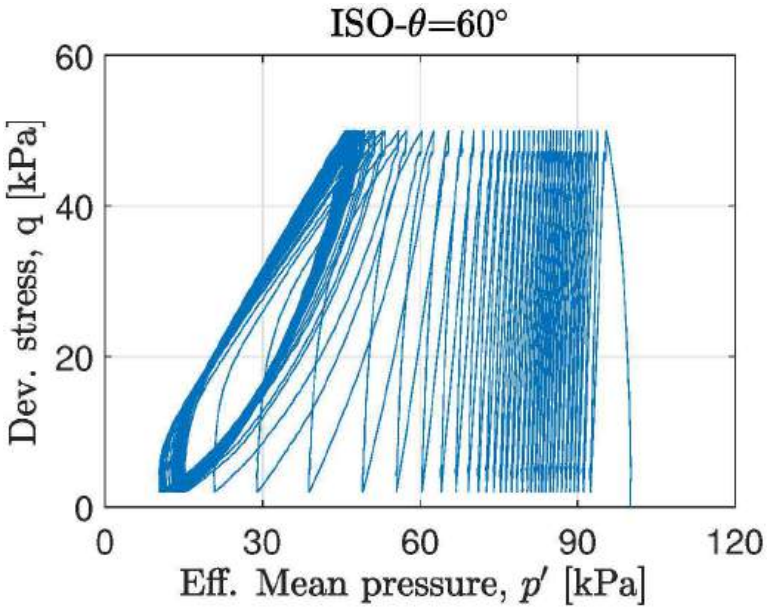
Keywords Intermediate Principal Stress, Undrained Cyclic Behavior, True Triaxial Test, Liquefaction

Until now, most experimental studies with undrained cyclic loading on granular soils have been limited to simple shear or axisymmetric triaxial conditions due to the difficulties involved in conducting tests with more complicated stress paths. However, the absence of information regarding the impact of intermediate principal stress led to the inspiration of studying the cyclic behavior under undrained true triaxial conditions using the Discrete Element Method (DEM) coupled with fluid method. The simulations were performed under isobaric conditions with different combinations of Lode angle and stress amplitude. The results revealed that an increase in Lode angle renders the soil more susceptible to liquefaction, decreases the cyclic resistance ratio, and leads to a more contractive behavior. Moreover, the shear strain amplitude during cyclic mobility increased with an increase in the Lode angle, indicating greater deformability of the soil. This study sheds light on the effect of intermediate principal stress on the undrained cyclic behavior of granular soils under true triaxial conditions, underscoring the importance of accounting for this effect in geotechnical design.



Impact of 1-dimensional granular chain

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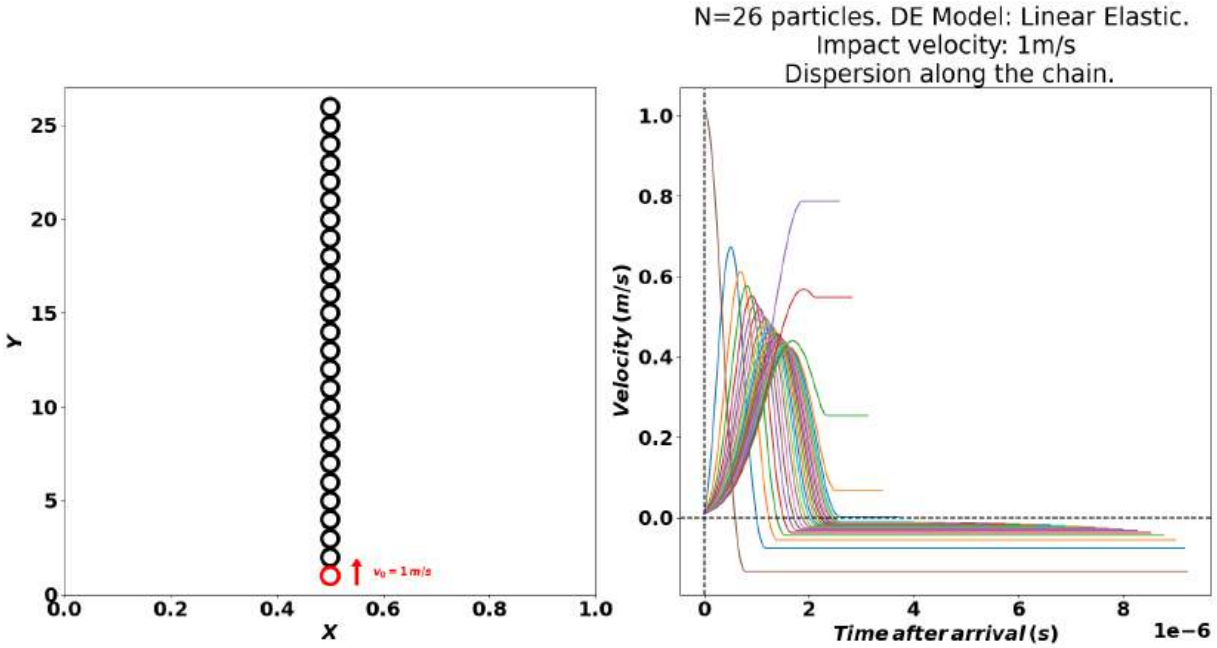
Keywords Wave Propagation, Granular Media, Discrete Element Simulations, Granular chain

Study of impact and subsequent wave propagation in granular media has attracted the interest of researchers across the globe over the last few decades. These investigations have relevance in fields of defense (Eg.: demining operations), automotive (Eg.: crash impact mitigation), acoustics (Eg.: noise damping), etc. For effective design of engineering objects for such applications, the study of wave propagation dynamics in granular media is necessary. In particular, dependence of various material and geometric properties of granular media on the wave speed, dispersion and attenuation is of considerable interest. We study the impact dynamics of a chain of spheres through Discrete-Element (DE) simulations. It is well known that the damping characteristics of materials are dependent on the strain rates they are subjected to. Keeping this in view, we have implemented a new DE model which employs a velocity dependent coefficient of restitution, ep(v). Using this DE model, we have simulated a 1-dimensional granular chain, which is imparted an input pulse on one end. We have investigated the subsequent wave that is setup in the chain. We report on the effect of input pulse profile (frequency, amplitude) on the wave speed, dispersion and attenuation along the length of the chain. The effect of various parameters such as pre-compression, chain length, density of constituent materials, size of the particles etc., on the wave dynamics has also been investigated. We have compared the performance of our velocity dependent damping DE model with other well known elastic (Hooke, Hertz) and inelastic (Linear Spring Dashpot) DE models. We conclude that incorporating velocity dependence of damping into the DE models helps us better capture the physics of wave propagation in granular media. This work serves as a step towards building better strain rate dependent DE models for future investigations in this field.



Optimising the rheology of dense granular suspensions using DEM modelling and machine learning

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Keywords Granular suspension, discrete elements, machine learning

Achieving optimal dense suspension rheology is key to meeting product quality requirements in a wide range of industries, but the traditional optimization approach, which is heavily reliant on physical trial-and-error, is prohibitively time-consuming and expensive. Virtual optimisation can lead to significant time and costs savings in this context. This work demonstrates an efficient virtual optimisation methodology that combines Discrete Element Method (DEM) simulation and machine learning to rapidly identify the optimal particle scale properties for a target suspension viscosity. The effect of the liquid phase of the dense granular suspension is obtained by combining a short-range hydro-dynamic force model with a fluid drag model. The optimization methodology consists of parametrizing the particle size distribution, morphology, volume fraction and surface frictional properties, automatically generating and running DEM simulations of dense granular suspensions subjected to simple shear for a well-distributed quasi-random sample of the parameter space and training a Reduced Order Model (ROM) on the resulting synthetic data using machine learning. A multi-objective genetic algorithm is then utilized to rapidly estimate the globally optimal parameter set from the ROM. This results in several orders of magnitude reduction in computational expense relative to the equivalent purely simulation-based approach and makes the virtual optimisation of dense suspension rheology from particle scale properties practical. The advantages and limitations of the proposed methodology are further discussed in the talk.

DEM modeling of the drained and undrained triaxial response of Karlsruhe fine sand

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Keywords Granular material, triaxial test, rolling resistance

In this study, our aim is to quantitatively model the mechanical behavior of cohesionless granular materials for drained and undrained triaxial conditions under monotonic loading. This to investigate in a later stage the susceptibility of granular materials to static liquefaction and triggering loading conditions. In the mining industry, static liquefaction is a common cause of failure of tailing storage facilities (TSF) [1], and therefore a fundamental aspect in the design and performance of such facilities. To capture the material response of Karlsruhe Fine Sand (sub-angular grain shape) [2], a rolling resistance linear contact model is used along with spherical particles and calibrated through an iterative process by adjusting the model parameters until the numerical response matches the experimental response. Finding a unique set of contact model parameters for both drained and undrained conditions is challenging since the stress-strain response is strongly influenced by the interplay of the different model parameters [3]. The DEM triaxial test simulations were performed using the open-source software YADE [4] on samples confined by rigid-wall boundaries. First, the model parameters were determined to replicate the drained triaxial tests response of Karlsruhe Fine Sand and a good agreement was obtained for both stress and volumetric response. For validation purposes, numerical simulations of undrained triaxial tests under monotonic and cyclic loading were also performed. Comparison of the numerical and experimental results showed that the numerical material behaved stiffer than the experimental material for undrained conditions. This led to the readjustment of the model parameters and to establish two different sets to better capture for each drainage condition the real material response. Future work will focus on the influence of more realistic modeling of particle shape to capture the response of the real granular material and to quantitatively investigate the onset and post-liquefaction response.

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Coupled effects of particle size and shape polydispersity on the mechanical behavior of granular media

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Keywords Shear strength, particle shape, grain size distribution, polydispersity, discrete-element modeling

Numerical and experimental studies have proven that particle size distribution (psd) does not affect the critical shear strength of granular media, with the condition that particle shape and roughness remain constant across sizes. On the other hand, particle shape is known to have a strong impact on the strength of these materials. While studies have primarily focused on the effects of particle size dispersity, the influence of grain shape variations within a granular media is still poorly understood. This research explores the mechanical behavior of samples presenting particles with size-shape correlations through three-dimensional discrete-element simulations. First, we investigate the effects on a geometrical particle shape descriptor related to grain angularity in the following conditions: (A) large grains are angular while small grains are spherical, and (B) large grains are spherical while finer particles are angular. Then, to characterize the mechanical properties of these materials, we perform triaxial tests on samples ranging from mono to highly polydisperse particle sizes, while the particle angularity varies by increasing the number of the vertex of polyhedral shapes from 6 (octahedra) to perfect spheres. We find that for material presenting size-shape correlation, the critical shear strength is no longer independent of the psd. For a given psd, the diversity of shapes in a granular sample substantially impacts its strength and solid fraction. Microstructural analyses help to understand how each class of grain shapes contributes to the macroscopic behavior as well as to provide insights into the micromechanical role played by particle shape based on their size.

Soft cohesive particles under compaction

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Keywords Material Point Method, Contact Dynamics, Granular materials, Compaction, Elastic particules

Soft granular materials are composed of disordered and highly deformable particles. The production of tablets, compacts or pellets from this type of particles is important in many industrial applications such as pharmaceuticals, cosmetics, food products and metal powders. Their compaction leads to complex behaviors due to particle shape change as well as particle rearrangements [1]. In this work we use the Material Point Method (MPM) for individual particles deformations, combined with the Contact Dy- namics (CD) method for the treatment of frictional contacts [2,3]. This approach was employed to investigate the compaction of elastic and plastic particle assemblies. In each case, we performed a sensitivity study of both friction and cohesion parameters by analysing packing properties (packing fraction, connectivity...). Finaly, a qualitative comparison will be performed between numerical and experimental results.

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Discrete element modeling of granular flows of polyhedral particles

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Keywords DEM, polyhedral particles, rotating drum, cascading regime, scaling

We investigate the flow behavior of granular materials composed of polyhedral particles using an in-house code based on polyhedral representation of particle shapes and a rigorous contact detection algorithm. This algorithm is able to distinguish different types of contact (face-face, face-edge, face-vertex, edge-edge, edge-vertex, vertex-vertex). A linear force law based on normal overlaps at the contact points between particles is used and face-face and face-edge contacts are represented by at least three and two contact points, respectively. Furthermore, to reduce the effect of sharp corners and edges, a small Minkowski radius is added. This approach is applied to simulate the flow behavior in rotating drums in the cascading flow regime. This geometry is extensively applied in industrial processes such as mixing, grinding, and granulation. Nevertheless, the rheology and scaling behavior for aspherical particles has not been investigated on a systematic basis. In fact, most previous studies have concerned either the rolling regime or the flow of spherical particles. In our simulations, we used icosahedral particle shapes and a broad range of the values of rotation speed, drum and particle diameters, and filling heights. We analyzed the evolution of flow variables including both macroscopic and microscopic properties such as the active layer thickness, the shape of free surface in terms of its average slope and the steepest slope, coordination number, forces, and shear rate of the active layer. We show that the flow behavior can be described in terms of a single dimensionless upscaling parameter combining different system parameters. We consider also the effect of particle coarsening on the flow characteristics. Interestingly, our simulations show that wall slip scales with the same upscaling parameter, meaning that wall slip should be treated with the same status as other flow variables.

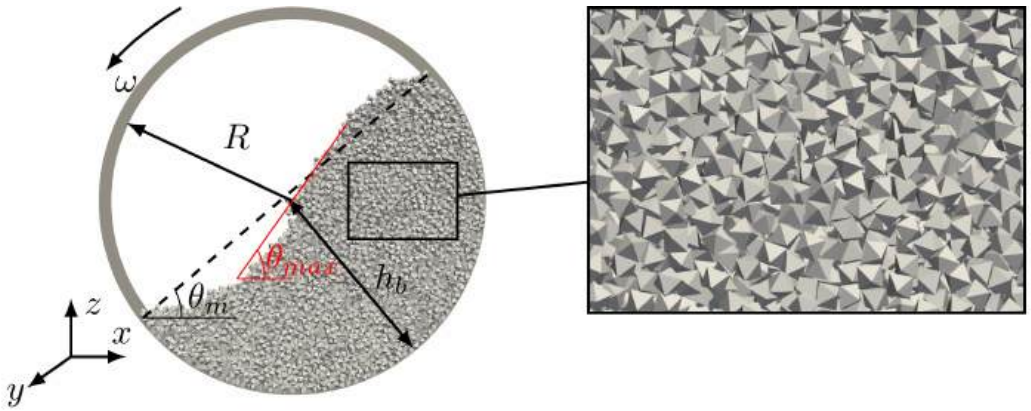

Figure 1: Snapshot of the flow of icosahedral particles in a rotating drum with periodic boundary condition along the y axis.

Segregation model for binary granular mixture during heap flow in quasi 2D system

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Keywords Segregation model, granular materials, macroscopic, binary mixtures

Flow of granular mixtures is encountered in most of the industrial processes. Modelling of such type of flow is very important to understand flow and segregation process. In this paper, segregation model equations are developed for two types of materials: flow of particles on the same materials (equal in size and density) and flow of binary mixtures (different in size). The system used is flow of particles between two vertical glass plates with a gap. The approach involves the use of macroscopic mass, momentum and species balance equations. The macroscopic balance equations are obtained by averaging the microscopic balance equations across the thickness of the layer. In the first part model equations are developed for flow of particles (equal in size) followed by flow of binary mixture (different in size). First model equation gives the direct relation between the velocity in the layer (u) and layer thickness (δ). While the second model equation gives the relation between number fraction of small particles (f) along the flow length x. The average velocity of particles withing the flowing layer is in well agreement with a predicted model.

