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- Emergencies off campus: 112
- Emergency Doctor appointments: +31(0)53 203 02 04
- Emergency Doctor appointments: +31(0)88 555 11 88 (Weekend between 17:00 – 08:00)
- Emergency Dental appointments: +31 (0)900 128 26 32
- Doctors service information number: +31 (0)900 431 33 33
- Twente Police Department: +31 (0)900 8844

Trains
In the Netherlands, traveling by train for long distances is most recommended. Taxis are relatively expensive compared to other countries. The easiest way to check train times is the NS Travel Planner (https://www.ns.nl/en). It will show you all available trains to your desired destination, the times and how often you need to change trains.

Buses
The University of Twente campus is connected with the bus network of the cities of Enschede and Hengelo. The nearest bus stop to get to either city is Westerbegraafplaats, see map on the previous page. OV9292 (https://9292.nl/en) provides information about traveling by public transport. In addition, Google Maps usually shows the most convenient routes with public transport as well.

Taxis
Here are some numbers of local taxi operators:
Taxi Maxx: +31 (0)53 450 05 00
DiTaxi: +31 (0)53 461 50 60
Schiphol Travel Taxi: +31 (0)900 88 76 (Airport Taxi)

Programme
The final programme is available online at https://mercurylab.co.uk/dem8/programme/. This will also be distributed separately.
Committee members

Local Organising Committee

Anthony Thornton – Universiteit Twente, The Netherlands
Thom W einhart – Universiteit Twente, The Netherlands
Stefan Luding – Universiteit Twente, The Netherlands
Donna Fitzsimmons – MercuryLab BV, The Netherlands
Hao Shi – MercuryLab BV, The Netherlands
Coby van Houten – Universiteit Twente, The Netherlands

International Organising Committee

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Mojtaba Ghadiri – University of Leeds, UK
Shunying Ji – Dalian University of Technology, China
Christoph Kloss – DCS Computing, Austria
Harald Kruggel-Emden – Technische Universität Berlin, Germany
Jeremy Lechman – Sandia National Laboratories, USA
Catherine O’Sullivan – Imperial College London, UK
Thorst en Pöschel – Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Franck (Farhang) Radjai – Université de Montpellier, France
Dingena Schott – Technische Universiteit Delft, The Netherlands
Subhash Thakur – Alkermes, OH, USA
Aibing Yu – Monash University, Australia
International Scientific Committee

Fernando Alonso-Marroquin – University of Sydney, Australia
Katalin Bagi – Budapest University of Technology and Economics, Hungary
Bruno Chareyre – Grenoble INP, France
François Chevoir – Laboratoire Navier, France
Paul Cleary – Commonwealth Scientific and Industrial Research Organisation (CSIRO), Australia
Raúl Cruz Hidalgo – Universidad de Navarra, Spain
Felix Darve – Grenoble INP, France
Tim Donahue – University of Newcastle, Australia
Itai Einav – University of Sydney, Australia
John Favier – Tech-to-Tech Consulting, USA
Yuntian Feng – Swansea University, UK
Indresan Govender – University of KwaZulu-Natal, South Africa
Nicolin Govender – University of Surrey, UK
Giovanni Grasselli – University of Toronto, Canada
Hans Herrmann – PMMH, ESPCI Paris, France
Mingjing Jiang – Tongji University, China
Petros Komodromos – University of Cyprus, Cyprus
Hans Kuipers – Technische Universität Eindhoven, The Netherlands
John-Paul Latham – Imperial College London, UK
Xikui Li – Dalian University of Technology, China
Michel Louge – Cornell University, USA
Joe Morris – Lawrence Livermore National Laboratory, USA
Antonio Munjiza – University of Split and Croatian Academy of Science, Croatia
Graham Mustoe – Colorado School of Mines, USA
Jin Y. Ooi – University of Edinburgh, UK
Bernhard Peters – Université du Luxembourg, Luxembourg
Luis A. Pugnaloni – Universidad Tecnológica Nacional, Argentina
Esteban Rougier – Los Alamos National Laboratory, USA
Mikio Sakai – University of Tokyo, Japan
Mark Sawley – École polytechnique fédérale de Lausanne (EPFL), Switzerland
Thallak G. Sitharam – Indian Institute of Science, India
Paal Skjetne – Stiftelsen for industriell og teknisk forskning (SINTEF), Norway
Rodrigo Soto – Universidad de Chile, Chile
Kiuchi Suzuki – Saitama University, Japan
Jukka Tuhkuri – Aalto-yliopiston, Finland
Ugur Tuzun – University of Surrey, UK
Dengming Wang – Lanzhou University, China
John Williams – MIT, USA
Dietrich Wolf – Universität Duisburg-Essen, Germany
Peter Wriggers – Leibniz Universität Hannover, Germany
Chuan-Yu (Charley) Wu – University of Surrey, UK
Zhanping You – Michigan Technological University, USA
Jidong Zhao – Hong Kong University of Science and Technology, China
Plenary talks

Monday 22\textsuperscript{nd} July, 9:20 - Thorsten Pöschel
Monday 22\textsuperscript{nd} July, 13:50 - Stefan Radl
Tuesday 23\textsuperscript{rd} July, 9:00 - Franck (Farhang) Radjai
Tuesday 23\textsuperscript{rd} July, 13:50 - Prashant Gupta
Wednesday 24\textsuperscript{th} July, 9:00 - Catherine O'Sullivan
Wednesday 24\textsuperscript{th} July, 14:10 - Benjy Marks
Thursday 25\textsuperscript{th} July, 9:00 - Christine Hrenya
Thursday 25\textsuperscript{th} July, 13:30 - Thomas Weinhart
Thursday 25\textsuperscript{th} July, After-dinner - David Pinson
Friday 26\textsuperscript{th} July, 9:00 - Jidong Zhao

Prizes

Both the best student talk and student poster will receive a prize of 150 € worth of Springer products.
Title
Simulation of Granular Packings by Ballistic Deposition

Abstract
We present an efficient event-driven algorithm for sequential ballistic deposition of complex-shaped rigid particles. Each of the particles is constructed from hard spheres (typically 5 \ldots 1000) of variable radii. The sizes and relative positions of the spheres may mutually overlap and can be chosen such that the surface of the resulting particle appears arbitrarily smooth. The proposed event-driven algorithm allows simulations of multi-million particle systems using desktop computers.

The algorithm is applied to investigate the structural evolution of a nanopowder by repeated dispersion and settling which can lead to characteristic fractal substructures with robust statistical properties. \cite{fractal}. It is also applied to very tall disc packings and very large heaps of simpler particles to reveal unexpected properties of the packing. The algorithm can be verified by means of Minkowski-Tensor characteristics.

Co-authors: Nikola Topic, Institute for Fluid Mechanics, Universität Erlangen, Germany; Jason A. C. Gallas, Institute for Multiscale Simulation, Universität Erlangen, Germany and Departamento de Física, Universidade Federal da Paraíba, João Pessoa, Brazil; Dietrich E. Wolf, Physics Institute, Universität Duisburg-Essen, Germany

Biography
Thorsten Pöschel is Professor for Multiscale Simulation at the Friedrich-Alexander-Universität Erlangen-Nürnberg since 2008. Before that, he held various posts at the University Bayreuth; Charite Berlin; University of California in Santa Barbara; University of Stuttgart; University of Chicago; Universidad de las Americas in Mexico; John von Neumann Institute for Computing (NIC) in Jülich; École Supérieure de Physique et Chimie Industrielle in Paris; and at Saarland University. He graduated in 1990 from the Humboldt-Universität, Berlin in Theoretical Physics. He is member of the editorial board of "Nature - Scientific Reports"; editor of “Revista Cubana de Física”, “Computational Particle Mechanics”, “Granular Matter”; associate editor of “BioSystems”; and member of the Board of the John von Neumann Institute for Computing at the Research Center Jülich. His current research topics are granular matter, fluid mechanics, statistical mechanics and simulation techniques.
Title
From No Physics to Full-Physics Simulation of Particle Drying

Abstract
Wet granulation and particle drying are unit operations that are of outmost importance for a number of industrial applications, especially in the food and pharma sector. In a typical application, a liquid is sprayed onto a bed of moving or fluidized particles, and subsequently evaporated or decomposed.