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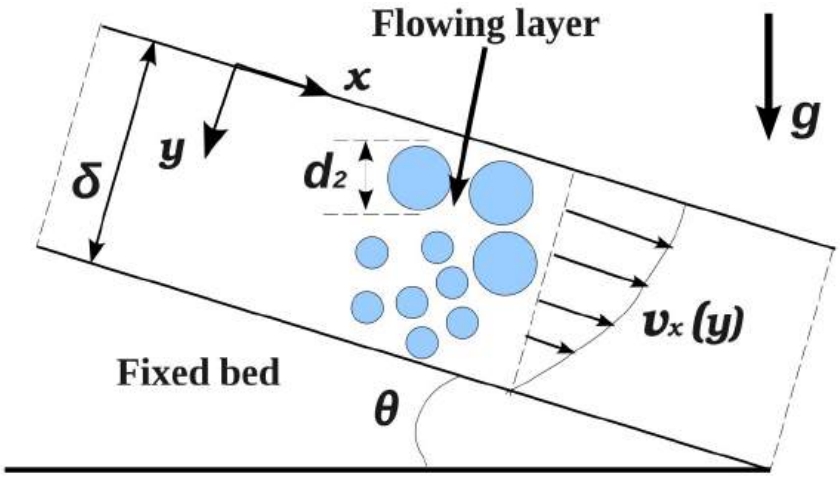

Numerical Simulation of vibro-fluidised inelastic particles with surface roughness using discrete element method

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Keywords Kinetic Theory of Granular Glow, Vibro-fluidised Bed, Rough particles, Granular Temperature

Vibration assisted fluidisation has wide application in process and pharmaceutical industries; however, the role of amplitude and frequency of vibration, on the macroscopic properties such as the density and the RMS velocities, is not well understood. Kumaran (1998) has derived the velocity distribution functions for the smooth and nearly elastic two-dimensional discs in a vibro-fluidised bed. Kinetic theory for nearly smooth and perfectly rough particles is derived in Rao and Nott (2008) for constant tangential coefficient of restitution. The objective of the present work is to simulate a vibro-fluidised bed of inelastic and rough particles and compare the results with the prediction within the range of validity. The objective also includes understanding the effect of parameters like amplitude and frequency of vibration on the particles' translational and rotational velocity distribution. To that goal, a three-dimensional vertical vibro-fluidised bed is simulated using LAMMPS. Inter-particle contact is simulated using linear spring-viscous dashpot model. Vibrational amplitude is set smaller than the particle diameter. Simulations are first performed for the range of parameters identified in Sunthar and Kumaran (1999) for comparing the results with the leading-order predictions of kinetic theory. Simulations were later extended for rough and inelastic particles. Distribution of the contact angle are obtained from the simulations to identify the regimes of contact. Contribution of the collisional part to the stress as compared to the streaming part is several orders of magnitude less as the simulations are performed mainly in the dilute regime. The effect of normal coefficient of restitution (COR) and the friction coefficient (μ) on the translational (TFE) and rotational fluctuation energy (RFE) is determined. TFE and RFE decreases and increases with the increase in μ, respectively (Figure 1). The amplitude and frequency of the vibrating base have very similar effects on the fluctuating energies.

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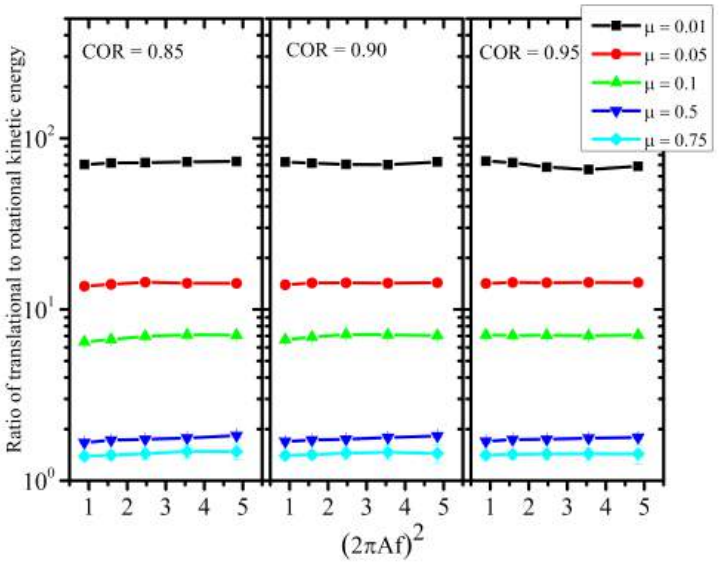

DEM investigation of separation performance and stress analysis of a five-deck industrial scale screen

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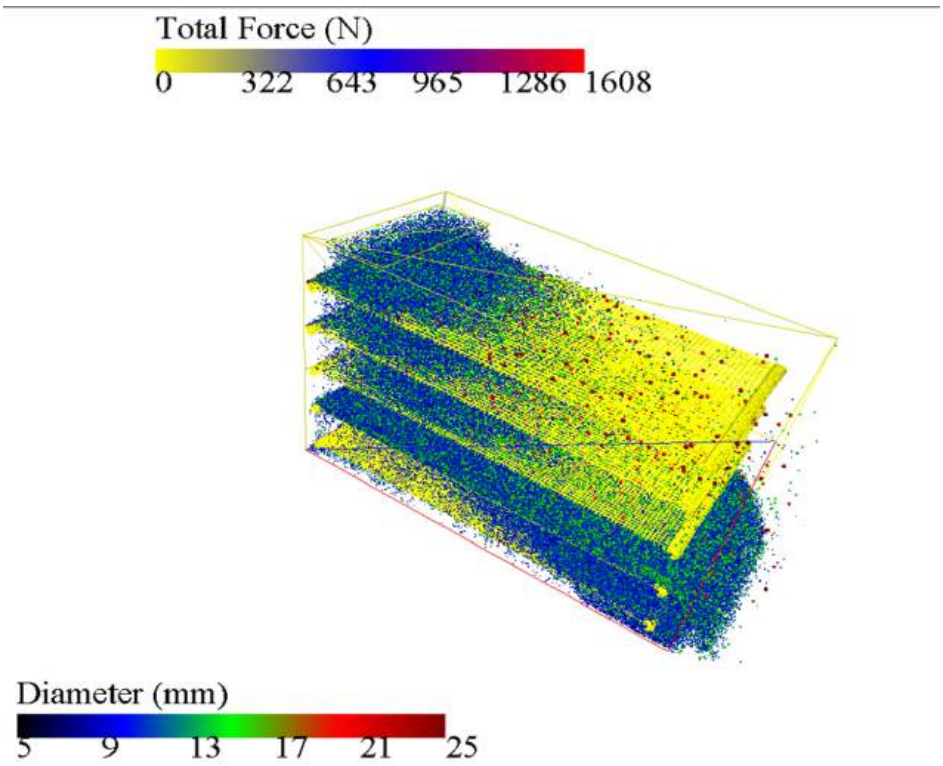
Keywords Screening, Discrete Element Method, Separation performance, Stress analysis

Screening is the most widely used method of sizing bulk materials. One of the vital roles of screens in a processing plant is to generate products of specified sizes as per the customers' requirement. During the Iron-Making process, optimal size range of pellets for effective reducibility and porosity inside the blast furnace is (-16+ 6) mm. To achieve this, two screens each of five decks with aperture sizes 25, 20, 17, 11 and 8 mm, made up of wire mesh media are used. DEM tool facilitated true replication of existing process including full screen geometry, its motion and high throughput. A comparative study of the plant data and simulation data facilitated validation of the model. Study of effects of vibration parameters i.e., frequency and amplitude, was done to find optimum values for maximum efficiency. The model provided an insight into the operation of each deck. It was observed that on increasing frequency, better stratification of the bed was achieved for the lowest deck and therefore lesser misplacement of -6.3 mm into oversize. However, increasing the vibration frequency beyond certain limit, increases the stress applied by flowing particles on the screen panel which may damage it. So, stress analysis on each deck were evaluated for six sub-parts along the screen length. Stress profile on each deck as well as along the length of deck varied as per the amount of feed and feed size distribution. Feed part of top screen experienced most of the impact force and breakage mostly occur in this part.



Hexapod particles: Random close packing texture and mechanical behavior

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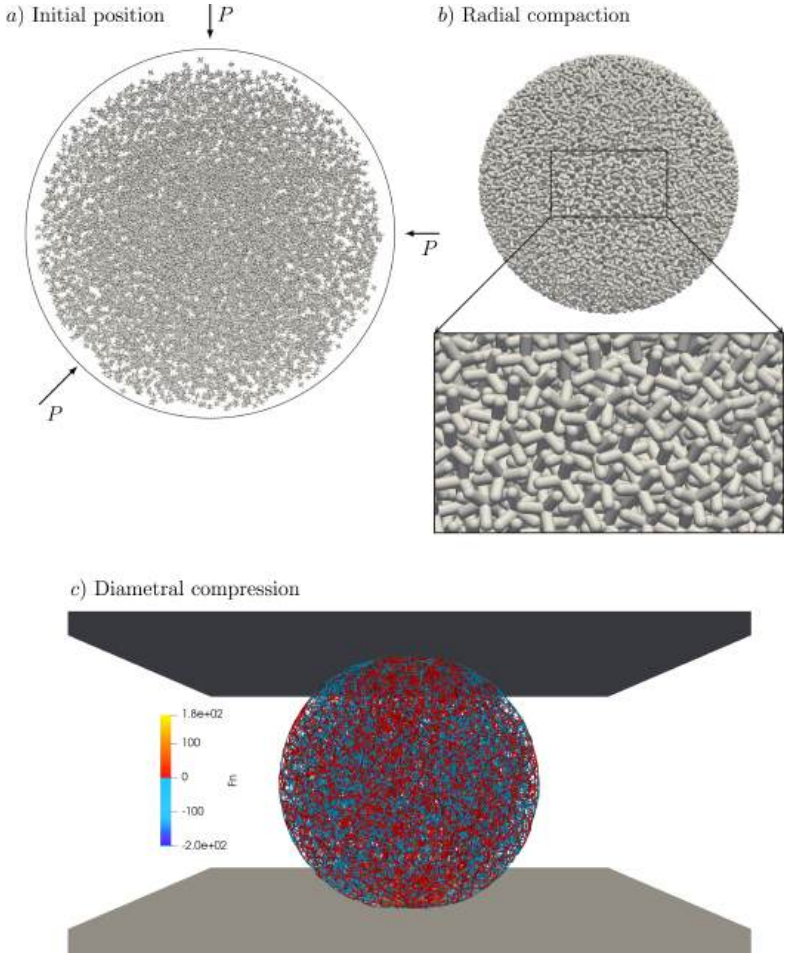
Keywords DEM, nonconvex particles, cohesion, compression, breakage

Many materials manufactured by means of the ceramic processes (grinding, pressing, sintering), have a granular microstructure composed of cohesive aggregates of various shapes, including nonconvex shapes. In this work, we investigate the mechanical and microstructural properties of agglomerates composed of hexapod- shaped aggregates using an in-house DEM code. The aggregates are characterized by their aspect ratio (ratio of their extension to thickness). By varying this parameter, the particle shape changes from sphere to thin hexapods. Spherical agglomerates are built by means of radial compaction for different values of aspect ratio and friction coefficient. We investigate the influence of aspect ratio and friction coefficient on the microstructure and geometrical properties such as packing fraction, connectivity and elastic bulk modulus. We also investigate diametral compression of these agglomerates and we analyze in detail the strength and fracture behavior as a function of aspect ratio, friction coefficient, and cohesive force between aggregates for both reversible and irreversible cohesive interaction. We show that for large enough aspect ratio, nonconvex shape considerably amplifies the cohesive strength of the agglomerate.



Modeling Irregular Particle Shapes in the N-Body Gravity SSDEM Code PKDGRAV

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Derek Charles Richardson

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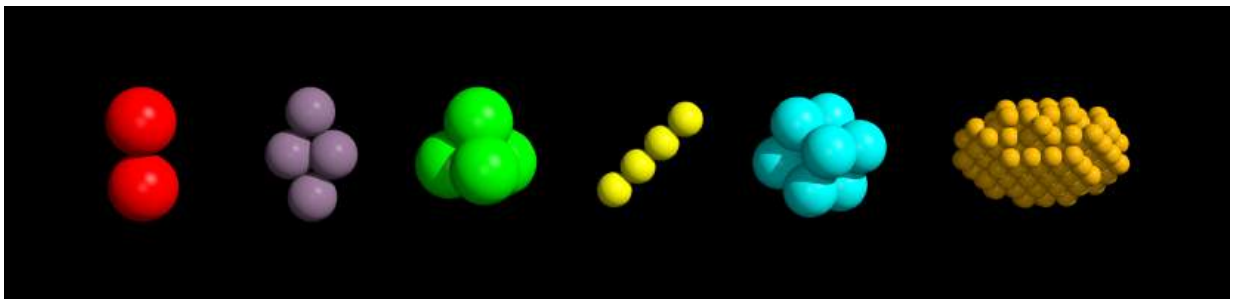
Keywords Soft-sphere, N-body, Small Solar System Bodies, Non-spherical particles, Planetary Science

We present a scheme for conducting high-resolution, soft-sphere DEM (SSDEM) simulations with non-spherical particles in the context of modeling rubble-pile bodies in the solar system. These bodies have surfaces with many thousands of discrete, irregular components and likely similar interiors. It is known that particle shape plays an important role in granular processes, but most DEM codes use spherical particles for the simplicity and computational efficiency they afford. Other codes include implementations of non-spherical particles, but their complexity can limit the numbers of particles that can be used in a simulation. We use the N-body code PKDGRAV, which is optimized for calculating gravitational interactions between very large numbers of particles. PKDGRAV uses a hierarchical tree algorithm that reduces the cost of finding particle neighbors and calculating interparticle gravitational forces and can be parallelized across an arbitrary number of processors.

Instead of constructing polyhedral particles with flat faces and edges, we make use of the existing capabilities of PKDGRAV and model non-spherical particles using a “glued-sphere” approach. We arrange arbitrary numbers of spherical particles in any desired shape and then fix their relative positions so that they behave as a unit, creating rigid, non-spherical aggregates. These arrangements can then be treated as “pseudo-particles,” capturing the physical realism of non-spherical grains, but without much of the computational complexity inherent in using polyhedral shapes.

As far as we are aware, PKDGRAV is the only code that combines a highly parallel N-body gravity solver and a soft-sphere contact model with an efficient “glued-sphere” approach to constructing non-spherical particles. This allows us to conduct high-resolution simulations of self-gravitating aggregates composed of non-spherical grains. While this technique has broad relevance to the study of small solar system bodies, we plan to use it to study spin-up, tidal effects, and granular convection and packing on rubble piles.



Hydrodynamics of filtration and retention of particles in slurries through saturated porous media

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Keywords Porous media, particle filtration, particle retention, slurry, CFE-DEM

Filtration of particle in porous media is in highly concerned due to its high efficiency of separations. The transport and retention of particles in slurry passing through porous media causes particle clogging, which resulted in the permeability reduction of porous media and the system failure in industrial applications. Particle clogging is primarily affected by the ratio of the particle diameter to pore-throat size of the porous media. A previous study reported that the filtration and retention of particles are affected by both the Stokes number and particle concentration in porous media, when the particle motion was driven by the fluid carrying passing through a homogeneous porous media.

Therefore, this research investigated hydrodynamics of the particle filtration in the heterogenous porous media, studying the hydrodynamics of the retention of slurry particles driven by fluid in the saturated porous media. Fluid-particle two-phase flow in porous media is numerically simulated using the computational fluid dynamics-discrete element method with a coupled resolved particle model. Particle clogging can be directly precited via the interaction between the particles and surface of the porous media by tracing the exact location of each particle. The study shows the hydrodynamic convention of the slurry during the filtration process, slows pore structure variation in affected by the particle retention. In addition, an increase of the particle concentration or diameter increased the possibility of the particles being retained in the porous media, and stokes number and gravity are also the key elements affecting the filtration.

Controllable Capillary Assembly of Magnetic Ellipsoidal Janus Particles into Tunable Rings, Chains and Hexagonal Lattices

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Keywords Controllable assembly, capillary interactions, Janus particle, liquid interface, discrete element method

Colloidal assembly at fluid interfaces has great potential for the bottom-up fabrication of novel structured materials. However, challenges remain in realizing controllable and tunable assembly of particles into diverse structures. Here, we apply a hybrid approach combining the lattice Boltzmann and the discrete element methods to investigate the behaviour of magnetic ellipsoidal Janus particles adsorbed at a liquid–liquid interface. Depending on their tilt angle, the anisotropic particles deform the interface and generate capillary dipoles or hexapoles. Driven by capillary interactions, multiple particles thus assemble into chain-, hexagonal-lattice-, and ring-like structures, which can be actively controlled by applying an external magnetic field. A field-strength phase diagram is predicted in which various structures are present as stable states. Owing to the diversity, controllability, and tunability of assembled structures, magnetic ellipsoidal Janus particles at fluid interfaces could serve as versatile building blocks for novel materials.

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A FEM-DEM multiscale approach in nuclear Mox fuel fabrication

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Keywords FEM, DEM, Multiscale, Macroscopic, Microscopic, EVR, Homogenization law

The nuclear fuel comes in the form of cylindrical pellets, the manufacture of such pellets is based on the powder metallurgy process called the Mox (Mix oxides) fuel manufacturing process. This process is composed of three main steps: powders blending, pellet shaping, and pellet sintering. Several crucial points have to be mastered to achieve manufactured pellets that meet the desired properties. For this reason, in addition to experimental approach (instrumented uniaxial compressions, shear trials), numerical simulations are used in two different scales: macroscopic and microscopic scale. Regarding the macroscopic scale, continuum approach based on the finite element method (FEM) is used to take into account the powder behavior during pellet shaping (Pressing) using soil mechanics plastic behavior. For the microscopic scale, the Discrete Element Method (DEM) allows to take into account the microstructure and the breakage agglomerate behavior depends on cohesion between aggregates and the porosity network [2]. To link microscopic and macroscopic scales, numerical homogenization techniques will be used to estimate the macroscopic elastic and plastic properties from the microstructure. This talk focuses on presenting numerical simulation tackled for each scale. In conclusion, we will propose a bibliographical analysis of numerical upscaling techniques.

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Correlating hard sphere model with material properties

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Keywords Hertz-Mindlin model, Tangential coefficient of restitution, angle of impact

There are mainly two approaches for simulating flow of granular materials, namely the hard and the soft sphere method. The earlier model is defined by two parameters, the normal and the rotational coefficients of restitution [1]. The soft sphere approach is based on the spring-dashpot-slider description of the particle contact and relates the material properties such as modulus of elasticity, Poisson's ratio to the post contact behaviour of the particles. The normal coefficient of restitution is correlated with the spring constant and the coefficient of viscosity. Kosinski et al. [2] proposed correlations between the rotational coefficient of restitution and tangential to normal spring stiffness, angle of impact, normal coefficient of restitution and coefficient of friction for linear springs. The objective of the present work is to develop correlations between the rotational coefficient of restitution and the modulus of elasticity, Poisson's ratio, friction coefficient and the impact angle for the particles following Hertz-Mindlin contact model. To that end, simulations are performed on LIGGGHTS and LAMMPS for inter-particle and wall particle contacts with proper implementation of Hertz-Mindlin model [3]. The results obtained from the correct implementation of the Hertz-Mindlin model is compared with the other existing models along with the experimental results published by Ganguli et al. [4]. Correlations between the rotational coefficient of restitution and the material properties, for the intermediate regime of contact, identified based on the contact parameter defined as a combination of the ratio of the normal and the tangential spring constants and the tangent of the impact angle, are obtained following four different regression methods. The correlations obtained in the present work along with the Walton's model for the sliding regime [1] may be used in the hard-sphere model to include the effect of material properties and impact angle.

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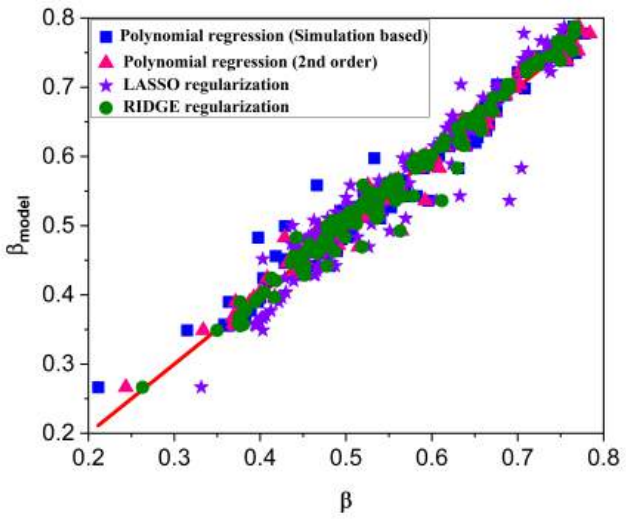

Direct form characterisation methods for 3D surface and volumetric meshes of particles

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Keywords Grain morphology, Particle shape characterisation, Fabric tensor, Surface Orientation Tensor, Volume Distribution Tensor

Particle shape has a profound effect on the mechanical behaviour of granular materials. Although current 3D imaging techniques can capture the geometry of individual particles accurately, the quantification of particle shape is not straightforward. Equivalent primitive shapes such as bounding boxes or fitted ellipsoids are often computed to determine the main particle dimensions. Spherical harmonics have been used to obtain analytical representations of particle geometry, while fractal analysis has been used to approximate the outline of 2D particle projections using linear segments of the same length. Considering these modified particle representations inescapably creates dependence of the characterisation results on the employed geometry processing technique.

This contribution presents two form characterisation methods which are applicable directly on the raw and unmodified 3D meshes of particles. The first one utilises the Surface Orientation Tensor (SOT) (Bagi & Orosz, 2020; Orosz et al., 2021), which is computed from the orientations and surface areas of the facets that make up a surface mesh, making it applicable to the imaging data derived via laser and light scanning. The second method computes the Volume Distribution Tensor (VDT) (Orosz & Bagi, 2021) calculated from the centroid positions and volumes of the segments of a volumetric mesh, which can be generated from closed surface meshes or voxelated images such as the ones derived via X-ray Computed Tomography. Both methods calculate Compactness, Flakiness and Elongation indices of individual particles and as well as their principal orientations.

Applications for convex and concave idealised geometries, as well as for real railway ballast grains will be presented. The correlation between the principal orientations (derived by the SOT and VDT) and the preferred contact orientations will be demonstrated via discrete element simulations of polyhedral particles subjected to gravitational and isotropic compression loading conditions.

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Rock failure mechanism in piston-bit-rock interaction: insight from 3D FDEM simulation

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Keywords Percussive drilling, FDEM simulation, strain rate effect, hard granite, impact energy

To reveal the rock failure mechanism in shallow percussion drilling, a single insert impact simulation was conducted at atmospheric pressure using the combined finite discrete element method (FDEM). When rocks are subjected to dynamic point loading, constant quasi-static rock mechanical parameters are insufficient to accurately represent the mechanical behaviour of the rock within a large strain rate range. To address this limitation, strain rate-dependent mechanical parameters were introduced. Specifically, the strain rate effect was implemented into the tensile strength and cohesion in the Mohr-Coulomb failure criterion, as well as the energy release rate I and energy release rate II in Griffith's fracture theory. The simulation results are in good agreement with the experimental findings reported in the literature. During the impact process, the initiation and propagation of conical-shaped side cracks were the first to develop followed by the propagation of radial cracks and a small number of fragments were generated beneath the insert. Subsequently, numerous fragments were generated, undergoing mutual friction and splattering out of the crater. Simultaneously, with the coalescence of side cracks and radial cracks, several large fragments (i.e., chippings) around the crater began to be generated. During the insert impact downwards stage, the impact force initially increased to its maximum value then decreased. As the insert rebounded upwards, the impact force had already decreased to approximately 10% of its maximum value. During the insert rebound stage, the breakage process is mainly the generation of rock chippings. Additionally, the simulation results did not show the initiation of median cracks beneath the crater, which is consistent with the main experimental observations reported. The influence of impact energy on the rock failure process was also explored.

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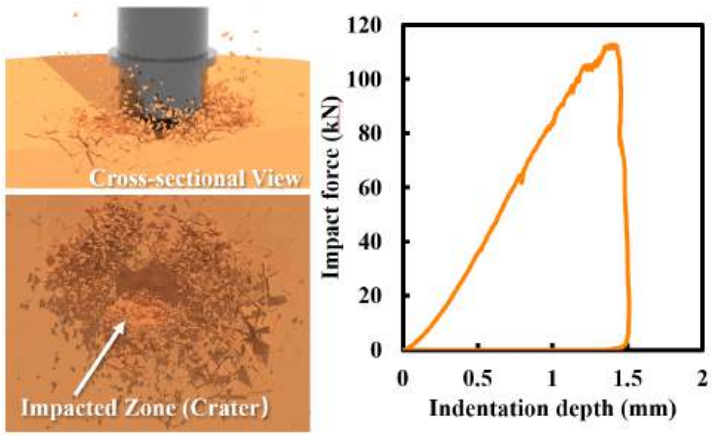

Material Point Method for Granular Materials

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Keywords Material point method, Contact, Damage

In this talk, we will present the modelling of granular materials using the material point method. When we view the granular materials as continuums, we present the algorithms for the impacting, solid-fluid coupling and multiscale modelling. When we view the granular materials as discrete matters, we concentrate on the modelling of contact and damage.

Discrete Element Modelling for Dosing Operation - Material Calibration and Validation

Thomas Forgber[1], Luca Orefice[1], Johan Remmelgas[1], Adrian Dobrowolski[2], Rakulan Sivanesapillai[2], Johannes Khinast[1,3]

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Keywords DEM, industrial application, feeding, dosing, machine learning, calibration, characterization

High-fidelity simulation techniques based on physical principles have proven extremely valuable in speeding up pharmaceutical development and increasing the availability of high-quality medicines. The Discrete Element Method (DEM) is one such technique that has found widespread use. Here, several particle-level contact parameters must be correctly specified or calibrated for the simulated powder to mimic the bulk powder's flow behavior (Coetzee, 2017). But even if multiple characterization tests are conducted, certain parameters might still be undefined, or a manifold of parameter combinations is possible. The current contribution extends a novel workflow for DEM calibration (Forgber et al., 2022), allowing us to identify sets of DEM parameters while matching the powder bulk behavior in standard characterization tests. We demonstrate the applicability of the workflow using a model cohesive powder for which groups of possible contact parameters are identified. A representative selection of these groups is used to predict the mass flow in a dosing device (Three-Tec ZD 5 FB). The results are validated for various screw types and speeds. The workflow and significant findings which will be addressed in the presentation are summarized in Figure 1.

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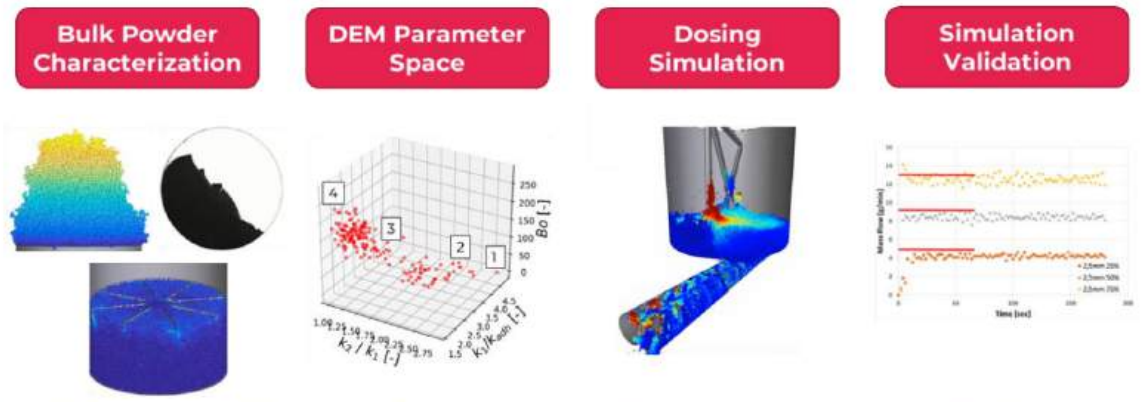

Figure 1: Summary of workflow with powder characterization, calibration, simulation, and successful validation of mass flow at different screw speeds and types.

A Total Lagrangian Smooth Particle Hydrodynamics Approach for Modelling of Soft Granular Powders

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Keywords TL-SPH, powder compaction, deformable particle, cohesion, CUDA

Most food items, pharmaceutical powders, and biological cells can be classified as soft particle systems. They are commonly characterized by substantial inter-particle contact and significant elastic or plastic deformations within the particles. Simulating large deformations and complex contact properties of high-density granular materials remains a challenge. To accurately model such systems, we propose an efficient numerical approach employing Total Lagrangian Smooth Particle Hydrodynamics (TL-SPH). TL-SPH is integrated with the hourglass control technique to effectively model plastic deformation within an individual particle. Concurrently, a penalty stiffness method, taking into account the contact direction at each surface point, is used to compute contact forces between particles. This contact algorithm accurately models both frictional and cohesive contacts commonly observed in various particle systems. The accuracy of the proposed approach is validated on its predictions of elastic and plastic deformation, friction, and cohesive contact. It is further applied to simulating the uniaxial compression of a 3D soft powder packing to examine the microscopic and mesoscopic mechanical properties during the compaction process, where a frictional, cohesive contact model is employed to describe the formation of cohesive bonds and solid bridges over the contact surface between two powder grains. The computational efficiency is further enhanced by Compute Unified Device Architecture (CUDA)-based GPU parallel computing.

DEM study on the particle breakage and uniaxial compression behaviors of bio-cemented calcareous sands

Jiawei Shen, Bo Zhou, Huabin Wang

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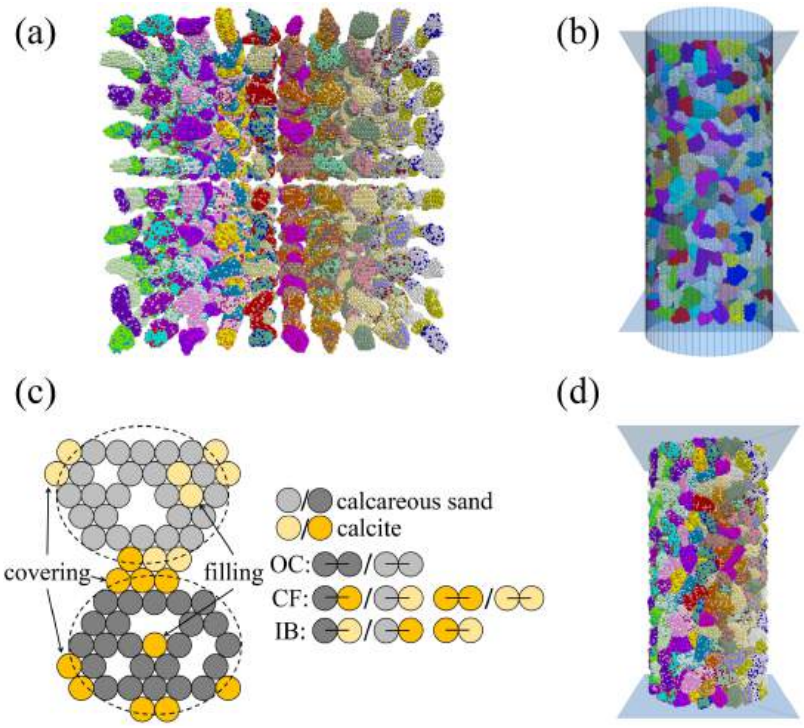
Keywords Calcareous Sand, Microbial-induced Calcite Precipitation, Discrete Element Method, Treating Effect

Calcareous sands possess irregular particle shapes and internal pores which lead to weak strength. Therefore, extensive particle breakage occurs under specific stress conditions. Recently, microbial-induced calcite precipitation (MICP) has become a popular green soil treatment technique to improve the mechanical properties of calcareous sands. However, the complex microstructures of calcareous sands make it challenging to understand the underlying mechanism and treatment effect of MICP. To address this issue, this study employed the discrete element method (DEM) to investigate the micromechanism of MICP treatment on calcareous sands. The study started by individually treating a group of calcareous sand particles via a proposed MICP process and then conducting single-particle crushing tests on the treated and untreated particles to further verify and calibrate the DEM models and parameters. The DEM model of MICP-treated calcareous particles was then established using a novel modeling technique on PFC3D. This model considered the inter-particle bridging and intra-particle pore-filling effects of MICP. Based on this method, a series of MICP-treated calcareous sand samples were simulated under uniaxial compression to study the effects of calcite content and its spatial non-uniformity on compression behaviors. Finally, the mechanism of MICP treatment on calcareous sands was elucidated by investigating the micromechanics of crack propagation and distribution obtained from DEM. This study aimed to provide insights into the micromechanical behavior of bio-cemented calcareous sands and shed light on the mechanism of this technique. The approach proposed and the findings can be useful for designing and optimizing green soil treatment techniques for improving the mechanical properties of weak soils.



Influence of contact topology on the fracture behaviour of particles

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Keywords Contact topology, Fracture behaviour, Micro finite element method

The initial area of the sphere-to-sphere contact is invariably a point and evolves to a circle under compression. In natural particulate materials, however, the contact topologies arising from the irregular-shape particles make their modelling non-trivial [1]. In this study, we present how the contact topology affects material fragmentation using a numerical approach. This approach is an extension of micro finite element method proposed in [1] incorporating cohesive interface elements to represent crack initiation and propagation [2]. The irregular particles are generated from micro-CT images and meshed using an in-house code. The mesh is enriched by adding zero thickness cohesive interface elements to enable random crack initiation and propagation. We visualise the crack initiation and propagation within the particle and quantify that the contact topology as it changes rapidly when the normal load is altered. Thus, for the same loading stage, the associated stress varies for various contact topologies and contributes to different fracture patterns. More flat contact topologies led to stress concentration at the central point, avoiding failures due to edge crushing and initial chipping. This study aims to establish a relationship between fracture behaviour and contact topology. It provides a new insight on predicting how particle breaks under complex contacts to inform multi-particle simulations.

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CFD-DEM modelling of the controlled chemical reduction of the iron ores with the adoption of coarse-graining

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Keywords Reduction of iron ore, reduction reaction modeling, CFD-DEM coupling, coarse-graining, kinetic parameter of reaction

The CFD-DEM based chemical reduction modelling of iron ores is often performed for direct reduced iron (DRI). A high-temperature value and high concentration of reductant gas (CO, H2) favor direction reduction to metal iron. Low-grade iron ores possess specific geological and mineralogical characteristics, such as the presence of hydrated clay minerals (e.g., goethite), making DRI and conventional beneficiation routes futile. Partial reduction of hematite (Fe2O3) to magnetite (Fe3O4) enables mineral beneficiation by significantly enhancing its magnetic properties. Unlike the DRI process, partial reduction requires a controlled environment regarding reductant gas concentration and temperature (Baur-Glaessner diagram) to prevent over-reduction to Wüstite or metal iron. The present work replaces the cumbersome process of experiment-based optimization by CFD-DEM based reaction modelling. The coarse-graining adoption was made to handle the computational limitations imposed by the large number of particles on DEM simulations. The accuracy of adopting coarse-graining in the complex environment of CFD-DEM coupling with reaction modelling was assessed by comparing the simulation results with the observations reported in the literature. The kinetic parameters for three reactions were determined by the calibration method. Though the adoption of coarse-graining leads to minor deviation from the actual results, it offers significant savings on the computational cost and wall-time of simulation. The extent of deviation was higher for larger values of coarse-graining factor. Further, the kinetic parameters of hematite to magnetite reaction for an Indian blue dust iron ore sample were determined by TGA-DSC studies, and validated with experiments performed in an incipient fluidization bed reactor. The coarse-grained simulation-based results were slightly different from the experimental observations. It can be concluded that the change in representative particle size caused by the adoption of coarse-graining affects fluid flow dynamics around the particle leading to scarcity of reductant gas, and thus, slower process of reduction.