In these applications a wet gas-particle suspension must be modelled, including the effects of heating and phase change (i.e., evaporation and eventually condensation). Simulations of these processes are extremely challenging due to (i) the large number of particles involved, and (ii) the lack of adequate closure models (e.g., rheological models of wet granular matter). Our present contribution has the purpose of (i) enabling coarse-grained parcel-based CFD simulation of wet gas-particle systems, and (ii) using the output of these intermediate-scale simulations to formulate device-scale models that can be readily coupled with, e.g., flow sheet models. This would enable a rational design, or optimization of wet particulate processes. Specifically, our present contribution will guide the audience through a journey on three levels of modelling detail:

- A detailed flow model considering primary particles, and that relies on an Euler-Lagrange approach (i.e., a classical soft-sphere CFD-DEM approach, see our previous work [1]), including closures that account for various modes of thermal transport. This is considered the full-physics level, since key physical phenomena can be directly predicted.
- A parcel-based (coarse-grained) model that relies on an Euler-Lagrange approach supplemented by novel interaction laws between parcels (i.e., groups of particles). This constitutes an intermedia level of modeling detail, mainly to reduce the computational cost at a moderate loss of model fidelity.
- A novel (0D) compartment model that can be readily integrated into a flow sheet model for fast predictions and optimization. This is clearly the “no physics” level of modeling, since gas-particle flow and exchange rates are no longer directly predicted, but hidden in model assumptions and correlations.
We will illustrate the above levels of modeling detail with a number of case studies, including fluidized and fixed beds, as well as simple shear flow considering various modes of thermal transport. Finally, we will review the progress made in the field of drying models, as well as outline future model applications in other fields, e.g., additive manufacturing.

References


Biography

Since August 2018, Stefan is an Associate Professor at Graz University of Technology (TU Graz, Austria) with a venia docendi for particle technology (habilitation thesis “Micro- and Mesoscopic Models for Flow and Mixing of Suspensions”). Before that, Stefan acted as an Assistant Professor at the same institution for five years.

After earning his Master and PhD Degree at TU Graz (supervisor: Prof. Johannes Khinast), Stefan received an “Erwin-Schrödinger” post-doctoral fellowship of the Austrian Science Fund, which he used to for a 13 months research stay at Princeton University (New Jersey, U.S.). During that time his research interest in suspension flow was shaped by Prof. Sankaran Sundaresan and Prof. Howard Stone.

Stefan was and is active in a number of national and international projects (e.g., the EC Marie curie ITNs “MatheGram” and “CALIPER”, or the EC FP7 project “NanoSim”) which are all centered around the modeling of particulate systems and suspensions. His research can be best summarized as Computational Particle Engineering, including topics such as (i) clustering in gas-particle suspensions, (ii) aggregation of cohesive particles and fibres, (iii) heat and mass transfer in suspensions, as well as (iv) the integration of suspension flow and process models.

Over the past eight years Stefan was involved in the supervision of 12 PhD students (seven already graduated), and mentored more than 20 Master students during their final diploma project. He was invited as a guest editor for an edition of the “Computers & Chemical Engineering” journal, and is active as a reviewer for leading journals such as the Journal of Fluid Mechanics, Physics of Fluids, the International Journal of Multiphase Flow, or the Chemical Engineering Journal.
Title
When does particle size matter in DEM simulations of granular materials?

Abstract
As a result of limited available computation time and memory, the tractable number \( N \) of particles in DEM simulations is often far below the real number of particles \( \sim (L/d)^3 \), where \( L \) is a linear dimension of the system to be simulated and \( d \) is the average particle diameter. As the equations of motion are solved for all particles and the mean values of particle displacement vectors and contact force vectors can be used to calculate the average strain(rate) and stress tensors (possibly by applying also smoothing operators) for a rather low number (say \( 10^3 \)) particles, it is tempting, for the sake of computational efficiency, to keep \( L \) at its real value but increase \( d \) in order to reduce the number of simulated particles or to apply the DEM to solve boundary-value problems (such as debris avalanches or rapid flows in complex powder treatment units). In this lecture, I discuss three aspects of this issue: 1) Finite-size effects and requirements for the size of the representative volume element (RVE), 2) Influence of wall boundaries, and 3) Influence of particle interactions. I show that with frictional contact interactions and rough walls the linear size \( L/d \) of the RVE is an order of magnitude larger than usually assumed. Then, I consider particle size effects for the elastic behaviour, brittle behaviour with cohesive forces, inertial flows, immersed flows in a viscous fluid, wet particle flows and gravitational aggregates. I show that in most cases a single scaling parameter can be used to elude particle size effects.

Biography
Farhang Radjai is Research Director at National Center for Scientific Research (CNRS) in France. He is the head of Research Team « Physics and Mechanics of Discrete Materials » at LMGC, University of Montpellier, and MIT research affiliate at the CNRS-MIT research group « Multi-Scale Material Science for Energy and Environment ». He graduated in 1995 in theoretical physics and received his PhD on modeling granular materials in University Paris-Sud. His research has mainly focussed on the rheology of granular materials using particle dynamics methods and statistical analysis by considering granular microstructure, stress transmission and kinematic fields as well as particle shapes, particle size distributions, cohesive contacts, solid bonding, fluid-grain interactions and particle fracture with applications to communition, powder compaction, inertial flows, avalanche dynamics and agglomeration.
Prashant Gupta – Procter & Gamble, UK

Title
Industrial applications of Discrete element method: challenges and opportunities

Abstract
Bulk solid handling of granular materials presents a great challenge to industries ranging from pharmaceutical to FMCGs. P&G is a world leader on the consumer good products ranging from detergent “powders” to hand dish “liquids”. Current work process for plant scale process design require large cost pilot scale with very less data obtained to make a decision. Industries dealing with fluid systems or motor industries have benefitted heavily moving to a virtual experiment space and invested heavily in R&D to understand these systems. However, there is a lack of a coherent approach to apply modelling and simulations tools to study the bulk solid systems. A key milestone which is yet to get achieved is to establish a suite of validated modelling and simulation tools to capture underlying physics governed at largely separated length scales.

Discrete element method (DEM) provides an approach to solve the microscopic details which could correctly capture particle level perturbation manifesting to evolving macroscopic bulk behaviour. The tool has worked wonders for academic understanding, however, its usage at industrial scale is difficult to establish. In this talk, we would like to a) demonstrate usage of DEM to solve industrial problems b) What can we not predict and is needed? c) Where do we see our future with DEM?

Co-author: Christopher Stoltz Procter & Gamble, USA

Biography
Dr. Prashant Gupta currently work as a scientist for Fabric and Home care division at Procter & Gamble Technical Centres Ltd, Newcastle Upon Tyne. His main area of expertise is process design for formulated product with leveraging modelling and simulation tools. Before joining the company in 2015, Dr. Gupta obtained his PhD in modelling hydrodynamics of multiphase flows from University of Edinburgh in 2014 and did a year of Post doc modelling large scale waste water treatment plants at Newcastle University.
Title
DEM, dams and dikes

Abstract
Embankment dams and flood embankments are probably the largest, man-made, structures that comprise particulate materials (soil). Recognising the particularly strong history of dike construction in the Netherlands, this presentation aims to demonstrate how DEM simulations can be used to inform the design, construction and ongoing maintenance of these critical elements of Dutch infrastructure. The talk will focus on internal erosion, a phenomenon where water seeping through the embankment can erode some of the embankment materials and pose a risk to embankment integrity.

Two key mechanisms will be considered: (1) the performance of filters which layers of sand and gravel placed to prevent erosion of low permeability, fine-grained material and (2) seepage induced internal instability, a mechanism which involves preferential erosion of the finer grains in the embankment filter and transition materials or in the embankment foundation.