Evaluation of the bearing capacity of mechanical anchors with grouting using DEM-CFD

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Keywords Bearing Capacity, Plate anchors, Discrete Element Method, Computational Fluid Dynamics

Geotechnical engineers face the ongoing challenge of increasing the bearing capacity of structures. In pursuit of this objective, extensive research and experimentation have been conducted to identify the key parameters involved. However, the effects of certain factors, such as grouting and velocity variations, have not been adequately investigated. This study aims to fill this research gap by evaluating the impact of grouting and different velocities on bearing capacity. To accomplish this, a combined approach of the Discrete Element Method (DEM) and Computational Fluid Dynamics (CFD), referred to as DEM-CFD, is employed. The experimental results highlight the correlation between velocity and bearing capacity, indicating that an increase in velocity positively influences the bearing capacity. Furthermore, the study examines the effect of rotating anchors from a vertical to a horizontal position along the grouting line. The findings reveal that this rotation significantly impacts the bearing capacity. The outcomes of this study provide valuable insights into enhancing the bearing capacity of geotechnical structures. The investigation of grouting and velocity variations using the DEM-CFD approach enables a comprehensive understanding of these parameters' influence on bearing capacity. This research contributes to the development of more effective models for measuring and predicting bearing capacity, thereby facilitating the design and construction of robust geotechnical systems.

DEM simulation on the settlement of municipal solid wastes

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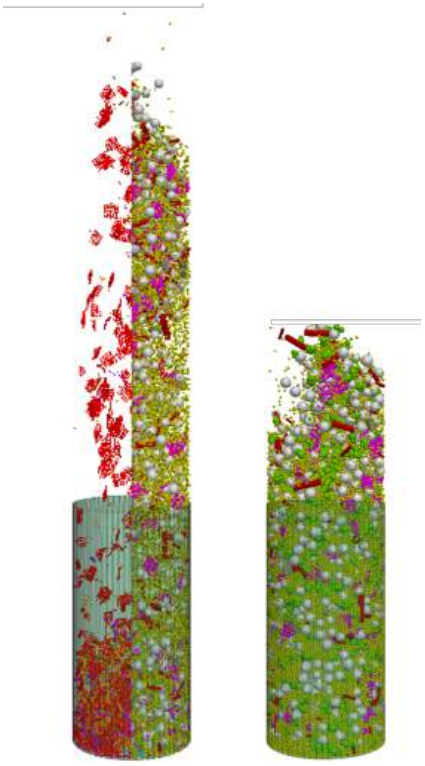
Keywords MSW, DEM, settlement, biodegradation

Municipal solid wastes (MSWs) settlement is important for the design, construction, operation and management of landfills. Due to the complex properties of different waste materials, the settlement prediction of MSWs remains a challenging topic. In this study, numerical modelling of MSWs under different degradation phases is conducted by a 3D discrete element method (DEM) utilizing the software PFC3D, which aims to reveal the mechanisms behind the settlement process of the composite material system. The model simulates the behaviours of MSWs by characterizing the wastes as 6 different types of materials, including wood, paper, food, metal, plastic, and soil. Those waste constitutions were modelled as clumps, rigid blocks, and bonded or unboned balls. At different degrees of biodegradation, the biodegradable materials can be shrunk or broken down to certain sizes according to the results of laboratory bioreactor tests. The corresponding settlement between the biodegradation phases can be measured, as well as the strain and stress field of MSWs during stabilization. Based on the analysis of measured and simulated results, the study reveals that settlements of MSWs are caused by two distinct mechanisms: structural rearrangement during mechanical compression and stabilization after biodegradation, and the geotechnical properties of MSWs change due to biodegradation. The materials exhibit softening behaviours in the early stages, followed by hardening in the later period. The main skeleton of the sample is formed during the period of 180-810 days, with plastics being the primary component that forms the force chain. These results demonstrate the complex nature of the settlement process in MSWs and highlight the importance of considering both structural and material properties in understanding their behaviour. Further investigation is required to fully understand the overall mechanical properties of the MSWs.



Discrete Element Modelling (DEM) of a granular material mixer: Zirconium sponge

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Keywords DEM, Sampling, Mixing index

Sampling is used in many industrial sectors to measure the physical and/or chemical characteristics of a granular material. However, in a rotating drum mixer, segregation increases heterogeneity and then the representativeness of the sampling. This phenomenon can be induced by differences in sizes, densities, or shapes of the particles. In the Zr alloy manufacturing field, the characteristics of the granular material from Zr sponge must be well controlled. Therefore, sampling plays a crucial role in ensuring the quality of the alloys. Preliminary analysis show that the particles constituting the Zr sponge are heterogeneous in terms of sizes, densities, and shapes. Consequently, this type of particles is particularly sensitive to segregation phenomena. To optimize the representativeness of sampling in a granular material, the number of samples can be increased and/or the homogenization quality can be improved. For practical and economic reasons, it may be more advisable to reduce the quantity of samples and thus improve the homogeneity of the medium. This work focuses on the numerical modelling of a rotating drum mixer for granular materials using the DEM method. The goal is to simulate real cases of particle mixing to propose technical solutions to improve the quality of mixing and to determine the optimal operating conditions of the mixer. To quantify the quality of mixing, Kramer mixing index was calculated at regular intervals. This approach allows tracking the evolution of the mixing index and thus monitoring the homogeneity of the mixture over time or as a function of the number of mixer rotations.

Analysis for dispersion and aggregation behavior of particles during wet ball milling

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Keywords Wet ball milling, DEM-CFD, aggregation, dispersion, grinding

Wet ball milling has been used in wide fields such as pigments, ceramics, and metal materials because it has an excellent feature that can grind to a single micron. On the other hand, recently, producing nanoparticles using wet ball milling has been demanding because nanoparticles can add new functions and improve the performance of the particulate materials. However, the wet ball milling has difficulty producing the nanoparticles due to re-aggregation occurring. The re-aggregation is the phenomenon that the ground particles form large aggregates even though the mechanical grinding conditions are constant. In the case of the wet ball milling, the re-aggregation occurs when the particle diameter becomes less than a single micron approximately. Moreover, controlling the reaggregation is generally difficult because the mechanisms of the re-aggregation have not been elucidated yet. As the background of this situation, the particle behavior is difficult being analyzed with experiments. On the other hand, the particle behavior could be analyzed by using the DEM simulation because the DEM simulation tracks the behavior of all particles in the calculation system. Thus, we analyzed the particle behavior during wet ball milling using the DEM-CFD coupling simulation. As a result, it was found that the re-aggregation occurred when the balls were approaching and departing, and the fluid compression force was a critical factor of the re-aggregation.

Acknowledgement
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Data-driven Dimensional Analysis and DEM based Coarse Graining Approaches for Modelling the Impact Dynamics of Granular Materials

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Keywords Granular materials, Discrete element method, Coarse graining, Data-driven dimensional analysis, Machine learning

Investigating the impact process and associated mechanical behavior of granular materials plays a crucial role in understanding the intricate physical laws governing particle collisions. The discrete element method (DEM) has proven to be a valuable tool for studying the impact buffering characteristics of granular materials. However, due to computational limitations, conducting research at the prototype scale poses significant challenges. Thus, the implementation of coarse-grained methods becomes essential for conducting simulations. It becomes crucial to assess the extent to which coarse-grained models can accurately represent the physical and mechanical properties of the original system. In this study, a data-driven approach based on dimensional analysis is employed to construct a network of response surfaces using a fully connected neural system, specifically the ridge function. The gradient of the response surface is computed through finite difference approximation for active subspace analysis. An effective methodology is proposed to determine the independent variables for calculating the response surface gradient. Additionally, an artificial neural network is employed to identify dimensionless quantities, enabling the identification of dimensionless numbers that influence the depth of the crater. Impact simulations using the discrete element method are conducted at different scales, and dimensionless numbers corresponding to various models are calculated to assess the accuracy of the coarse-grained approach.

Unresolved CFD-DEM simulation of a pilot-scale pneumatic conveying system

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Keywords Pneumatic transport, CFD-DEM, particle-fluid flow, unresolved method

Pneumatic transport is an extensively used operation to transport granular solids from one point to another in a large number of industrial processes, often having a key role in them. Consequently, the transport operation has been the subject of numerous studies, using a wide variety of methods. Several recent studies have been focused on the use of numerical approaches, such as the coupling of computational fluid dynamics (CFD) and the discrete element method (DEM), to model and predict the gas-particle behaviour during transport and thus improve the performance of the industrial process. However, further research is still necessary to continue developing and to improve the accuracy and efficiency of the CFD-DEM approach. This work focuses on the unresolved CFD-DEM modelling of a pilot scale pneumatic transport system. The simulations were performed using the open-source code CFDEM® Public. We analysed the applicability of the different models available to this case. We also investigated the effect of solids insertion on the transport hydrodynamics as well as the selection of sub-models and parameters. The validity of the simulation was assessed by comparing the results (e.g., the predicted pressure drop) with experimental data. The main objective of this project is to develop a reliable and efficient CFD-DEM model for the simulation of the pneumatic transport of biomass and recycled solids at industrial-scale, an important operation in many waste recovery processes.

Permeability Evolution of Methane Hydrate-Bearing Sediments: A CFD-DEM Coupling Study

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Keywords CFD-DEM coupling, Methane hydrate-bearing sediments, Permeability, Permeability stress sensitivity

Permeability plays a crucial role in marine hydrate-bearing sediments (MHBS), impacting production efficiency and governing geotechnical engineering problems and geohazards. However, limited experimental conditions have hindered a comprehensive understanding of the dependence of permeability on hydrate saturation and effective stress. This study verifies the effectiveness of a coupled computational fluid dynamic (CFD) - discrete element method (DEM) model by comparing it with experimental results. The validated CFD-DEM model is then employed to investigate the permeability evolution of pore-filling type MHBS with different hydrate saturations (10%, 15%, and 20%) during various depressurization production scenarios. The numerical results demonstrate that the hydrate saturation significantly affects the MHBS permeability, with good agreement between numerical simulations and experiments. The correlation between permeability and effective porosity can be described by a modified Chapius and modified Kozeny-Carmen model, and the effective porosity decreases exponentially with increasing effective stress in which the porosity stress sensitivity index decrease with increasing saturation. Furthermore, permeability stress sensitivity analyses confirm a positive correlation between permeability stress sensitivity coefficient and saturation, consistent with previous findings. The influence of depressurization exploitation on MHBS permeability is quantitatively evaluated using a scale number defined as the ratio of permeability before and after hydrate dissociation. The results indicate a negative correlation with depressurization pressure and a positive correlation with saturation. This study provides valuable insights into the permeability evolution of MHBS during exploitation using the CFD-DEM approach.

Towards DEM in AutoPas – An extension of the auto-tuned simulation framework

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Keywords Discrete Element Method, Auto-tuning, Automatic algorithm selection, Dynamic Tuning, HPC

Simulations applying the Discrete Element Method (DEM) are a powerful tool enabling the investigation of many phenomena relevant in a variety of fields. However, the high computational costs associated with the need for accurate predictions of particle-particle interactions (i.e. the pairwise particle forces) encountered in such processes is often times the prohibiting factor of simulations containing a large number of particles. It is therefore imperative for the simulation software to provide optimal performance throughout all stages of the computation. The scope of the present work is to extend the open-source Molecular Dynamics (MD) framework of ls 1 mardyn and AutoPas towards DEM. While the former code is optimized for massively parallel computations on large high-performance computing (HPC) architectures and relies on an efficient dynamic load balancing algorithm, the latter one aims to provide optimal performance on the node level of the supercomputer. AutoPas achieves this by taking over the computationally expensive particle-particle interactions of the MD simulation and automatically tunes a large set of algorithmic configurations in form of data structures, solvers and parallelization strategies at runtime. In order to utilize this framework for DEM predictions the molecular interaction force is replaced by one suitable for solid particles, i.e. in the simplest case a spring force can be used. Furthermore, hierarchical grids are introduced in AutoPas for simulating poly-disperse particle systems. An auto-tuning approach is applied, i.e. the properties of the hierarchical grids are adapted at runtime of the simulation in order to provide optimal performance during all simulation stages. The performance is investigated relying on different test scenarios, e.g. a cubic particle system or particles falling into a box. It is shown that the tuning capabilities of AutoPas can lead to an improved performance compared to non-tuned simulations, depending on the scenario of interest.

Integrating the Combined Finite-Discrete Element Method with Fluid-Solid Interaction Solutions

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Keywords FDEM, fluid-structure interaction

The combined finite-discrete element method (FDEM) [1] is a hybrid method introduced by Munjiza in the 1990s and since then it has become a tool of choice for numerically addressing a wide range of problems involving fracturing and fragmenting solids [2], [3], seismic wave propagation [4], rock breaking phenomena [5], earthquake rupture dynamics [6], bolide impact physics [7], [8], etc. FDEM is designed to handle finite displacements and finite rotations while simultaneously incorporating large-strain-based deformability models [9], [10]. These techniques are merged with objective discrete crack initiation and crack propagation solutions that exhibit a great deal of fidelity in reproducing complex fracture patterns and eventual fragmentation. Recent developments [11] now allow for problems involving the simulation of the interaction between fluid and solid domains to become increasingly achievable and therefore relevant for various applications. However, when trying to solve these types of problems, an additional complexity is introduced if one must consider that the solid domains can also fracture and fragment under the action of loads imparted by the fluid. A hybrid approach, where the material is allowed to transition from continuum to discontinuum (i.e., fracture and fragment) is ideal for these types of applications. This presentation will concentrate on summarizing the latest advances obtained at Los Alamos National Laboratory in regards to FDEM-based fluid structure interaction solvers.

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Stress Variation in Cohesive Granular Column

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Keywords DEM, Cohesion, Janssen stresses, SJKR2 model

We perform DEM simulations of frictional, inelastic, monodisperse spheres filled in a container of rectangular cross section under the influence of gravity. In order to avoid history dependence and achieve full friction mobilization at the walls, the base wall supporting the material is moved by a few particle diameters at a constant velocity. Various components of the stress tensor following this protocol are obtained. The Simplified Johnson Kendall Roberts (SJKR2) cohesion model is employed and the effect of particle-particle cohesion and particle-wall cohesion on the stresses in the column investigated. Increasing the particle-wall cohesion reduces the normal stress at base as shown in Fig.1. Since, the elastic properties also play an important role, we also explore a range of Young's modulus for a fixed cohesive energy density (C). In contrast to cohesionless grains, the stress in the cohesive granular column seen to be affected by the Young's modulus. In addition, the initial height from which material is poured into the container also seems to be important despite following the Janssen's protocol for full friction mobilization at the walls. The results obtained give an insight about the important effects that need to be considered during the storage of cohesive grains and many more interesting features which will be presented in this talk.

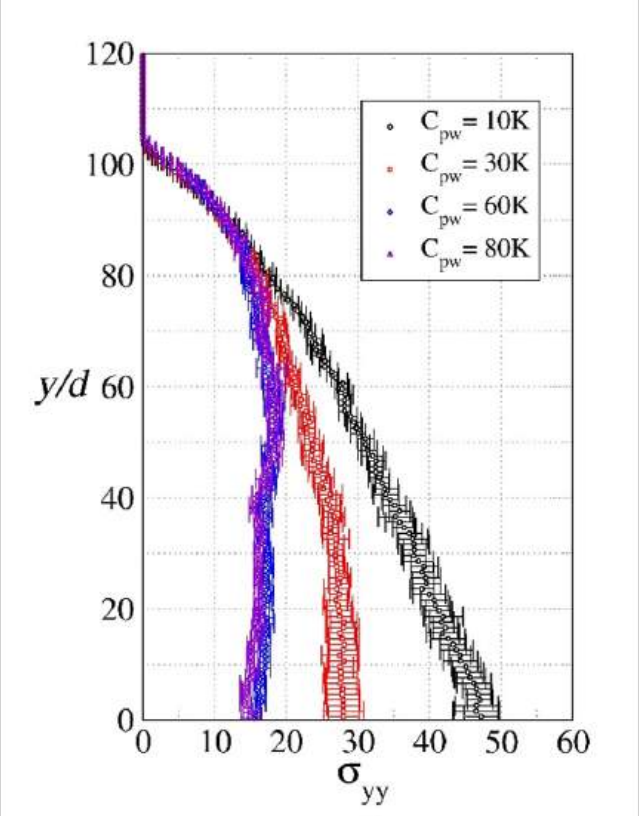

Fig.1: The stress variation profile of C_{pp} = 60 KJ/m^3 for different particle-wall cohesion values.