Considering firstly filter performance, engineers have long recognized the importance of the size of the narrowest points in the void space, which are called constrictions or pore throats. Hitherto attempts to estimate constriction sizes have relied on a number of unproven hypotheses. DEM enables a direct measurement of the sizes of the constrictions in virtual filter samples. Micro Computed Tomography data can be used to confirm the relevance of DEM-derived data. Network analysis can be used to understand the basic mechanisms involved in filter performance.

In a gap-graded material, where there are a mixture of coarse and finer grains, there can be significant inhomogeneity. The amount of the overall stress transmitted by the finer grains can be very small, particularly when the proportion of finer grains in the material is small. Consequently these materials can fail lower hydraulic gradients that are typically considered safe in engineering design. DEM simulations have been used to examine in detail the relationship between this stress inhomogeneity and both the proportion of finer grains and the size of the coarse grains relative to the finer grains. Coupled DEM-CFD simulations have then confirmed that the proportion of stress in the finer grains influences the likelihood that these grains will be transported under the action of seepage flow.
**Biography**

Catherine O’Sullivan is a Professor of Particulate Soil Mechanics in the Department of Civil and Environmental Engineering at Imperial College London. She is a civil engineer specializing in geotechnical engineering and studied in both University College Cork, Ireland, as well as the University of California at Berkeley. Her research has primarily focussed on the behaviour of sand at the scale of the individual particles using discrete element method simulations complemented with experimental studies. She has considered the load:deformation behaviour of sand at both large and small strain levels and internal erosion of dams and flood embankments. She is an editor of the ASCE Journal of Geotechnical and Geoenvironmental Engineering and Associate editor of Soils and Foundations and Granular Matter. She has contributed to over 85 papers in international journals and has received funding for her research from the Engineering and Physical Sciences Research Council, the Leverhulme Trust and the Institution of Civil Engineers. She delivered the prestigious Géotechnique lecture in 2015 and was awarded a best paper award by the Japanese Geotechnical Society in both 2018 and 2019.
Title
Hyperspheres in hyperspace

Abstract
The Discrete Element Method has proven to be capable of serving three distinct purposes. First and foremost, it has been successfully used to probe the mechanics of granular media and describe scaling laws for its behaviour. Secondly, it has been used to simulate directly systems with 'small' numbers of particles. Finally, the method has been used to augment experimentally inaccessible regions of phase spaces. Here, we propose a new and vastly unexplored region of this phase space, namely systems of hyperspheres in spaces with arbitrary numbers of spatial dimensions. The description of these particles requires new numerical and technological tools, which will be described in an interactive presentation. The challenges of visualising higher dimensional spaces will be explored using virtual reality, and will require significant audience participation.

Co-author: François Guillard, The University of Sydney, Australia

Biography
Dr Marks is a Lecturer in the School of Civil Engineering at The University of Sydney. His research is based in the mechanics of granular media, in particular the processes of segregation, mixing and grain crushing. He is involved in developing new X-ray based techniques for investigating the interior of landslides, and creating new mathematical and computational tools for understanding their behaviour.

Dr Marks also is part of the team running the Immersive Learning Laboratory at The University of Sydney. This Lab works to deliver Virtual Reality solutions to educators around the whole University, both developing content for individual classes and also managing a physical space where large classes can learn in VR.
Thinking outside of the DEM box

Abstract

DEM is an invaluable tool for the particle technology researcher. Arguably the most common usage is to simulate a system setup inspired by an industrial operation (mixing, granulation, heat transfer, etc.) or a natural phenomenon (avalanches, asteroid dynamics, etc.). Oftentimes, the computational overhead of the ultimate system of interest is impractical with today’s resources, so we are forced to perform simulations containing fewer particles. Instead of viewing this a drawback, here we describe a series of case studies illustrating alternative and novel uses of DEM simulations, both on its own and in conjunction with other tools. We’ll also consider how this meshes with current industrial needs, based on a recent survey of a wide range of companies.

Biography

Christine Hrenya is a Professor of Chemical Engineering at the University of Colorado at Boulder. She holds chemical engineering degrees from The Ohio State University (B.S. 1991) and Carnegie Mellon University (Ph.D. 1996). Her interests lie in the field of multiphase and solids flows, using a combination of theory, simulation, and experiments. Recent emphases of the research program include multiphase flow instabilities, cohesive particles, and gas-solid heat transfer. Prof. Hrenya currently leads a $3.5M U.S. Department of Energy grant targeted at discrete-particle simulations for the energy industry, including exascale computation. To date, her research program has resulted in 110 journal papers and 130 invited lectures, and $13M in funding from the U. S. DOE, NSF, NASA, ACS and industry. Recent recognitions include the 2014 AIChE Lectureship Award in Fluidization and the 2013 University of Colorado Excellence in Teaching Award. Professor Hrenya currently serves as an Associate Editor for the AIChE Journal and as an Editor for Granular Matter. She recently served as the Chair of the 2016 AIChE Annual Meeting, and has previously served as Chair of the 2006 Gordon Conference on Granular Flow (Oxford University) and as co-Director of a 2001-2004 GAANN program in Micro- and Nano-Particle Technology.
From discrete particles to continuum fields

Abstract

Micro–macro transition methods are used to both calibrate and validate continuum models from discrete data, obtained from either experiments or simulations. Such methods generate continuum fields such as density, momentum, stress, etc., from discrete data, i.e. positions, velocity, orientations and forces of individual elements. Performing this micro–macro transition step is especially challenging for heterogeneous and dynamic situations.

Here, we present a mapping technique, called coarse-graining, to perform this transition. This novel method has several advantages: by construction, the obtained macroscopic fields are consistent with the continuum equations of mass, momentum and energy balance. Additionally, boundary interaction forces can be taken into account in a self-consistent way and thus allow for the construction of locally accurate stress fields even within one element radius of the boundaries. Similarly, stress and drag forces can be determined for individual constituents, which is critical for several continuum applications, e.g. mixture-theory based segregation models. Moreover, the method does not require ensemble-averaging and thus can be efficiently exploited to investigate static, steady and time-dependent flows. The method presented in this paper is valid for any discrete data, e.g. particle simulations, molecular dynamics, experimental data, etc.; however, for the purpose of illustration we consider data generated from discrete particle simulations of granular mixtures flowing over rough inclined channels. We show how to practically use our coarse-graining extension for both steady and unsteady flows using our open-source coarse-graining tool MercuryCG. The tool is available as a part of an efficient discrete particle solver MercuryDPM (http://www.mercurydpm.org/).
Biography

Thomas Weinhart is Assistant Professor in the Department of Thermal and Fluid Engineering at the University of Twente. He studies granular processes on all scales: he developed and experimentally validated contact laws for wetting, friction, cohesion and sintering; established coarse-graining as micro-macro method for extracting local macroscopic quantities from discrete particle data; modelled granular systems on the macroscale; and used FEM simulations to predicting the flow behaviour of large-scale systems. He now develops coupled methods for solving multi-scale, multi-physics problems, such as liquid migration, segregation of cohesive powders, sintering, 3D printing, tabletting, and wet granulation. In 2009, he co-founded MercuryDPM, a cutting-edge open-source software for particle simulations, together with AR Thornton, and leads the development team. The code has several unique features that make it particularly apt to simulate complex industrial systems. All his research codes are publicly available in the software. For commercial use of the software, he co-founded MercuryLab, a spin-off company providing custom software, training and advice to companies on the design of process equipment.
A nice picture is truly a great validation

Abstract

Particle simulation approaches to granular research have developed into sophisticated research and process simulation tools. The detailed particle/contact scale information available offers an unprecedented level detail when needed and the ongoing development of coarse graining techniques permits extraction of engineering scale data as required. However, both laboratory and industrial problems often lack the ability to measure system properties – or at least measure with the resources available. However, industrial engineers often come to us with problems where they can visually observe the phenomena they want modelled, but no means (or budget) for any quantification. In that case, being able to exploit quantitative information from imaging methods for system validation is critical. In primary ironmaking, a majority of process problems are really particle problems. Considering some of the interesting applications of visual comparison and quantification and their improvement over time hopefully we take new inspiration for how the growing world of cheap and ubiquitous imaging technology supports particle scale research.

Biography

Dr Pinson has worked on projects for the ironmaking industry for more than 20 years which is dominated by large-scale multiphase particulate processes. Over the same time period, particle scale simulation has grown into a fantastic problem solving and design tool in both a plant operation and asset management context. In these areas he has worked on many problems of coupled particle-fluid problems, wide size ranges, cohesive materials and very large time and physical scale problems. These include blast furnace burden distribution, raceway phenomena, hearth drainage and raw materials handling. Close collaboration with academic researchers and a long list of hard-working students has made it possible to tackle the wide range of industrial problems that occur in primary ironmaking.
Title
Multiscale Modeling of Particle Breakage for Granular Media

Abstract
Particle breakage underpins the operation and performance in a wide variety of engineering and industrial processes and applications involving loading, processing, granulation, crystallization, solidification, transportation and storage of particulate materials. Typical examples include milling and grinding in minerals and mining engineering, tablet/pill design for transportation, storage and comfort use in pharmaceutical industry, rock-fill dam construction and maintenance in hydraulic engineering, fault gauge breakage and slip in geoscience and earthquake engineering. In geotechnical engineering, the mechanical behaviors of crushable granular sands, such as yielding, deformation, dilatancy, failure and mobility, are closely related to the breakage of granular sands, which bear direct relevance to the design and installation of geo-systems such as piles. Numerical modeling of particle breakage in granular materials is challenging. Commonly adopted modeling techniques, such as those based on discrete element method, frequently involve various over-simplifications on aspects such as crushing criteria and patterns and crushed particles shapes which limit their robustness and efficiency.

This talk introduces a totally new numerical strategy in modeling particle breakage for granular media. An integrated computational multiscale framework is formulated to simulate the breakage of granular media subjected to mechanical loading. It features rigorous coupling of two relatively new computational methods for engineering community, Peridynamics and Physics Engine. The breakage of individual particles in a granular assembly, subjected to in-situ multiple contacts, is analyzed and simulated by Peridynamics without artificial presumptions on the probable fracture paths, crushing patterns and crushed child particle sizes. Rigid body motions of irregularly shaped particles generated during the crushing and their inter-particle interactions are effectively modeled by the Physics Engine based on a non-smooth contact dynamics approach which has been popularly used in video game and animation industries. The hybrid framework enables rigorous modeling of particle breakage and allows reasonable simulation of irregular particle shapes during the continuous breakage process, overcoming apparent drawbacks/challenges faced by many existing methods. The predictive capability of the proposed method is further demonstrated with simulations of one-dimensional compression and triaxial shear on crushable sand, where Weibull statistical distribution on the particle strength is implemented. The simulation results compare favorably with experimental observations in terms of mechanical responses, particle size distribution,
fractal dimension, as well as particle morphology. We further explore the possibility of further implementing the proposed method into a hierarchical multiscale modeling framework to simulate engineering-scale boundary value problems where particle breakage may play a critical role.

**Biography**

Dr. Jidong Zhao is Associate Professor of Geomechanics in the Department of Civil and Environmental Engineering at Hong Kong University of Science and Technology. He earned both his bachelor’s degree and PhD from Tsinghua University and was a postdoc fellow and university lecture at the University of Newcastle, Australia, before relocating to Hong Kong in 2008. Dr. Zhao’s research is focused on multi-scale, multi-physics modeling and characterization of granular media pertaining to applications in geotechnical engineering, energy extraction, mining, chemical and pharmaceutical industries. He received financial supports from Australia Research Council, Research Grants Council of Hong Kong, Natural Science Foundation of China and Croucher Foundation for his research. He was a recipient of “University of Newcastle Research Fellowship” award (2007), “Computers and Geotechnics Outstanding Paper Award” (2018) and “Granular Matter Top 5 Cited Article Award” (2018). He serves as an Editor for Granular Matter (Springer), Associate Editor for Journal of Engineering Mechanics (ASCE) and an editorial board member for Computers and Geotechnics (Elsevier) and International Journal for Numerical and Analytical Methods in Geomechanics (Wiley). He is a core member of two technical committees of International Society for Soil Mechanics and Geotechnical Engineering (ISSMGE): TC105 Micromechanics and TC103 Numerical Methods in Geomechanics and is a current member for the Granular Mechanics Committee of Engineering Mechanics Institute (EMI).
Abstracts listed by ID
Large-scale direct numerical simulation for investigating the mesoscale structure in gas-solid flow

Limin Wang, Wei Ge

Institute of Processing Engineering, Chinese Academy of Sciences, Beijing, China

Keywords LBM-DEM, particle cluster, drag, DNS, gas-solid flow

Abstract A coupled Lattice Boltzmann Method and Discrete Element Method (LBM–DEM) approach is usually a kind of particle-resolved direct numerical simulation (DNS) algorithms for modeling gas-solid two-phase flows, in which the size of fluid grid is generally one magnitude smaller than particle diameter and force acting on particles directly calculated by integrating both viscous force and pressure gradient force on the particle’s surface. It has been regarded as the most accurate numerical method for simulation of gas-solid flow. However, the main disadvantage is its huge computational cost resulting from small grid size and time step limited by Kolmogorov length and time scales. Only hundreds of particles scale is reported for DNS of gas-solid flow in the latest literature, which is very different from the number of particles in the real gas-solid flows. In order to solve the problem of computational speed and scale, an immersed boundary method in framework of LBM has been adopted to realize the fluid-solid coupling to avoid a stair-step representation of the solid particles’ surfaces (Wang et al., 2010; Zhou et al., 2011) and the multi graphics processor units (GPUs) parallel computing of LBM–DEM approach has been implemented. Taking advantage of the inherent parallelism of LBM and the attractive Flops/Price ratio of GPU, we have implemented 576 GPUs parallel computing on a Mole-8.5 system and conducted the largest scale DNS of gas-solid suspensions so far, with 1,166,400 solid particles in an area of 11.5cm x 46cm for a two-dimensional system and 129,024 solid particles in a domain of 0.384cm x 1.512cm x 0.384cm for a three-dimensional system (Xiong et al., 2012). The scale of DNS data has been reached the size in traditional computational grid, which implies the really meaningful statistical results from large-scale DNS of gas-solid flows were obtained for the first time. The effects of mesoscale structure on the interaction force between gas and solid phases (Zhou et al., 2014) and the statistical properties of particles (Liu et al., 2017) were explored, which may provide the corresponding constitutive relation and detailed microscopic information for discrete particle simulation and two-fluid model.

References
10: From DEM to continuum theory for both solid and fluid states

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Keywords
DEM, micro-macro, constitutive modeling

Abstract
In order to understand the fundamental micro-mechanics of particulate and granular matter, one can use particle simulation methods like DEM, where often the fluid between the particles is important too. However, large-scale applications (due to their enormous particle numbers) have to be addressed by coarse-grained models or by continuum theory. In order to bridge the gap between the scales, so-called micro-macro transition methods are necessary, which translate particle positions, velocities and forces into density-, stress-, and strain-fields. These macroscopic quantities must be compatible with the conservation equations for mass and momentum of continuum theory. Furthermore, non-classical fields are needed to describe the micro-structure (fabric, force-chains) or the statistical fluctuations, e.g. of the kinetic energy, before one can reach the ultimate goal of solving application problems. In this talk, recent progress on DEM based continuum theory and constitutive modelling will be given, with focus the transition from fluid-like to solid behavior (jamming) and the reverse (unjamming).
Numerical simulation of one dimensional consolidation test of montmorillonite/kaolinite mixtures using discrete element method

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Keywords

one dimensional consolidation test, montmorillonite, kaolinite, discrete element method