Exploring transition in granular flow through an outlet in a silo

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Keywords Flow transition, Granular flow, Silo

Grains draining through an aperture in a silo exhibit a variety of phenomena, which have been a subject of investigation for decades. Here, we focus on understanding markers of transition in granular flow as grains approach the outlet. Several studies have been reported in the past aiming to understand the physical mechanism governing flow transition in the neighbourhood of an exit. The study of Rubio-Largo and colleagues [Phys. Rev. Lett. 114, 238002 (2015)], for instance, provides a picture of flow transition in light of the spatial non-monotonic trends of kinetic pressure. In this work, we explore flow transition from the viewpoint of energy dissipation, employing computations based on the discrete element method.

Influence of grain sphericity on collapse mechanics

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Keywords Grain shape, liquefaction, steady state, collapse, rotational-resistance

Grain shape plays an important role in the volumetric and strength behavior of granular materials. The results from experimental investigations on natural materials carry simultaneous effects from gradation, grain shape and mechanical properties of grains which limits judgement about the isolated influences of grain shape. In this DEM study, the grain size distribution, contact parameters and modelling protocol was kept the same in order to study the isolated effects of grain geometry under notionally undrained (or constant-volume) shearing. Convex polyhedrons were modelled to simulate different grain sphericities. During shearing, strength showed an initial peak (at instability state) followed by a collapse untill its lowest value (transitional state) which was either sustained or led to re-hardening depending on the initial state of sample. On e-p' (void ratio vs. mean effective stress) plane, the steady state (SS) line moved upwards with the decrease in grain sphericity. This means at the same void ratio, the net contractive potential decreases or dilative potential increases with the decrease in grain sphericity. The stress obliquity mobilized at the SS increased with the decrease in grain sphericity which shows that this state is influenced by the grain-interlocking and rotational-resistance. For isotropic consolidation lines starting from the same initial e, the compressibility increased with the increase in grain sphericity which was due to the ease of rearrangement through rolling. At the same e and state parameter, the stress ratio at instability state increased with the decrease in particle sphericity which promotes interlocking. At the same e, the lowest mobilized strength increases and the post-collapse dilation increased with the decrease in grain sphericity which was due to correspondingly increasing coordination number and eccentric grain geometry. This shows that the grain sphericity is of high interest for the mechanics relevant to liquefaction both at its initiation and collapse following it.

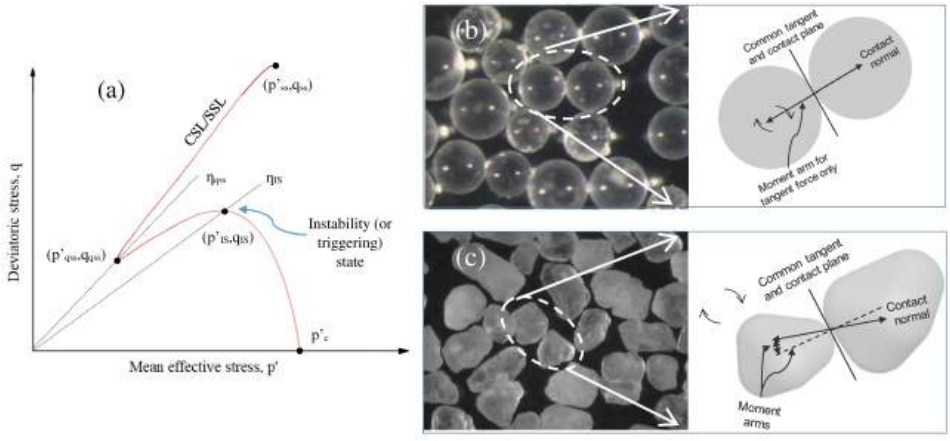

Figure. (a) Key behavioral states to study the influence of grain sphericity (b) Interaction between freely rolling spheres with contact normal vectors coincident with the branch vector & (c) Interaction between non-spherical grains with moment/torque transmission through contact normal force vectors [Note: IS=instability state, QSS=quasi-steady state & SS= steady state or alternatively as CS= critical state]

Residence time calculation algorithm for long-duration processes

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Keywords Residence time, upscaling, time extrapolation

Residence time is an important process parameter in many industrial applications. Processes with bulk material that include heating, drying, chemical reactions, and many more, usually require knowing the residence time of the particles. Calculating the residence time is not always trivial, and the use of DEM simulations can help achieve this. However, industrial applications often involve millions of particles and last for hours or more. In these situations, a full DEM simulation of the process can be unfeasible. An algorithm has been developed that allows the estimation of the residence time for long processes based DEM simulations of a fraction of the process time. Taking two steady state snapshots a given time t apart, we can track particle X from its initial position in State 1, x1, to its location in State 2, x2. We can then use x2 to locate a particle Y in State 1 that occupied that position. That particle can be tracked to its new position in State 2, and so on until the particle leaves the domain. Since when a steady state is reached in the simulations, further simulation time does not produce more information, this allows the estimation of the residence time for an hours-long process by running a few minutes of simulation time. The comparison with two experiments shows that the simulation with a runtime of about two minutes was capable of predicting residence time of hours of process.

Tomographic Imaging-Based Finite Element Analysis of 3D Mixed-Mode Cracks

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Keywords 3D cracks front, FEM, Tomographic Images

When a brittle material is subjected to tensile stress, fractures propagate perpendicular to the maximum direction of the principal stress [1]. However, when out-of-plane shear stress is applied under such conditions (mixed-mode I+III), the crack front becomes unstable and breaks down into leaves that twist relative to the mother planar crack [2]. Unfortunately, the underlying physical mechanisms responsible for this phenomenon remain unclear due to the lack of a full 3D theory of crack propagation [3-4].

In this study, we generate hydraulic fractures in hydrogel using an in-house setup and subsequently obtain a 3D tomographic image of the crack. Additionally, we employ finite element analysis to infer fracture mechanics parameters that otherwise will be inaccessible by experimental methods. By combining the experimental data with numerical simulations, we aim to shed light on the complex behavior exhibited by mixed-mode I+III cracks front in brittle materials.

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MBD-DEM co-simulation of operations of hydraulic excavators for polydisperse bulk materials and different configurated buckets

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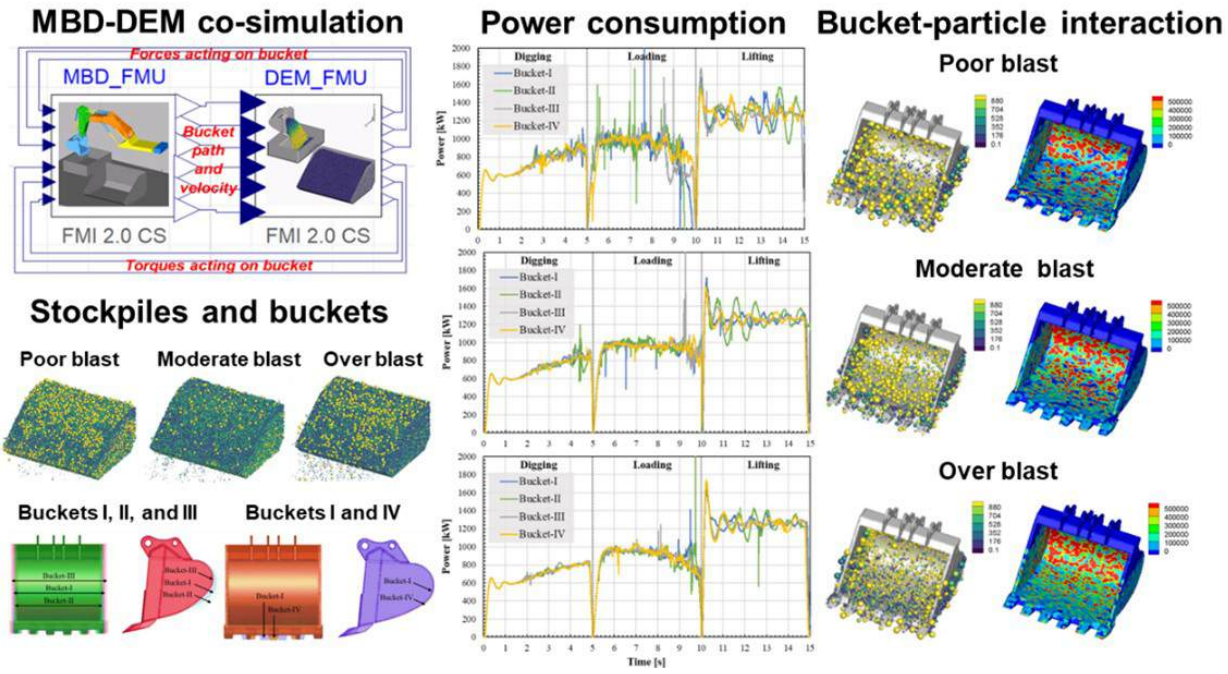
Keywords Multibody dynamics, Discrete element method, Hydraulic excavators, Particle size distribution, Bucket geometry

Excavator is a common construction machinery, which is widely used in all kinds of open-air earthmoving operations. During the operation of excavators, the interaction between materials and bucket has a great influence on the performance of excavators. However, the studies on excavator performance so far are very limited in the literature. Some fundamental questions are still not well answered. For example, why do excavators perform differently in environments with different material properties? How do manufacturers design and improve bucket performance by adjusting bucket structure instead of increasing bucket weight? This work aims to address these questions through a coupled technique of multibody dynamics (MBD) and discrete element method (DEM), which can replicate the whole working cycle of excavators, capture the interaction forces, and further investigate the excavator performance under different operating conditions. The results show that with the increasing material density, the hydraulic power consumption and interaction force increase. During the digging, loading, and lifting, the power and interaction force change greatly, with stress concentrations first appearing at the bucket teeth, followed by large stresses at the bottom of the bucket. A high lifting does not imply a high payload due to more spillage during bucket swinging. From poor blast to moderate blast to over blast, the power fluctuation is reduced, the particle-to-bucket stress becomes more uniform, resulting in an increased area of the bucket being stressed. The narrower but deeper bucket has a higher payload than the base bucket and is suitable for moderate blast and over blast. The bucket with one less tooth station has a lower payload, but the power fluctuation is effectively reduced, which is suitable for poor blast.



DEM study of a piston indentation into granular assembly

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Keywords Strip foundation, force chain network, geometry optimization

The constant piston indentation can mimic, to some extent, the settling strip foundation problem, which has been intensively investigated over time. The focus has been mainly on the bearing capacity of such a foundation or deformation of the subsoil (primarily its settlement) to meet practical needs. Despite many years of research, the problem is still the subject of study because it can provide valuable data on the physical basis for forming failure mechanisms and deformation patterns in granular materials, which still need to be fully understood. The DEM method is presently the most helpful tool to recognize them better. Furthermore, this method enables the straightforward performance of numerous sensitivity analyses, limited only by computational resources, while an experimental campaign encompassing such analyses would be costly and time-consuming.

The proposed paper aims to optimize the geometry and dimensions of the experimental setup for the piston indentation problem, which will be tested in the laboratory. The experiment aims to investigate the evolution and structure of the force chain network developing below the piston as a reaction to its embedding into the granular system consisting of glass beads. The sensitivity analyses encompass different sizes of the box containing the granular material to avoid the influence of boundaries on the results and different grain sizes. The final structure of the sample is subjected to image processing to obtain the displacement fields and strain maps. The results of the presented analyses enable not only the determination of the appropriate and the most optimal dimensions of the experimental setup but also bring significant knowledge about the real engineering problem: the safe design of strip foundations.

Investigating Lunar Regolith with Discrete Element Simulation: Insights from Chang'E-5 Mission's Soil Particle Morphology

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Keywords Lunar soil, particle morphology, triaxial compressed tests, macro- and micro-mechanical properties, image-based discrete-element method

To align with the current strategic planning of "survey, mining, and development" in China's lunar exploration mission, and to obtain more accurate physical and mechanical properties of lunar regolith, this study focuses on the influence of lunar regolith particle shape based on particle images from the lunar regolith of the Chang'E-5 mission. A discrete element numerical simulation method that considers lunar regolith particle morphology is proposed by linking particle shape characteristics with gradation. Initially, the shape characteristics and size information of the particles are extracted from the lunar regolith images. The particles are subsequently categorized into six groups based on their sphericity, establishing the corresponding relationships; Secondly, the study utilizes a three-dimensional (3D) lunar regolith contact model and calculates rolling and twisting resistances at inter-particle contact by incorporating shape parameters to account for lunar particle shape effects. Subsequently, the model considers particle size characteristics within the discrete element analysis. Ultimately, a discrete element numerical model that incorporates the particle shape characteristics of the Chinese lunar regolith is developed; Comparison with the results of Apollo lunar regolith laboratory tests reveals that the variability of grain shape in lunar particles can be directly incorporated into the discrete model. Additionally, the benefits of considering the grain shape characteristics of lunar regolith were discussed in comparison to numerical samples that neglect the characteristics. The results show that the method can effectively capture the main characteristics of the mechanical behavior of lunar regolith, and provide a basis for the lunar resource exploration and exploitation methods.

DEM-PFV analyses of suffusion phenomena during permeation grouting treatments

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Keywords Permeation grouting, micro-scale, DEM-PFV coupling, seepage, suffusion

During permeation grouting treatments in highly graded soils, parasite suffusion phenomena occur [1, 4] even if low injection pressures are imposed: finer particles, not involved in force chains, are washed out by seepage, without any change in volumetric strain. Then, both particle size distribution PSD and intrinsic permeability k of the injected soil starts evolving with time, leading to highly heterogeneous spatial distributions. This complex phenomenon is so characterised by a solid-to-fluid transition of washed-out particles. Its numerical simulation requires a discontinuum approach and the DEM-PFV coupled method, implemented in YADE [2, 3], is here employed, conjugating the capability of pore-scale modelling and computational efficiency. Once validated the conceived model on seepage laboratory test results, the suffusion mechanisms occurring at the micro-scale, i.e. fine particle flushing throughout pores and clogging/deposition due to not large enough pores and constrictions, are numerically investigated as well as the role played by injection conditions, soil and Newtonian fluid properties. PSD turns out to play the major role. Injection pressure and fluid viscosity mainly affect the time length required from the initial homogeneous configuration to the final heterogeneous steady-state one. This numerical strategy can be employed as a useful tool at the pre-design phase of permeation grouting treatments by predicting the suffusion mechanisms prone to occur at various distances from the injection source and providing a quantification of the changes in terms of PSD and k. For instance, if a soil turns out to be susceptible to a significant fine fraction transport characterised by a considerable travelling distance, to enhance grout permeation, the earlier fine particles' removal from the zone to be treated, by means of water injections, can be suggested. Conversely, when clogging zones are expected, grout permeation is obstructed and low viscosity solutions, e.g. colloidal silica grouts, are preferred.

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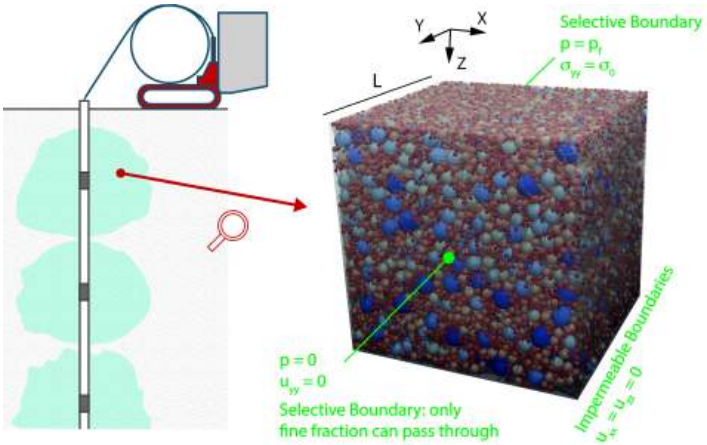

Experimentation for the Validation of Discrete element method (DEM) numerical simulations for mixing/grinding of powders

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Keywords Nuclear fuel - Discrete Element Method (DEM) – Simulation – Fragmentation – Validation

The fabrication of nuclear fuel is currently carried out using a powder metallurgy process of UO2/PuO2 (MOX) that involves several stages including: mixing and grinding. This Work focuses on validating a discrete element method (DEM) numerical approach for simulating the manufacturing physical processes in nuclear fuel fabrication. The study investigates the fragmentation behavior of model aggregates under different loading conditions, including quasi-static, impact, and dynamic loads. The model fragmentable systems investigated in this study comprise cohesive particle agglomerates with varying shapes, including spherical or polyhedral shapes. Experimental validation is conducted through carefully designed experiments on model systems with controlled geometries, comparing the results with DEM simulations. The study considers different scales, materials, and mechanical tests to assess the generality and limitations of the numerical approach. Characterization techniques such as tomography, image analysis, and analytical tests are employed. The findings contribute to enhancing the understanding of aggregate fragmentation in sight of optimizing manufacturing processes in the nuclear fuel industry.

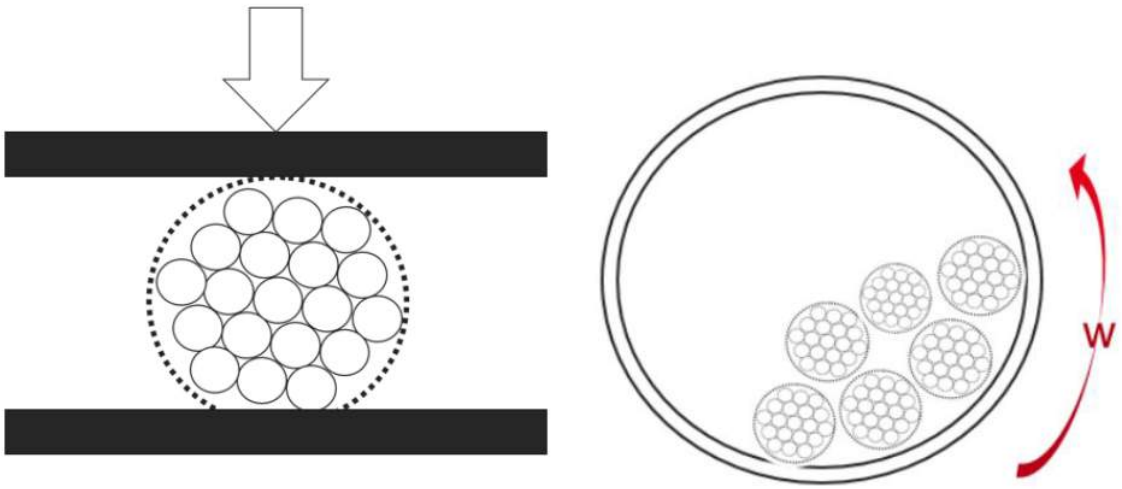

Figure : Some mechanical tests to be performed on the manufactured aggreagtes: uniaxial compression (left), rotating drum (right)

The framework of constitutive model of interface between hydrate block and clay accounting for macro and micro paraments based on DEM analysis

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Keywords Deep-sea energy soil, discrete element simulation, interface characteristics, constitutive model, damage law

Deep-sea energy soil (soil containing hydrates) is a type of problematic soil highly sensitive to temperature and pressure. Hydrates often exhibits block in shallow clayey deep-sea energy soil. The frictional performance and significant differences in stiffness between hydrates and soil exert substantial control over the mechanical characteristics of the energy soil. This work firstly establishes a discrete element simulation method for block hydrates based on the correlation between macro and micro mechanical properties under different temperature and pressure conditions. Additionally, the simulation method for the clay is established. Then, using the principles of thermodynamic conservation, the relationship between specimen volume variations before and after hydrate decomposition under the influence of temperature is established. On this basis, the undrained shear test of the hydrate-clay interface is simulated, and the influence patterns of relative stiffness and temperature on the mechanical properties and volumetric strain of the interface are analyzed. Finally, based on the results of the discrete element simulation, a damage law considering the evolution of the energy of shear zone is established, and this damage law is incorporated into the disturbance state model to establish the constitutive model framework for the interface between hydrate and clay.

Study on the discrete element method for forming ridges of whole film-mulching and double ridge–furrow

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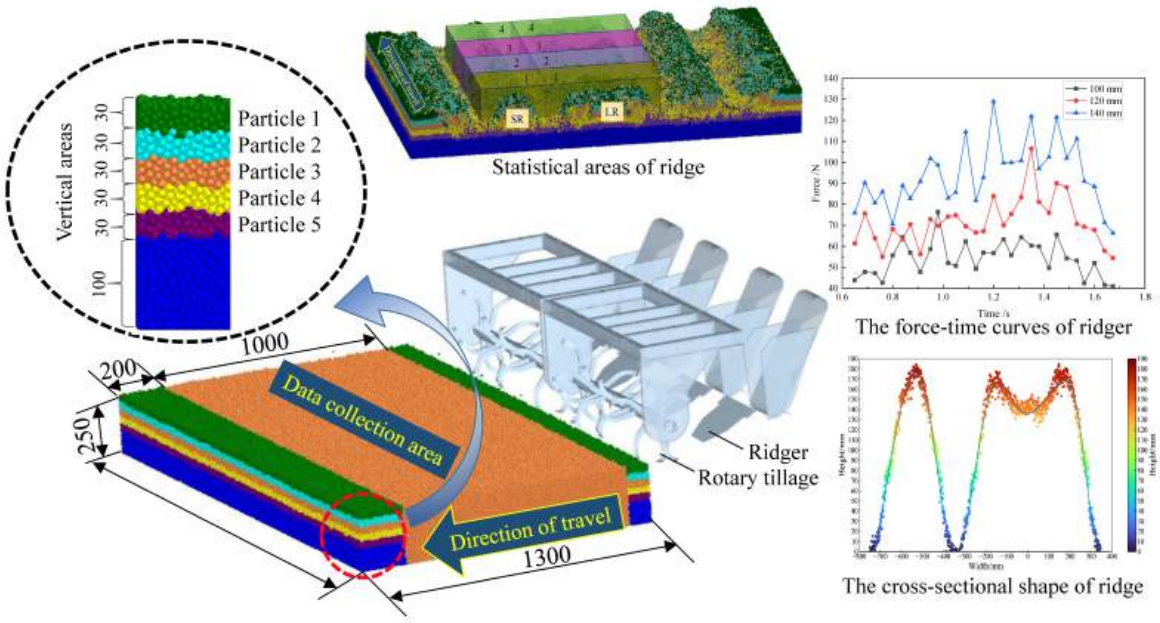
Keywords Discrete Element Method, Ridger, Whole film-mulching and double ridge–furrow, Large ridge, Small ridge

The Northwest of China is a typical production mode of rain-fed agriculture, which mostly adopts the whole film-mulching and double ridge–furrow technique to address the difficulty of surface water storage. However, the quality of ridge formation directly affects the water storage on both sides of the ridges, the reliability of plastic film mulching, and the crop growth. This study focused on the process of rotary tillage ridging, took different inclination angles and depths of ridger as variable factors, explored the influence of different operation parameters on the quality of ridge forming. The soil viscoplastic model was established in the study using the discrete element method. The changes in ridger resistance, ridge structure, and soil particle disturbance were analyzed in detailed, respectively. The results indicated that as the inclination angles and depths of ridger increased, the resistance of ridger also increased. The height of the ridges significantly influenced by the inclination angles and depths of ridger, and under the same inclination angles of ridger, the height of the ridges was directly proportional to the depth of ridger. Under different combinations of operational parameters, the height of the small ridges had good agreement with the ridging agronomy. As for the large ridges, when the depth of ridger was 100mm and the inclination angles were 15°, 30°, and 45°, the working parameters met the agronomic requirements for ridge forming. In terms of soil disturbance, the soil located within a range of 30-90mm from the surface was most susceptible to disturbance from the rotary tillage and the ridger, and the soil disturbance was stronger in the small ridges compared to the large ridges. The results of study contributed to a deeper understanding of the rotary tillage ridging process and provided insights into the factors influencing the quality of ridge forming.



Research-led Teaching of Discrete Element Simulations

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Keywords Discrete element education, engineering education, research-led teaching, open-source software

The Discrete Element Method (DEM) is an essential numerical tool for the simulation of particulate systems. Yet, systematic DEM education is missing from the curricula of most STEM programmes worldwide compared to methods for continuum modelling, such as the Finite Element Method (FEM). This contribution highlights the teaching activities organised at the Institute for Multiscale Simulation (MSS) of the Friedrich-Alexander-Universität Erlangen-Nürnberg to provide DEM education at a postgraduate level. The teaching content is underpinned by previous and ongoing research of the MSS and the wider DEM community. Theoretical and practical sessions are combined with the goal of gaining actionable knowledge on numerical simulations, applicable to real-life problems of discrete systems. Focus is given on the main elements of a DEM simulation, including the selection of appropriate material parameters, contact models and timestep, as well as contact detection schemes and particle shape. The open-source DEM software YADE is employed to provide a user-friendly Python interface, which allows for easy scene generation, as well as various types of particle shape and contact laws for viscoelastic, adhesive and capillary behaviour. This course imparts an understanding of the physical phenomena arising in many-particle systems and the importance of microscopic parameters on macromechanical behaviour. Through this educational activity, we aim to contribute towards a more standardised DEM education.

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A microscopic approach to fatigue failure of brittle rocks based on stress corrosion model

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Keywords Time-dependent cracking, Creep, Damage, Brittle rocks, Micromechanical modelling

A numerical model for brittle creep and stress relaxation is proposed for the time-dependent brittle deformation of heterogeneous brittle rock under uniaxial loading conditions. The model accounts for material heterogeneity through a stochastic local failure stress field, and local material degradation using an exponential material softening law. Importantly, the model introduces the concept of a mesoscopic renormalization to capture the co-operative interaction between microcracks in the transition from distributed to localized damage. Our model also describes the temporal and spatial evolution of acoustic emissions, including their size (energy released), in the medium during the progressive damage process. The model is first validated using previously-published experimental data and is then used it to simulate brittle creep and stress relaxation experiments. Our model accurately reproduces the classic trimodal behaviour (primary, secondary and tertiary creep) seen in laboratory brittle creep (constant stress) experiments and the decelerating stress during laboratory stress relaxation (constant strain) experiments. Brittle creep simulations also show evidence of a 'critical level of damage' before the onset of tertiary creep and that the initial stages of localization be early as the start of the secondary creep phase, both of which have been previously observed in experiments. Stress relaxation simulations demonstrate that the total amount of stress relaxation increases when the level of constant axial strain increases, also corroborating with previously-published experimental data. Our approach differs from previously-adopted macroscopic approaches, based on constitutive laws, and microscopic approaches that focus on fracture propagation. The model shows that complex macroscopic time-dependent behaviour can be explained by the small-scale interaction of elements and material degradation. The fact that the simulations can capture a similar time-dependent response of heterogeneous brittle rocks to that seen in the laboratory implies that the model is appropriate to investigate the non-linear complicated time-dependent behaviour of heterogeneous brittle rocks.

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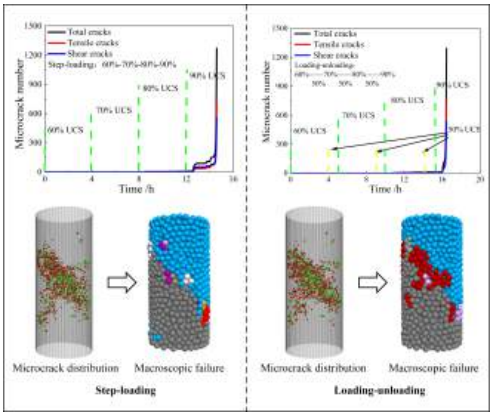

Developing SPIRAL: A stable particle rotation integration algorithm

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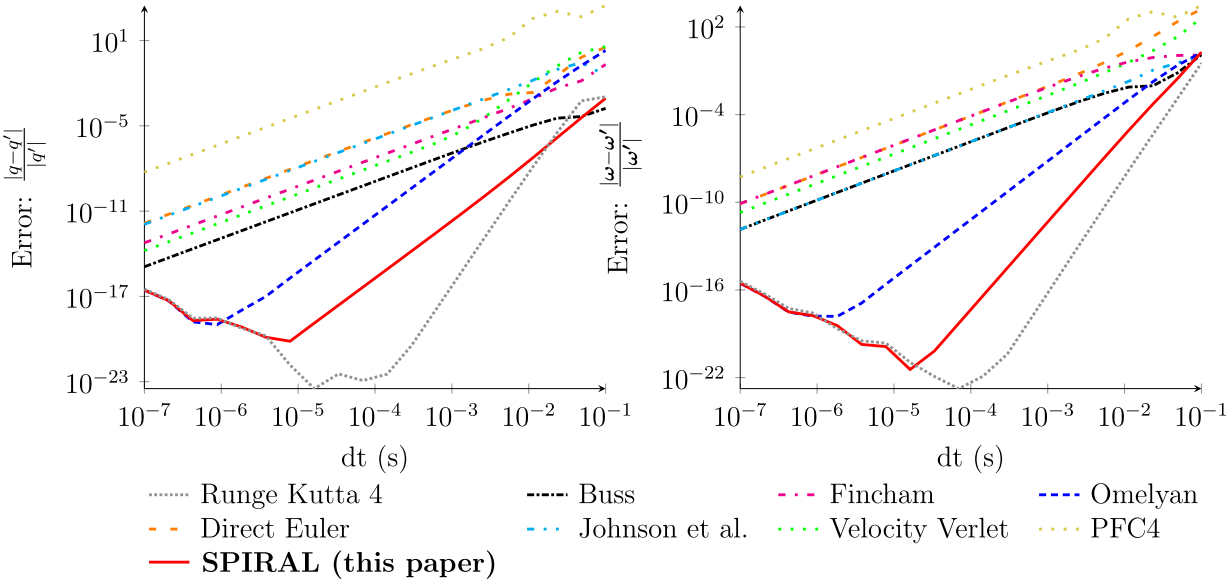
Keywords Discrete element method (DEM), non-spherical particles, simulation accuracy, numerical integration algorithm for rotation, molecular dynamics (MD)

We introduce SPIRAL, our newly developed third-order integration algorithm, which resolves many of the issues with existing ones and outperforms them in all tested metrics with only minor increases in computational cost. The algorithm does not require quaternion normalization for each timestep and is compatible with both leapfrog and non-leapfrog schemes, making it easy to adapt to most existing simulation frameworks. The integration of rotational motion is a key part of many applications, such as embedded systems, sensors, aircraft control systems, molecular dynamics (MD), and discrete element method simulations (DEM). However, current methods for integrating the rotational motion of particles in simulations are not optimal, particularly for non-spherical particles. This study compares various integration algorithms using a range of metrics, including accuracy against an analytical solution, performance, numerical stability, and energy conservation in a challenging undamped system.



Meshless algorithm for heat flow modelling in DEM simulations

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Keywords Heat flow, Yade software, large deformations, meshless approach, heat pipe concept

The possibility of heat flow modelling greatly extends the capabilities of the DEM simulations, allowing for thermal analyses, thermo-mechanical coupling and accounting for variable temperature-dependent material parameters. Hence, various frameworks for reflecting this phenomenon have been developed for the past three decades. Advanced algorithms consider numerous phenomena (radiation, conductance, pore fluid influence). Those, however, complicate the simulation framework and come with a significant computing cost. The current distribution of the Yade software provides an advanced algorithm allowing for thermo-hydro-mechanical coupling. This work presents an alternative approach - a simple meshless algorithm for heat flow modelling in DEM simulations and its implementation to Yade software. It is dedicated to simulations where pore fluid is absent or negligible. The principle is based on the concept of heat pipes and heat reservoirs, where bodies in simulations exchange heat flux via contacts. The single iteration consists of two loops. In the first loop, each pair of interacting bodies exchange the heat flux flow based on the contact properties and temperature gradient. In the second loop, the temperature of all bodies is updated due to the accumulated thermal energy and capacity. By default, the contact area is computed from the geometry of overlapping bodies. Nevertheless, the user can create 'dummy interactions' to prescribe a specific contact area or create a thermal connection between non-overlapping bodies. It is beneficial in the case of advanced contact models, where the contact area is not simply derived from the geometry of bodies (e.g. Hertz-Mindlin law, partially fractured cohesive contacts, etc.). It makes the algorithm versatile despite its simplicity. The algorithm has been tested with problems such as heat flow for spherical packings, clumps, large deformation problems and cohesive fractured media. It will be further developed, e.g. to incorporate temperature-dependent conductant properties of the materials.