Abstract

In this study, the investigation of volumetric changes in soil containing montmorillonite and kaolinite and mixtures of the two has been carried out using the discrete element method (DEM). In order to achieve this goal, seven clay samples containing montmorillonite and kaolinite were prepared using the DEM by modeling all physicochemical forces between particles during consolidation testing. Particles were simulated in both flexible and non-flexible modes. The consolidation coefficients along the loading and unloading paths were found to be dependent upon the montmorillonite content of a given mixture. The results of analysis were then compared with those from laboratory testing.
Analysis of Multi-phase Flow in a Packed Bed

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Keywords
Extended Discrete Element Method, multi-physics, multi-scale

Abstract

Multi-phase flow in packed or moving beds such as trickle bed reactors with either co-current or counter-current flow of gas, liquid and solid phases is apparent in many natural and engineering applications e.g. chemical and petroleum industries. These applications belong to the most challenging flow scenarios including a complex interaction between the individual phases. Flow regimes depend on solid, liquid and gas flow rates in conjunction with physical properties and determine pressure drop, liquid hold-up, pulsing or trickling transitions at low and high temperatures or/and pressures. However, these phenomena are difficult to measure due to sometimes more than hostile operating conditions. Therefore, numerical approaches are a complementary path to follow and to gain a deeper understanding of the underlying physics.

The objective of the current contribution is to present a numerical model that resolves the flow of liquid and gas phases in a packed bed of particulate material. This is achieved with an Euler-Lagrange framework referred to as the extended discrete element method (XDEM). It is an extension to the classical discrete element method and describes additionally the thermodynamic state of individual particles. Particles of a packed bed experience a strong interaction with gas and liquid phases in the void space of a packed bed through heat, mass and momentum transfer. Liquid and gas phases are described by computational fluid dynamics as inter-penetrating and continuous phases. For each phases set of differential conservation equations is solved and thus, allows treating a wide range of engineering applications. In the current contribution, the approach is employed to the lower part of a blast furnace including cohesive zone, dripping zone, dead man and hearth. An analysis of predicted results contribute to an increased knowledge of the phenomena taking place during iron production and thus, aim at controlling and improving the blast furnace process.
A combined DEM and XFEM approach for breakage modeling of angular rockfill materials

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Keywords
Particle breakage; Rockfill; Discrete element method; EXFEM; Crack propagation

Abstract
Particle breakage in two-dimensional angular rockfill materials is simulated using a combined DEM and XFEM approach. In this approach, the interaction of particles is simulated by DEM and breakage analysis is carried out on each particle using XFEM. Simplifying assumptions for the breakage path are eliminated in this approach and the history of cracking is considered for each particle in the breakage analysis. Simulation of various laboratory tests on rock samples and biaxial tests on rockfill assemblies show the ability of the proposed model to capture different aspects of particle breakage and the behavior of granular materials.
Abstract
In this research, hydrodynamics of a spouted fluidized bed with different injection patterns was studied using computational fluid dynamics coupled with the discrete element method (CFD–DEM). The gas flow was modelled by a k-ε turbulent model and the motion of particles was predicted using the DEM. Dimensions of the bed were 1 (m) height, 0.15 (m) width and 0.02 (m) depth which was filled with about 36,500 particles with 2.53 (mm) diameter. Results of CFD-DEM simulations were validated with experimental data. After the validation, three different bubble injection patterns were investigated. First, the motion of a single bubble injection from central inlet was studied. Second, the motion of multiple sequential bubbles injection from central inlet and interactions between bubbles was investigated. Finally, the motion of two adjacent bubbles injection from two inlets and their interactions was simulated. These configurations are shown in Figure 1. The hydrodynamics of the bed with the mentioned injection patterns as well as the pressure signals from the bed were studied in this work.
Segregation of ternary granular mixtures during heap formation in a simplified model of blast furnace

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Keywords
Segregation, granular materials, heap, blast furnace

Abstract
Segregation is an important phenomena from industrial point of view. It occurs mainly due differences in size, shape and density. In this paper, we studied the size segregation of ternary granular mixtures during heap formation in a simplified model of blast furnace (2D system). Steel balls of different sizes (1, 2, 3 & 4 mm) are used as model granular materials. The heap formation take place by repeatedly pouring a fixed mass of the mixture. The parameters varied in the experiments are the composition of the mixture, the mass of the mixture poured at a time, the height of the feeding point above the bottom of the bin and size ratio. Images are captured using high speed video camera. Images are analyzed to detect the position of each particle in the heap using image analysis technique (in house code). Results are plotted along the flow direction to get better insight of segregation pattern formed in each case. In each layer formed by a pouring, segregation results in the fine (small in size) particles being deposited first, coarser one in the middle and bigger particle travel more distance and settle in the opposite end. Each experiment repeated three times to get an average data.
Mathematical programming based DEM in geomechanics

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Keywords
Discrete element method; second-order cone programming; computational geomechanics

Abstract
In this paper, a discrete numerical model using second-order cone programming is presented. The formulation naturally leads to a standard second-order cone program, which can be solved using efficient optimisation solvers, and a purely static method is derived that does not require artificial damping parameters. Notably, the approach unifies two distinct discontinuum approaches: the soft-particle model and the hard-particle model. The capabilities of the proposed method are demonstrated through a series of numerical tests.
Effect of bond strength on pulverization behaviour of crushable particles under confined compression

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Keywords
Crushable particles, confined compression, DEM, contact bond strength, pulverization behaviour

Abstract
This paper presents a discrete element model (DEM) to simulate the pulverization behaviour of crushable particles under confined compression. The purpose of this study is to explore the effect of bond strength on the pulverization behaviour of crushable particles. The compression system included a thin-walled circular cylinder with a solid bottom, and a top platen. The circular cylinder was filled with 1000 crushable particles. Each particle consisted of 12 spheres, which were bound together in HCP crystal structures by contact-bond model. A load was applied to the assembly of crushable particles contained in the cylinder by driving the top platen down at a constant displacement rate. The numerical results reveal that the loading stiffness and the contact force intensity increase with bond strength, whereas the crack number and the solid fraction decrease with the increase of bond strength. In addition, the vertical normal stress increases with bond strength. However, the probability distributions of the contact forces for the inter-particle and particle-wall contacts do not change with bond strength.
Simulation of wet sieving using the coupled DEM-SPH method

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Keywords
Wet sieving; Coupled DEM-SPH method; Particulate solid-liquid flow

Abstract
Wet sieving is commonly used for accelerating the separation of smaller particles from other coarser particulate fractions. While sieving under dry conditions is a well comprehended process, which can be performed in batch or continuous mode, sieving under wet conditions is yet only understood to a limited degree as the underlying physical mechanisms become more complicated.

Modelling of dry sieving can be readily performed using the discrete element method (DEM). Liquid bridge forces should be taken into account when moist particles are considered. However, the coupled analysis of the solid phase (particles) and the liquid phase should be considered in case of wet sieving [1]. By coupling the DEM with appropriate methods of Computational Fluid Dynamics (CFD) like the Smoothed Particle Hydrodynamics (SPH) [2] it gets feasible to account for sieving under wet conditions.

In the present study, numerical simulations of wet sieving using the coupled DEM-SPH method [3] are performed (Fig. 1). For validation purposes, a comparison with simulations derived using Finite Volume Method coupled with DEM is performed. A detailed representation of the sieve is considered on the DEM side. However, a simplified representation of the sieve is used on the SPH side as a consequence of the spatial resolution used to represent the fluid. The effects of operational conditions are investigated by a series of numerical experiments. The velocity field, the particle spatial distribution and the residence time are analyzed. Obtained results form the possible basis to derive process models later on to describe sieving under wet conditions.