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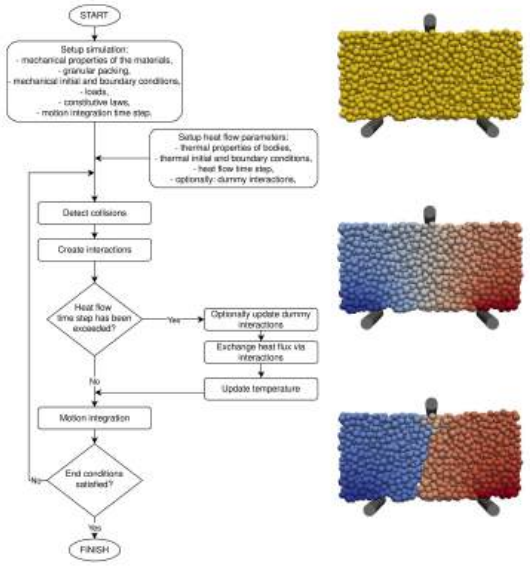

How to locally increase the resolution when simulating fractures with DEM: A 3D MechSys implementation

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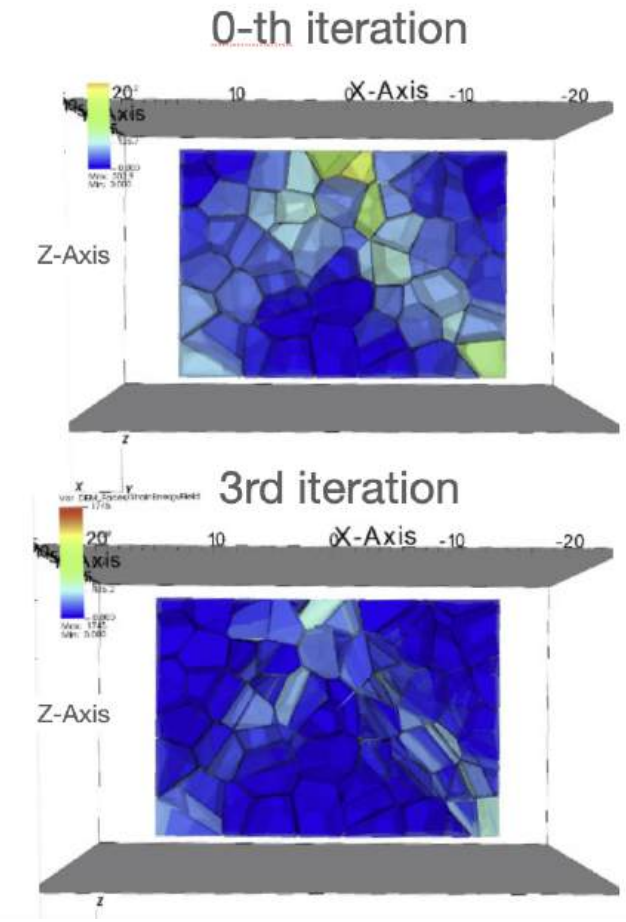
Keywords Fracture, resolution, strain energy field, MechSys

Discrete element methods (DEM) have been broadly used to simulate fractures, but reaching a good resolution is usually performed by setting a small size for all elements, with enormous computational costs. Hereby we introduce a general procedure to increase the resolution just where the fracture will take place. First, the DEM simulation runs up before the fracture limit and measures the Strain Energy Field (a scalar field derived from the strain) on every element, identifying those with high SEF. Next, those elements are split at the initial condition, and the DEM simulation runs again. When implemented on MechSys for discrete elements joined by beams (Fig. 1), the procedure runs stable and increases the resolution only at the fracture, with CPU times that are significatively smaller than those for running DEM with the larger resolution on the whole material. The procedure is general and could be implemented on almost any DEM model for fractures.



Analysis for the effect of the mixing of particles with different sizes on shear thickening in concentrated slurries

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Keywords Concentrated slurry, Shear thickening, Shear flow

The processes for dealing with concentrated slurries are in many industries such as ceramics, pharmaceuticals, and fuel cells (Blair & Ness, 2022). The viscosity of the slurry has a significant influence on the operability and energy costs of those processes. Therefore, understanding the viscosity change of concentrated slurries is very important. It has been widely reported that concentrated slurries show complex viscosity change with shear rate. For example, the phenomenon called shear thinning is a decrease in viscosity with increasing shear rate, and the phenomenon called shear thickening is an increase in viscosity with increasing shear rate. In particular, the mechanism of shear thickening has been still substantially discussed. Interestingly, in recent studies, it has been observed that shear thickening is suppressed by mixing particles of different sizes in several cases (Nakamura, 2021). This suppression is considered to be caused by changes in the contact state of particles. Nevertheless, changes in particle behavior during the suppression have not been observed because it is difficult to visualize the inside of the slurry in the experiment. Therefore, the mechanism of the suppression of shear thickening by mixing particles of different sizes is not clear.

Thus, the simulations that analyze particle behavior in shear flow were carried out to investigate the effect of mixing particles with different sizes on shear thickening. The simulation results show that the increase in viscosity of shear thickening tends to be suppressed when the volume of small particles in the slurry is increased. In addition, it has been observed that the contact force between particles to resist shear flow is less likely to increase when particles of different sizes are mixed. Therefore, when particles of different sizes are mixed, it is considered that contact between particles is less likely to occur or contact between particles is weak.

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Tree Codes for Neighborhood Algorithms in Discrete Element Simulations

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Keywords Discrete Element Method, Neighborhood Algorithm, Tree-code, Parallelization

Traditional algorithms in the field of DEM simulations like Verlet tables have a computational overhead (recomputation of the tables in Ne2-loops), while neighborhood tables lead to a memory overhead (unoccupied empty table spaces). The more recent sort-and-sweep algorithm has no such overhead, but the re-sorting of bounding boxes is necessary even for particles which cannot interact.

Tree codes were originally conceived to reduce the computational complexity of point-particle systems with 1/re2 interactions from O(Ne2) to O(N logN) (Barnes & Hut, 1986). Tree codes allow to deal with only neighboring particles which can actually have an interaction due to their geometric alignment. However, the straightforward application of this algorithm to discrete element methods (DEM) was hampered by the finite size and the shape of the particles.

We explain the algorithmic intricacies which are necessary to implement tree-codes for the neighborhood computation of DEM-particles, like the treatment of elongation, polydispersity and walls, as well as the efficient updating approach for the tree from one timestep to the next. We also show benchmark comparisons with the sort-and-sweep approach.

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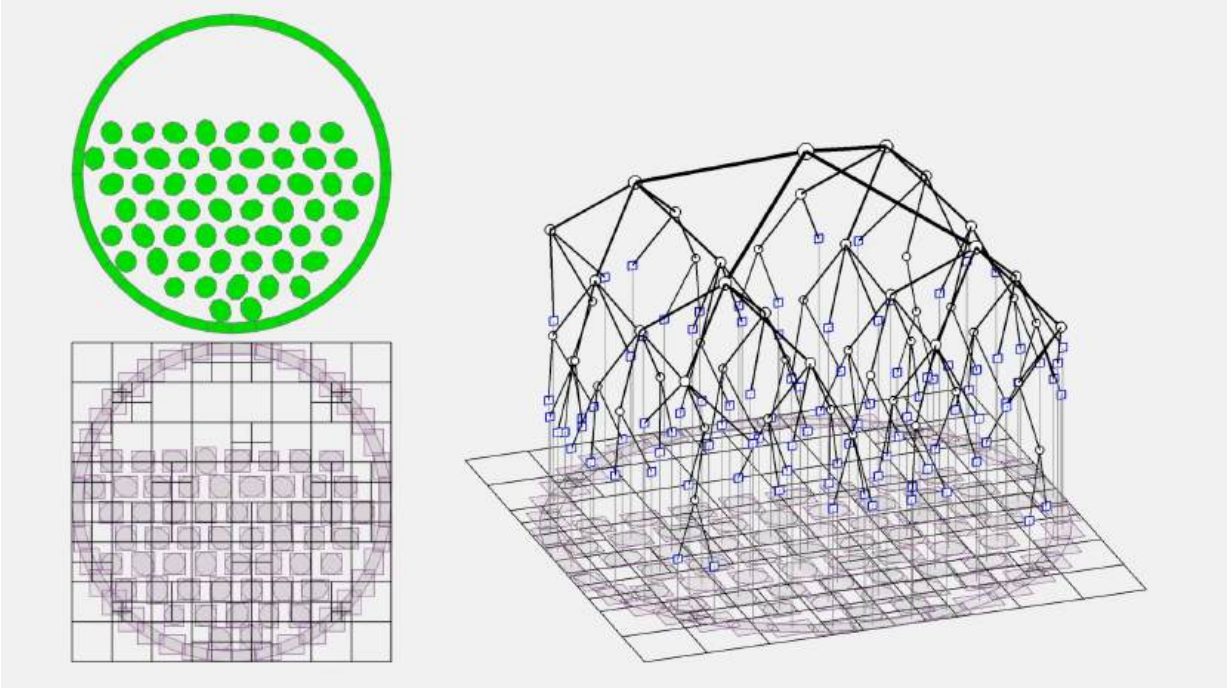

Simple and efficient methods on local structure analysis in dense poly-disperse hard disk systems

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Keywords Methods on local structure analysis, Poly-disperse hard disk systems, Free volume, Pressure, Inherent structure

In many-particle systems, the free volume (FV) of a tagged particle constructed from excluded volume by surrounding particles was crucial to describing the macroscopic properties in the history of liquid state theory. Several numerical algorithms for calculating the FV have been invented [1-4], such as Monte Carlo (MC) sampling and Voronoi tessellation. However, MC is an approximate calculation, and the Voronoi tessellation requires high computational costs (especially for poly-disperse systems). As an alternative algorithm, we developed the simple, efficient, and precise method, Neighbors for Enclosing Local Free Area (called NELF-A), which is easily applied to dense poly-disperse hard disk systems often used in the granular (jamming) and glassy model systems [5]. Particle trajectories in the dense molecular system can be decomposed into the pure structural positions (PS, generally called inherent structure) and thermal fluctuations around them (e.g. [6]). As one of an application of the NELF-A, we implement an alternative method to obtain the PS using a centroid of FV (CFV) by introducing the recursion form for convergence (ReCFV) instead of short-time averaged coarse-graining trajectories (TCG). The typical distributions of FV in the equilibrium state and PS by this method in the mono-disperse hard disk system are exhibited in Figure (I), where the isotropic shape of FV located on a triangular lattice is observed, indicating a perfect crystal structure. In a typical bi-disperse hard disk system, the difference in probability density functions of FV in PS obtained by ReCFV and TCG are shown in Figure (II). We confirmed that the distribution by ReCFV is reasonably consistent with TCG's. At the conference, we will present our algorithm in detail and remark on the substantial advantage of ReCFV over conventional TCG. We also discuss comparing the equation of state (compression curves) by FV-based algorithms and other conventional methods regarding precision and efficiency.

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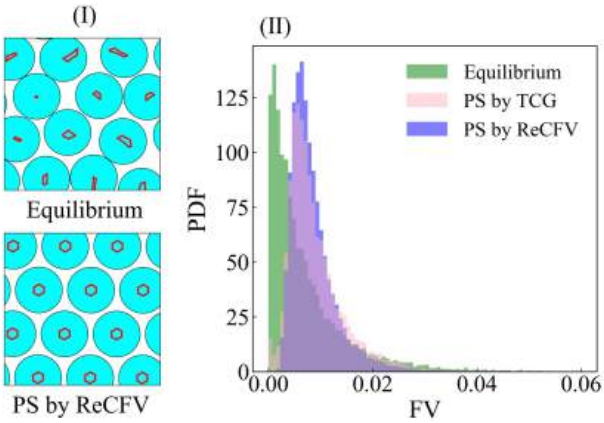

Free energy analysis of the molecular transport into micelles using molecular dynamics simulations

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Keywords Micelle, molecular dynamics, free energy profile, molecular transport

Micelles are self-assembled structures of surfactants that have the ability to transport insoluble substances in solvents: water-in-oil or oil-in-water. To control the transport and solubilization of molecules using micelles is important in many fields like pharmaceutical or analytical sciences. In this talk, I show the free-energy analysis of the transport of a molecule in micelle and reverse-micelle systems by molecular dynamics simulations.

In the micelle system, we controlled the diffusion of surfactant molecules to make a sharp boundary. By calculating the free-energy profile in transporting of a hydrophobic molecule into the micelle, we investigated the effect of boundary roughness on the transport property. The results reveal that a sharp boundary induces the free energy barrier at the interface and the stableness of a molecule in the center of micelle.

In the reverse-micelle (RM) system, we investigated the effect of the water content in the RM on the transport of water. From the analysis in the hydrogen-bond lifetime, it is found that the lower content of water leads to the longer lifetime of hydrogen bonds. This means that the RM with less water have more rigidity. In the talk, I will discuss the relationship between the rigidity of the RM structure and the free energy profile of water transport.

Cooperative phenomena in active matter systems with alternative interaction of neighbors

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Keywords Active matter, Vicsek model, neighbor interaction, metric-free, SANN

Recently, the active matter has been actively studied by physicists, who explore the universal laws of untrivial cooperative phenomena driven by the self-propelled interaction between particles. One of the well-known models is the Vicsek model [1], which has been mainly studied by numerical simulation such as the molecular dynamics method. In the original Vicsek model, the directions of the elements are evaluated by the sum of directions of neighbors located within the fixed cut-off radius. However, it is eventually recognized that the macroscopic behavior in the Vicsek-like models strongly depends on the definition of neighbors due to the inhomogeneity in the distribution of elements. To be more realistic, "metric-free" topological interactions such as the Voronoi construction [2] and the kNN [3,4] for detecting neighbors have been studied recently. In this study, we introduced alternative metric-free interaction for detecting neighbors by SANN (Solid-Angle Nearest Neighbor) method [5] to the Vicsek model. The SANN has distinct advantages over conventional methods for applying the non-equilibrium system. It is expected to be exceedingly feasible as the actual cooperative behavior in the Vicek-type model, which decides the optimal cut-off radius adjusted by the configurations and density of surrounding elements at a simultaneous time. In this study, to figure out the macroscopic phase changes by neighbor interactions described above, we implemented the efficient algorithm of SANN in two dimensions, in which the computational costs in CPU time are comparable to that of the conventional cut-off method. At the conference, we would like to present the difference in the macroscopic behaviors (e.g., polar order parameter, diffusional characteristics) in the Vicsek model by changing microscopic interactions between elements and discussing its validity as the active matter model.

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Analyzing Asteroid Anchoring Characteristics using Discrete Element Method under Diverse Working Conditions

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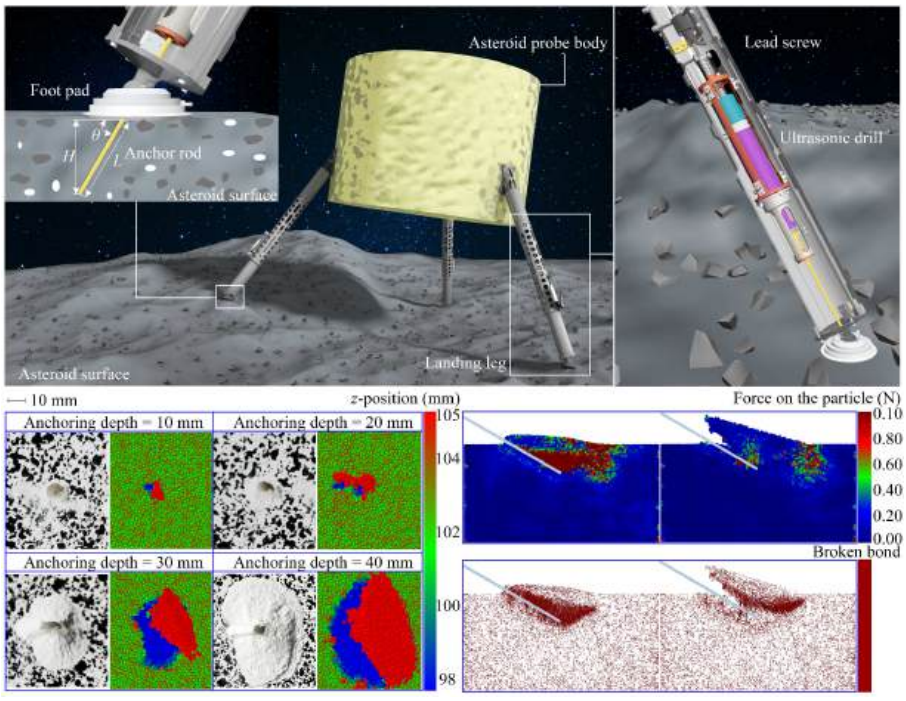
Keywords Discrete Element Method, Asteroid anchoring, Bonding model, Particle force, force chain

Due to the microgravity environment on the surface of asteroids, an anchoring device is essential for the asteroid probe to realize in-situ detection. However, there is currently a significant lack of research on asteroid anchoring, while the discrete element method (DEM) allows for studying the anchoring characteristics of the device and revealing the anchoring mechanism more comprehensively. Thus, the DEM is employed to investigate the anchor rod-asteroid surface interaction. Several geomaterials are selected to imitate the asteroid surface, and their DEM parameters are calibrated using uniaxial compression and angle of repose tests. The anchoring experiments verify the accuracy of the DEM model. Based on the DEM simulation and the central composite design method, the influence of the drilling depth and anchoring angle on the anchoring force is investigated. The failure mechanism of the anchoring is revealed according to the force on the particles, the force chains, and the fracture of the bonds. As the drilling depth increases, the optimal anchoring angle increases gradually. At the same drilling depth, the optimal anchoring angles vary for different geomaterials; however, they generally fall within the range of 50°–60°. The stressed particles and fractured bonds occur predominantly above the anchor rod, forming the damaged area in the geomaterial, and the damaged areas obtained by simulation meet those observed in experiments. The tangential force of the force chain between particles is significantly greater than the normal force of the force chain, indicating that the geomaterials mainly undergo shear failure during the anchorage failure process, which is consistent with the assumption of the failure surface theory. By investigating the anchoring process through DEM simulation, this work contributes to the understanding of the mechanism involved in anchoring on asteroids and provides guidance for the design and implementation of effective anchoring systems in such missions.



Random packings of Meissner Tetrahedra

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Keywords Meissner tetrahedra, packing, X-ray computed tomography

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

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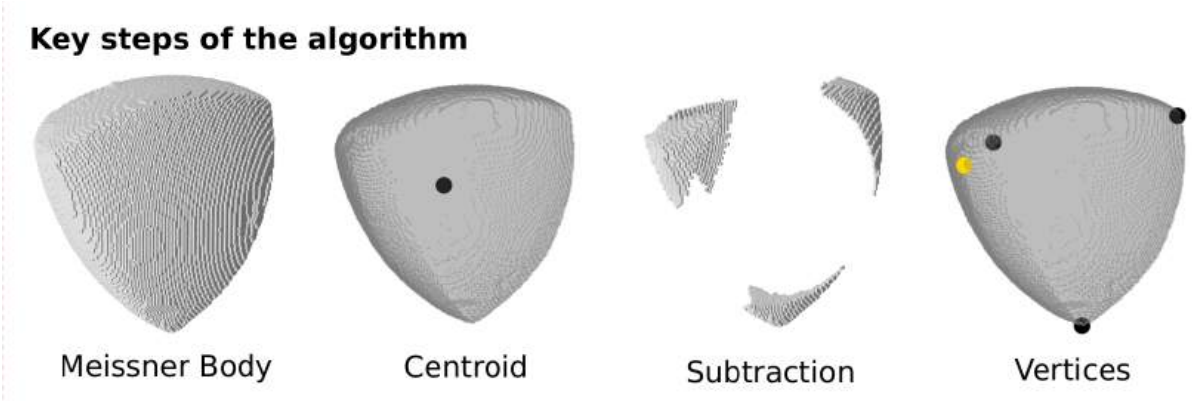

Particle simulation by a sphere with points positioned outside of the sphere

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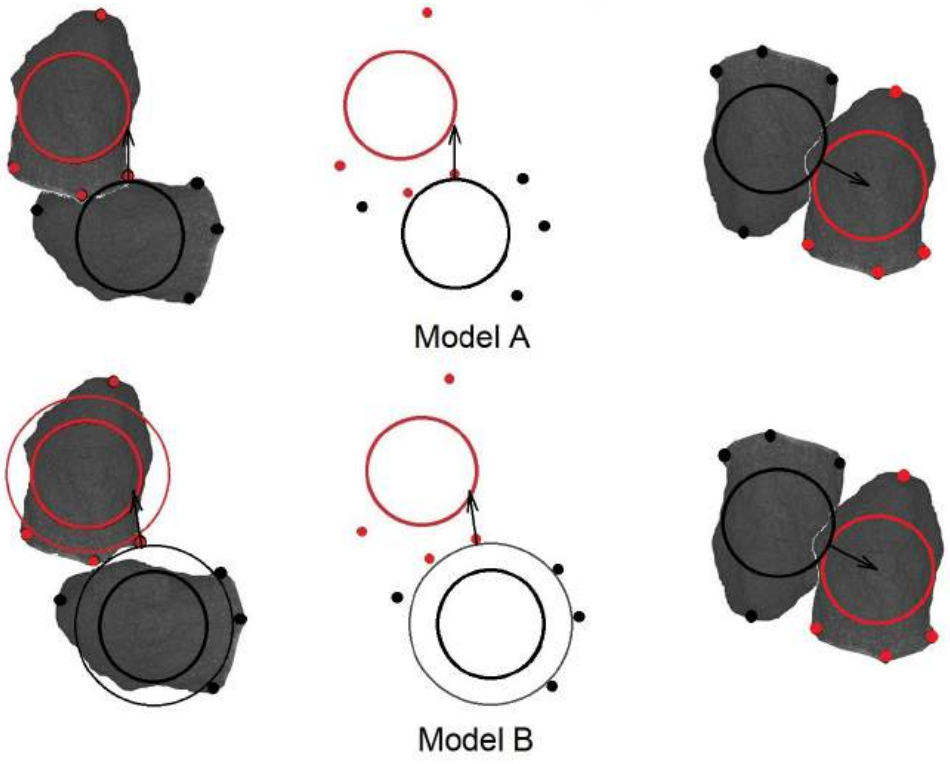
Keywords Particle, granular, simulation, sphere, vertex

To simulate particles similar in shape to those of crushed stone, sand, at least 50 spheres are required. It is necessary to use a particle model with a minimum and sufficient number of constituent elements to reduce the computer time of simulation. Authors proposed the following method for particle simulation. The particle model consists of a sphere and rigidly positioned points in the sphere's relative coordinate system. To develop a particle model, a sphere is inscribed into a real particle's shape. The vertices of real particle that are the most distant from the center of particle are determined, and points of the model are positioned on these vertices. One particle's points can contact with the other particle's sphere. In the proposed simulation, the point–sphere contact simulates the contact type of two real particles, vertex–face, edge–edge, edge–face. The sphere-sphere contact simulates the face-face contact type of two real particles. The following hypothesis is used. To simulate real particles, it is sufficient to use the number of points equal to the number of vertices of real particles. Two series of numerical experiments were performed. In the first one, the particle model consists of 89 spheres located on the octahedron surface. 8000 particles were used in the simulation. Particles' packing was studied, the quantitative ratio of contacts' types (vertex-face, edge-edge, edge-face), the location of contact points relative to the centers of mass of interacting particles were found. In the second series, the particle model consists of a sphere and six points. The diameters of spheres and positioning heights of points were selected to find the properties of the granular material similar to those from the first series. Simulation of particles by spheres and points reduced the computer time by 23 times.



A Novel Image-Informed Data-Driven Multi-Scale Modelling Method for Granular Materials

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Keywords Granular Materials, X-ray Computed Tomography, Segmentation, Reconstruction, Discrete Element Method, Fabric Evolution Law, Data-Driven Modelling

Understanding the microstructural characteristics of granular materials and the development of an accurate multi-scale model still remain open questions. This study proposes a data-driven assisted framework to bridge the multi-scale mechanical behaviours of granular materials. A random forest based segmentation and enhanced level-set based reconstruction algorithms are tailored to process X-ray micro-computed tomography (μCT) images of extremely irregular and porous granular materials. The reconstructed particles are subsequently fed to the level set discrete element method (LS-DEM) to achieve one-to-one particle mapping for mechanical modelling. Finally, a data-driven fabric evolution law is developed based on the simulations of LS-DEM with the inputs of identified particle-scale characteristics from μCT images, which can be integrated with the framework of micromechanics to model engineering- scale problems. The results indicate that the new segmentation and reconstruction algorithms ensure 81% of particles are reconstructed, outperforming conventional methods with a 20% improvement. Moreover, the one-to-one mapping LS-DEM simulation accurately captures the fabric evolution and macro-scale mechanical behaviours of granular materials, showing strong agreement with the experiment data. The novel data-driven fabric evolution law is robust to be integrated with micromechanics-based models and exhibits stable convergence for numerical modelling.

Development of discrete element software for multidirectional coupled simulations at the Budapest University of Technology and Economics

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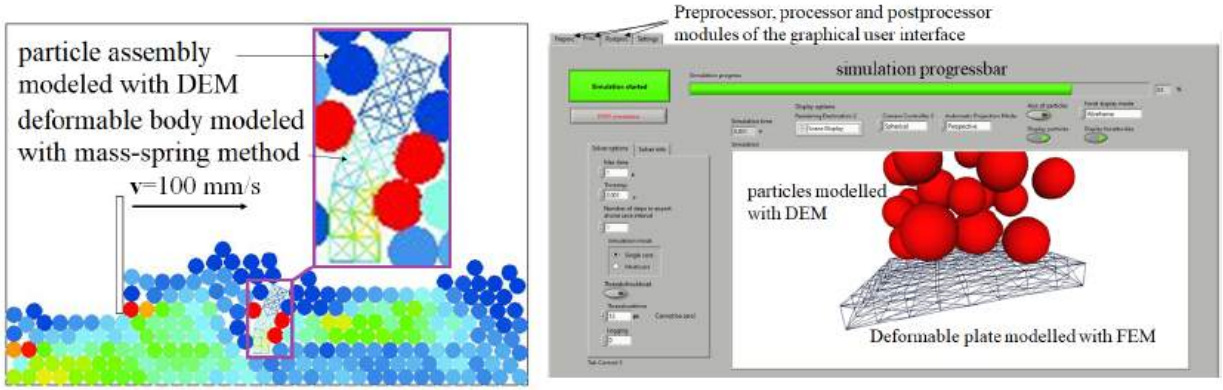
Keywords Software development, coupled DEM simulation, LabView, soil-tool-stem interaction

In the DEM calculations, the solid bodies in contact with the particles are generally considered rigid, thus in the event of contact forces causing a significant deformation in the solid body, which already affects the movement of the particles, the discrete element simulation alone is not sufficient, another calculation procedure is required to model the deformation of the solid body, which can cooperate in parallel with the discrete element calculation. The aim of our research is to develop simulation software that integrates the discrete element method, as well as numerical methods that enable the calculation of the deformation of solid bodies and are able to cooperate with the discrete element method in parallel. The research project was started with the development of a two-dimensional discrete element software (BMEDEM2D) (Figure 1 a) in LabView. We provided this with an easy-to-use graphical user interface that allows the user to define and run simulations even without programming knowledge. Later, the so-called mass-spring method was incorporated into the software, which models deformable, tear-able solids with mass points connected by springs and damping elements. The combined use of DEM and the mass-spring method makes it possible, for example, to take into account the roots and stem residues modeled by the mass-spring method in soil modeled with a discrete element assembly in tillage simulations. Furthermore the development of a three-dimensional discrete-finite element software (BMEDEM3D) in C++ is also in progress (Figure 1 b), in which the DEM and FEM calculations are executed parallel. DEM calculates the motion of particles, and FEM calculates the deformation of solid bodies. The software also has a graphical user interface for easy application. Moreover the mass-spring method is also planned to be incorporated to provide an other possibility for modeling deformable bodies, and to enable the tear of the solid bodies.



a) b)

Studies for Flowability in Hopper with Multiple Outlet using Particle Image Velocimetry and Discrete Element Method

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Keywords Multiple outlet hopper, PIV, DEM, particle flowability

A hopper is the most representative example used for the storage and transportation of powder and particles. In general, the fluidity and the flow type inside hopper are determined by the material properties of the particles and the container, and container design. The flow of powder inside a hopper or silo with single inlet and outlet can already be predicted using several theoretical equations such as kinematic theory, and accordingly, the fluidity of the hopper can be identified. However, these theoretical equations are mainly applicable only to hoppers or silos with single inlet and outlet, and are not applicable to hoppers with multiple outlets. In particular, such multiple outlets are often used in silos for storing coal or iron ore in the steel industry. Therefore, in this study, the flow in a hopper for the steel industry with multiple inlets and outlets is analyzed using Particle Image Velocimetry, and the internal flow of the hopper is reproduced using the discrete element method. Ultimately, through the discrete element method simulation, the fluidity of the powder with given properties in the hopper is improved by changing the design of the hopper.

Acknowledgement
This research was supported by the MSIT(Ministry of Science and ICT), Korea, under the Innovative Human Resource Development for Local Intellectualization support program (IITP-2023-2020-0-01612) supervised by the IITP(Institute for Information & communications Technology Planning & Evaluation).

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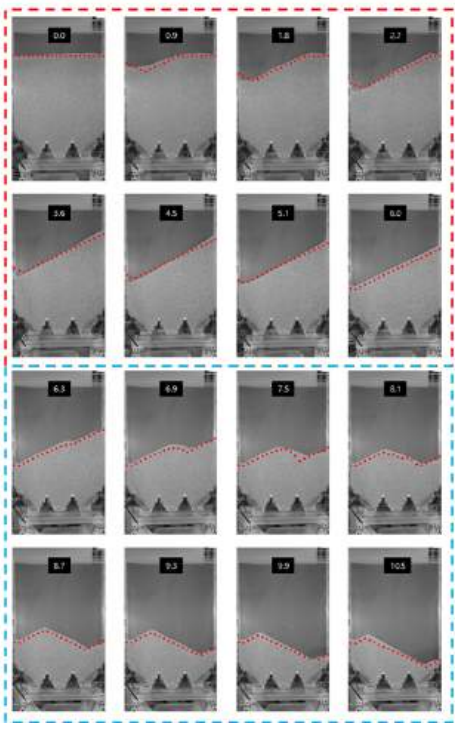

Developing a Fabric Model with JKR and Liquid Bridge Models for Accurate Dynamic Simulation of Clothes with the Effect of Water in Drum Washing Machine

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Keywords Drum Washing Machine, DEM, JKR, Liquid-Bridge, Fabric

In the previous study, the washing process of Drum Washing Machine was analyzed using spherical particles without considering the effect of water. However, there are limitations to modeling the behavior of flexible objects such as towels and clothes, and it is not possible to consider the effect of surrounding water on particle-particle contacts. In this study, we developed a Fabric Model that connects particles with 2-D springs to simulate the behavior of flexible objects such as towels and clothes and create a cloth-like shape. We also applied the JKR Model and Liquid Bridge model to the program for calculating the effect of water during washing process. To validate the Fabric Model, we conducted a vibration analysis using a membrane. We compared the results and frequencies with Zheng Zhou-Lian's (2009) findings. We also conducted an experiment to compare the program's performance to consider the effect of water. The experiment used contaminated cloth, in which two cloths were soaked in water and attached to each other. Additional weights were added to the lower cloth, and the weight at which the cloth fell off was measured. Both in the experiment and simulation, the contaminated cloth fell when an additional approximately 60g of weight was added. In conclusion, to overcome the limitations of previous studies, we applied the Fabric, JKR and Liquid Bridge Models to the program. When compared to their theoretical equations, all models had an error of less than 2%. We also compared the program's results to actual experimental results. These findings confirm the program's performance to accurately simulate particle-particle contact with the effect of water.

Acknowledgement
This research was supported by the MSIT(Ministry of Science and ICT), Korea, under the Grand Information Technology Research Center support program (IITP-2023-2020-0-01612) supervised by the IITP(Institute for Information & communications Technology Planning & Evaluation).

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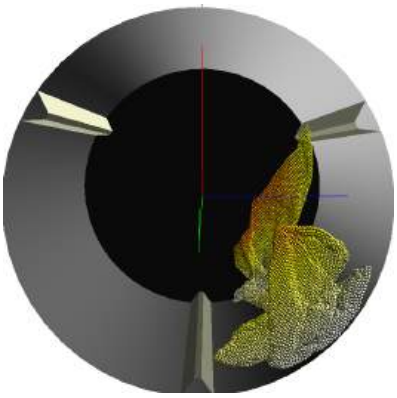

Beyond the Black Box: How DEM Gives a New Approach to Vertical Stirred Milling

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Keywords Vertical Stirred Mill, Process Optimisation, Grinding, CFD-DEM, GPU Computing

With the increased capability and speed of computing from technology such as GPU's and HPC's, industrial systems can now be studied in greater accuracy and depth than ever before. One process which has really benefited from these advances is vertical stirred milling; a complex system that requires large-scale DEM simulations, often coupled with CFD, to predict fine particle grinding. This has enabled research to go beyond the "black box" theory of only being able to demonstrate milling effectiveness from grinding output, and allowed for study on a regional and even collisional level. Almost every industry relies on particle size reduction methods, with grinding from mining alone contributing almost 2% of global energy [1]. Therefore, a better understanding of these machines could improve efficiency and reduce energy consumption. The talk demonstrates how we can develop a validated DEM mill using experimental technique. Laboratory data collected using the Positron Emission Particle Tracking (PEPT) method shows that, despite being able to collect significant data, there are limitations with current physical techniques. This is where the model gives us an ability to assess the full design space. Once built, evolutionary algorithms were used to refine the material parameters until an optimal set of conditions were found. In certain cases, it was also found that the complex and computationally expensive CFD-DEM coupling could be reduced or even removed due to the nature of the system

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Modeling of powder dynamics in additive manufacturing

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Keywords Powder dynamics, CFD-DEM coupling, Additive manufacturing, Powder-liquid/gas interactions, Binder jetting

Powder-based additive manufacturing (AM) techniques, such as powder bed fusion (PBF), powder-feed directed energy deposition (DED), and binder jetting (BJ), are very promising with high manufacturing flexibility and accuracy. However, the powder dynamics are very complex, where computational modelling is powerful to understand the underlying mechanisms. We have developed a series of models to study various phenomena in these AM techniques. In powder-bed-based AM processes (PBF and BJ), powder spreading is the first procedure, and we have used the discrete element method (DEM) to simulate various powder spreading conditions and validated against experiments quantitatively in terms of surface roughness and packing density. Furthermore, we have developed a CFD-DEM coupling model to reproduce the powder spattering and denudation phenomena during laser melting, by simulate the interactions of vapour jet, ambient gas and powder particles. In powder-feed DED, we have developed a model to simulate the interactions between the powder and gas to understand powder streaming, as well as the laser heating powder on the fly to study laser power attenuation. In BJ, we have developed a two-way coupling model of binder-powder interactions to reproduce both the binder flow (spreading and penetration) and powder dynamics (splashing and agglomeration).

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