References
CFD-DEM model and simulation of fluidization of non-spherical particles in fluidized bed

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Keywords
Non-spherical particle, Super-ellipsoid model, CFD-DEM, Fluidization

Abstract
The fluidization of non-spherical particles is common in some industrial fields such as biomass utilization. It is well known that CFD-DEM (Computational Fluid Dynamics - Discrete Element Method) is a powerful tool for studying the fluidization of particle. However, few researchers have investigated the fluidization of non-spherical particles using CFD-DEM. In this study, a robust and efficient CFD-DEM algorithm is proposed for the fluidization of non-spherical particles, in which the non-spherical particles (including rod-like particles, disk-like particles, tablet particles, and non-spherical particles in other shapes) are described by super-ellipsoid model, multi-super-ellipsoid model, and multi-sphere model. The void fraction of the CFD cell and the drag force between the non-spherical particle and the fluid are calculated by dividing the particle into more than 100 parts to realize the two-way coupling between the non-spherical particles and the fluid more accurately. To validate the prediction accuracy of the CFD-DEM model, the simulation results are then compared with the corresponding experiments. The results demonstrate that the proposed CFD-DEM model has a rather high efficiency and accuracy for modeling the fluidization of non-spherical particles in fluidized bed.
DEM simulation of the coating process of tablets in a pan coater

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Keywords
DEM, Tablet, Super-ellipsoid, Coating, Non-spherical particle

Abstract
Tablet coating is an important unit operation in the pharmaceutical industry. In this study, the tablet coating process is investigated based on the Discrete Element Method (DEM), where the spray droplets are simulated using the Discrete Droplet Method (DDM). The corresponding experiment is performed in a lab-scale pan coater using the ellipsoidal tablets to validate the numerical model. Here, the super-ellipsoid model is adopted to describe the tablets with different shapes (including ellipsoidal tablets, disk-like tablets, bi-convex tablets, etc.), and the accuracy of the model to simulate the coating process is verified. Moreover, the effect of coating time, pan rotational speed, pan tilt, spray angle, spray flow rate and spray droplet diameter size on coating was studied based on DEM simulations. The simulation results show that the coating variability decreases with the increase in coating time, pan rotational speed, pan tilt and atomizing gun’s spray angle, while that increases with the increase in spray rate.
Analysis of Multi-phase Flow in a Packed Bed

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Keywords
XDEM, CFD-DEM coupling, multi-physics, multi-scale

Abstract

Multi-phase flow in packed or moving beds such as trickle bed reactors with either co-current or counter-current flow of gas, liquid and solid phases is apparent in many natural and engineering applications e.g. chemical and petroleum industries. These applications belong to the most challenging flow scenarios including a complex interaction between the individual phases. Flow regimes depend on solid, liquid and gas flow rates in conjunction with physical properties and determine pressure drop, liquid hold-up, pulsing or trickling transitions at low and high temperatures or/and pressures. However, these phenomena are difficult to measure due to sometimes more than hostile operating conditions. Therefore, numerical approaches are a complementary path to follow and to gain a deeper understanding of the underlying physics.

The objective of the current contribution is to present a numerical model that resolves the flow of liquid and gas phases in a packed bed of particulate material. This is achieved with an Euler-Lagrange framework referred to as the extended discrete element method (XDEM). It is an extension to the classical discrete element method and describes additionally the thermodynamic state of individual particles. Particles of a packed bed experience a strong interaction with gas and liquid phases in the void space of a packed bed through heat, mass and momentum transfer. Liquid and gas phases are described by computational fluid dynamics as inter-penetrating and continuous phases. For each phases set of differential conservation equations is solved and thus, allows treating a wide range of engineering applications. In the current contribution, the approach is employed to the lower part of a blast furnace including cohesive zone, dripping zone, dead man and hearth. An analysis of predicted results contribute to an increased knowledge of the phenomena taking place during iron production and thus, aim at controlling and improving the blast furnace process.
Strength properties of cohesive self-gravitating aggregates

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Keywords
Granular Asteroid, Discrete Element Modeling, Scaling Behavior, Strength

Abstract
Recent space missions and observations have established that most of the Near Earth Objects (NEOs) are gravitational aggregates likened to a pile of rubble comprising particles of various sizes (from microns to meters) and irregular shapes, with low, though non-negligible, internal cohesive strength and varying macro-porosity. This has led to the definition of a “Granular Asteroid” and the emergence of a new interdisciplinary field of investigation involving Planetary and Granular Matter scientists. Granular asteroids have large interior voids, which allow them to support large plastic deformations. Their macroscopic behavior and internal structure are still not well known and how to predict their mechanical strength, based on their microstructure and dynamics, is still an open question. However, in view of their discrete nature, it is reasonable to use the theoretical concepts and numerical tools developed for granular media to study them.

In this work, we used three-dimensional contact dynamics simulations, to analyze the strength properties and microstructure of a granular asteroid, modeled as a self-gravitating cohesive granular aggregate composed of spherical particles, and subjected to diametrical compression tests (See Fig.1). By systematically varying the parameters of the system (shear rate, cohesive forces, asteroid diameter), we show that both macro- and microstructures can be described by an extended inertial number that incorporates inter-particle cohesion and gravitational forces, which leads to a generic dependence of the normalized yield strength and microstructure. From a micromechanical description of the contact and force networks (See Fig.2), we propose a model that accounts for solid fraction, local stress, particle connectivity, and granular texture. In the limit of small inertial numbers, we find a very good agreement of the theoretical estimate of compressive strength, evidencing the major role of these structural parameters for the modeled granular asteroids.
Numerical simulation of fracturing behaviour of pre-cracked crystalline rock using a cohesive grain-based distinct element model

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Keywords
Discrete element modelling (DEM), Cohesive grain-based model (CGBM), Crystalline rock

Abstract
Understanding the cracking response of crystalline rocks at mineralogical scale is of great importance during the design procedure of mining structures. A grain-based distinct element model (GBM) is employed to numerically study the cracking response of Barre granite at micro- and macro-scales. The GBM framework is augmented with a proposed distinct element-based cohesive model to reproduce the micro-cracking response of the inter- and intra-grain contacts. The cohesive GBM framework is implemented in PFC2D distinct element codes. The microstructural properties of Barre granite are imported in PFC2D to generate synthetic specimens. The microproperties of the model is calibrated against the laboratory uniaxial compressive and Brazilian split tensile tests. The calibrated model is then used to simulate the fracturing behaviour of pre-cracked Barre granite with different flaw configurations. The numerical results of the proposed model demonstrate a good agreement with the experimental counterparts. The GBM framework proposed thus appears promising for further investigation of the influence of grain microstructure and mineralogical properties on the cracking behaviour of crystalline rocks.
DEM Analysis on Crack Propagation of Rock-Like Material Containing a Single Flaw Under the Coupling Effect of Water Pressure and Uniaxial Compression

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Keywords
Rock-like material; Crack propagation; DEM; Flow network; Internal water pressure

Abstract
For a better understanding of the evolution mechanism of crack propagation in brittle rock mass, the deformation and failure mechanism in rock-like materials (cement mortar specimens) with a pre-existing single flaw applied by jointly uniaxial compression and internal water pressure rising from 1 to 4 MPa is investigated based on the discrete element theory. An improved fluid flow model for low permeability media is proposed and coupled with a bond-based DEM model to simulate crack propagation induced by injecting fluid exerting on internal interfaces of the pre-existing flaw under uniaxial compression by means of modifying the calculation method of interaction between fluid and particle and optimizing parameters in the fluid domain. The results reveal that the occurrence of secondary crack without acting water pressure features instant and a large quantities of micro-cracks with wider than wing crack. Additionally, initiation stress and peak stress witness a slight rise by around 15% in spite of the dramatic decreasing number of micro-cracks with the increasing internal water pressure to effectively release the accumulation of energy between particles in the process of loading, indicating that higher water pressure can significantly promote crack initiation and propagation. While axial stress remains dominant in terms of crack propagation and failure patterns at lower internal water pressures.
Development of an automated mobile DEM calibration unit

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Keywords
Discrete Element Method, Bulk Good, Calibration, Multi-objective Optimisation, Mobile Unit

Abstract

The use of the Discrete Element Method (DEM) for simulating bulk good processes is already an accepted tool in industry. It is used to analyse behaviour of machines, plants and processes all over the world with a great diversity of bulk good materials. But to guarantee valid simulation models, precise and tedious calibration procedures are required. The desired bulk good is usually transported to qualified laboratories and calibration scenarios are undertaken for the respective material. Due to changed conditions between the laboratory and the usage site with e.g. different temperature, humidity or changed material properties caused by transportation, the whole calibration yields to insufficient results. To overcome this concern, we present an automated mobile calibration unit which enables proper calibration on site. The entire unit consist of recent calibration scenarios to determine the corresponding density, static and dynamic angle of repose, the friction values and a validation test bench. All calibration scenarios are embedded into a transportable housing which contains all necessary equipment. The automated mobile DEM calibration unit is equipped with an HMI which leads through the different calibration procedures with instructions and default values. All test scenarios are controlled and observed automatically by an IPC. This shall simplify the complete calibration procedure and ensure an equivalent calibration independent from the operator and its background knowledge. After gathering all important information on site, a multi-objective optimisation algorithm based on recent machine learning algorithms finds the corresponding material properties like Young’s Modulus or coefficient of restitution etc. By ensuring only a small number of simulation runs, the optimisation algorithm finds appropriate physical property values which are later compared with the validation test bench. The novel development of an automated mobile DEM calibration unit combines established calibration scenarios wrapped into a mobile device for determine physical parameters on site and calibration with a suitable optimisation algorithm.
**Discrete element damping models and their contribution in the particles flow**

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**Keywords**

Discrete element, damping models, coefficient of restitution, ice particles, piling

**Abstract**

The Discrete Element Method (DEM) presents a numerical tool widely used for simulation of various particle systems in many technological areas. Proper evaluation of the inter-particle contact model plays a critical role in predicting the behavior of the particle assemblies. In order to increase the simulation accuracy, especially by entering into new application areas, careful reexamination of existing approaches is required.

Presentation concerns dissipative contact behavior of the spherical viscoelastic particles and its contribution to the granular flow. The problem is very complex, and several semi-empirical approaches describing damping in terms of different dashpot constants \(C_d\) are applied in DEM models. The common feature of the existing models is that the energy dissipated during particles contact is used to be evaluated by the non-dimensional parameter, the coefficient of restitution (COR), obtained by impact experiments. Here, a general damping model governed by single non-negative parameter power factor of contact displacement is elaborated. It will be shown that the most popular Lee-Herrmann, Kuwabara-Kono (Brilliantov) and Tsuji damping models are particular cases of universal model. Moreover, new models may be derived in order to fit experimentally observed variation of the COR. The new model is implemented into original DEM code running in GPU environment.

To illustrate the issue of different damping models and the contribution of velocity-dependent effects, the behavior of ice particles exhibiting remarkable sensitivity to impact velocity is demonstrated by numerical solution of multi-particle systems. Series of numerical experiments were performed by considering packing, piling and avalanche flow on the rough inclined plane were performed. Compositions of mono-sizes and bi-dispersed multi-particle systems containing large number up to \(10^6\) particles were considered.
Powder Characterization Flowability at preheating temperature in Additive Manufacturing

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Keywords
Additive Manufacturing; powder flowability; preheating temperature

Abstract
Powder flowability characterization methods are important for powder powder spreading in Additive Manufacturing. These traditional methods for characterizing powder flowability are all designed for a specific condition and have a strong experience which are not suitable for powder flowability characterization in Additive Manufacturing. The temperature has an important effect on powder flowability. Considering the important effect of temperature on powder flowability, the present study aims to powder flowability at preheating temperature in AM. In this work, an experimental platform with a heated rotating drum was built, the camera was used to study the flow pattern of powder in the heated rotating drum. The nylon and 316L stainless steel powder flowability at different temperatures are assessed by the statistical analysis of avalanche angles, median avalanche time, the powder surface fractal and surface linearity, which provides the basis for the characterization method of powder flowability at preheating temperature.
Effect of particle size distribution on compactness of Nylon powder in Additive Manufacturing

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Keywords
Keywords: Additive Manufacturing; DEM; nylon powder; preheating temperature

Abstract
Nylon powder is a commonly used powder material in Additive Manufacturing whose fluidity is closely related to temperature. Exploring powder fluidity at preheating temperature in Additive Manufacturing is the basis for studying the fluidity and spreading properties of powder in selective laser sintering (SLS) process. Choosing nylon powder in SLS technology as a raw material and the flow behavior of nylon powder is studied by Discrete Element Method (DEM), which is a hot topic of numerical simulation and powder spreading process optimization in Additive Manufacturing. Based on Hertz-Mindlin model, Hamaker theory model and Coulomb’s law, Van der Waals and electrostatic force are introduced to describe the contact dynamics of nylon powder at preheating temperature. The DEM model of nylon powder at preheating temperature was established based on the mechanical parameters and the rationality of the model was verified by comparing with the experimental results. The effect of powder gradation on the quality of powder bed will be revealed, and the particle gradation optimization model will be established to improve the quality of powder bed aiming at promoting the technological progress of AM.
The model to simulate interface behavior in the particulate DEM: The particulate interface model

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Keywords
interface, joint model

Abstract
This research proposed an interface model in the particulate discrete element method to simulate the mechanical behavior of an interface. The interface is simple to reproduce qualitatively in the particulate DEM, however, it is hard to simulate quantitatively due to the randomness of particle arrangement. This research investigates what’s happen during interface shearing in the particulate DEM and proposed modifications to develop a new interface model. The simulation results are verified with direct shear test and block sliding test. The former present the performance in quasi-static state and the latter shows the simulation behavior under dynamic condition. The simulation results show the particulate interface model can reasonably reproduce designed interface behavior and is highly agree with the analytical solution. Compared to the ordinary contact and the smooth-joint model, it is obvious that the particulate interface model has a better performance in the validations.
Effects of interparticle friction coefficient on the dynamic shear flow behaviour of granular material in the FT4 Powder Rheometer

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Keywords
Dynamic friction coefficient, Powder rheology, DEM

Abstract
In quasi-static granular flows, inter-particle frictional forces are dominant due to the extensive particle coordination but are less dominant for dynamic, rapid flows, due to increasing bed dilation. However, the coefficients of static and dynamic friction are often assumed to be the same in Discrete Element Modelling (DEM) of granular materials. The macroscopic friction value applied in DEM is routinely obtained by iterative variation until the simulation results mimic experimental data. Although the micro-contact particle characteristics affect the macro-scale response of granular assemblies, there are limited experimental studies to quantify the frictional response for particle-particle and particle-wall micro-contacts, particularly the effect of sliding velocity.

This study focuses on experimentally determining these frictional contact properties for particle-particle and particle-wall contacts for a range of sliding velocities. Micro-mechanical sliding tests are conducted using monolayers of dry spherical glass particles with radii of 63, 125 and 850 μm under constant normal force. The experimental setup is replicated in DEM, albeit using perfectly spherical particles; as such requiring the coefficient of sliding friction to be tailored in DEM to match the experimental shear response. The developed relationship is implemented into a velocity dependent friction model, to simulate the shear response in the FT4 Powder Rheometer under a range of strain rates, spanning the transition from quasi-static to dynamic flow regimes. The predicted torque and force measurements are compared to experimental measurements of the FT4 Powder Rheometer for validation.
36: DEM Simulation of Mechanofusion System

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Keywords Discrete Element Method, Mechanofusion, Particle Dynamics, Stress Analysis, Energy Consumption

Abstract Mechanofusion is a dry coating method for fine powders in the micron and sub-micron particle size range\cite{1}. The bulk powder is compressed against a retaining wall by a high centrifugal force field and is sheared at a high strain rate by a fixed ‘pusharm’, engaging with the bed, thereby further increasing the compressive force, and shearing it. The use of the centrifugal field does not allow the bed to get aerated, and therefore the shearing forces acting on individual particles can be sufficiently high and suitable for dry coating of fine powders by smearing their surfaces with coating powders, flow aids, lubricants and glidants \cite{2}. It could also even alter the physical and chemical characteristics of the surfaces. Its application in pharmaceutical engineering has been explored by Zhou et al. \cite{3} by assessing the extent of coating of fine lactose powders by magnesium stearate (MgST) powder. The use of MgST is ubiquitous in the pharmaceutical industry as it enhances powder flowability and tableting. Therefore the vast range of applications for fine powder processing raises the demand for detailed knowledge of the system dynamics and factors affecting the energy requirements and process efficiency. In this study, the mini-mechanofusion system of Hosokawa Micron is modelled using Discrete Element Method (DEM) at four different operational speeds. Particle dynamics around the pusharm and velocity profiles before the pusharm and at the highest compression zone are analysed. Stresses on the pusharm are also quantified and correlated to the operational speed. The expended energy for this extreme shearing condition is also quantified and correlated to operational speed.

![Figure 1](image1.png)

**Figure 1:** (a) Particle dynamics in Mechanofusion process at 2500rpm, compressive forces on each particle is shown by shade of blue and fixed from 0 to 0.5N; (b) Velocity profiles of four rotational speed at shown 1 to 18 bins.

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Rock failure analysis via DEM-FDM hybrid method during deep tunnel construction in composite formation

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Keywords tunnel excavation, DEM-FDM, composite formation

Abstract With the further exploration of the underground space, the tunnels are developed toward to deeper and longer. However, the complex geological conditions in deep ground, such as the composite formation, will likely bring a series of disaster such as squeezing large deformation and jamming of Tunnel Boring Machine (TBM) in the process of tunnel excavation.

In this study, a hybrid model, which combines Discrete Element Method (DEM) and Finite Difference Method (FDM), is developed to investigate the failure mechanism of tunneling in composite formations. The close and far regions are respectively calculated by DEM and FDM, and the two regions are coupled in each time step to satisfy the compatibility conditions along coupled boundary. A new bond contact model is employed in DEM, which considers the bond width and thickness, as well as the micro-strength envelopes obtained from experiments. The tension-compression strength ratio and rock brittle characteristic can be simulated more properly by this new bond model than the Parallel Bond Model (PBM).

A circular tunnel excavated in composite formation is simulated by hybrid DEM-FDM model. Two types of composite formation are employed, i.e., soft and medium hard rock composition, medium hard and hard rock composition. To investigate the mechanism of rock failure around tunnels, the failure patterns, bond breakage distribution, contact force distribution and deformation patterns are analyzed under conditions of various soft/hard rock combination ratio (Q) and lateral pressure coefficient (K₀).

The result reveals that rock failure all occurs in more soft rock, and the bond breakage number increases with the increase of combination ratio; with the increase of lateral pressure coefficient, the different failure pattern is observed, and the failure zone is smallest in case of K₀ = 1 in soft-medium rock composition cases. Meanwhile, in order to find out the influence of liners on tunnel deformation, the liner with different thickness is installed on tunnel boundary. The liner region is simulated by FDM and coupled with DEM region. The results indicate that both the rock failure and the bond breakage are effectively controlled.
Load distribution within railway ballast: A DEM study considering realistic particle shapes

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Keywords
Railway Ballast, Load Distribution, Polyhedral Particles, Realistic Particle Shapes

Abstract
Railroad constitutes a significant part of the linear transportation infrastructure worldwide, with the majority of regular train tracks lying on ballast layers. To date, ballast is the least understood element of a rail track and its contribution is considered by the engineering practice in a qualitative and conservative manner. In this study, new insights are sought concerning the load distribution within a ballast layer, employing the discrete element method (DEM). In the simulations performed, a sleeper is placed on a ballast layer. Ballast is modelled using polyhedral particles, with shapes based on real grains, so that particle to particle interactions are approximated in a realistic manner. The model is constructed as a 3D plain strain slice of a standard ballasted cross section, bound by periodic boundaries along the longitudinal direction of the rail line. The mechanical characterisation of the material is derived via calibration to available drained triaxial tests on ballast specimens. The DEM results are compared with the load distribution assumed in the British Standards and the level of conservativeness of the latter is now assessed in a quantified manner.
A strength formula for soilbags considering the maximum vertical strain

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Keywords
DEM, Soilbags, Vertical strain, Tensile force, Strength formula

Abstract
Soilbags buried in subgrade can improve the bearing capacity of subgrade and also limit the vertical settlement. In order to explore the relationship between the compressive strength of soilbags and the maximum vertical strain, a strength formula for soilbags that takes the vertical strain into account is derived. A way of modeling flexible bags in DEM simulations is proposed. The soilbag under vertical compression is numerically simulated by DEM to verify the derived strength formula. The results indicate that the derived formula can predict the relationship between the compressive strength of soilbags and the maximum vertical strain, providing a theoretical basis and design methods for the promotion and application of subgrades built with soilbags. The study is also beneficial to the development of the reinforced soil technology.
A combined discrete-finite element method is proposed to simulate the interaction between the pneumatic tire and pebble road, where the spherical discrete element method is used for the pebble particles and the finite element method is used for the pneumatic tire. Then, based on the self-developed software CDFP, the travel performance of the pneumatic tire on pebble road at different slip ratios are simulated. In order to verify the correctness of simulation results, an soil bin test facility was developed. The results show that the simulated sinkage and gross tractive force are basically corresponded with the experimental results, and verify the effectiveness of the proposed discrete-finite element method in studying the interaction between pneumatic tire and granular terrain.
42: Faster, more flexible, particle simulations: The future of MercuryDPM

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Keywords Discrete Element Method; Granular Materials; Open-Source; Simulation

Abstract We focus on the main new developments underway in MercuryDPM. New features include:

- **Deformable clusters (agglomerates)**: Elementary particles are “glued” together, but their relative position is not fixed, making the agglomerate deformable and breakable.
- **Experimental coarse-graining**: Wrappers now exist to analyse data from optical, positron emission particle tracking, and reflective index matched scanning experiments. Allowing a much closer (grid-free) comparison with simulation data.
- **Melting particles**: This is an extension to the previous solid-state sintering model and allows the particles to form melt layers that can interact. On cooling these melt layers solidify potentially forming permanent bonds between the particles.
- **Particle-solid interaction**: MercuryDPM can now be coupled with oomph-lib. One of the new features this allows is surface coupling with FEM walls, i.e, the walls deform in response to the forces exerted on them by the particles.
- **Multi-resolution particle-fluid coupling**: A second feature the coupling with oomph-lib enables is a multi-resolution fluid particle coupling. Meaning it adapts between full, partial and under resolved situations allowing the simulation of particle-fluid coupling with arbitrary large particle size-distributions.
- **Pressure-controlled Lees-Edwards Boundaries**: This new boundary allows the user to specify both a target stress tensor, and a strain rate tensor, at the same time.
- **Better hybrid openMP-MPI parallelisation**
- **STL/STEP readers for reading in industrial geometries**

Some of these new features will be demonstrated for industrial relevant examples: (1) industrial mixers, (2) selective laser sintering, and a (3) tunnel boring machine.

Figure: (left) Industrial mixer with smooth geometric features (centre) melting of additive manufacturing powder (right) Tunnel boring machine and soil simulated with MercuryDPM
Fast, Flexible Particle Simulations: An Introduction to MercuryDPM

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Keywords Discrete Element Method; Granular Materials; Open-Source; Simulation

Abstract We introduce the open-source package MercuryDPM we have been developing over the last few years. MercuryDPM is an object-oriented C++ algorithm with an easy-to-use user interface and a flexible core, allowing developers to quickly add new features. It is parallelised using MPI and is released under the BSD 3-clause license. Its open-source developers’ community has developed many features, including moving and curved walls (polygons, cone sections, helices, screw threads, level-set defined, nurbs, etc); state-of-the-art granular contact models (wet, charged, sintered, cohesive, etc); specialised classes for common geometries (chutes, hoppers, etc); non-spherical particles (multisphere, superquadric and bonded particles) general interfaces (particles/walls/boundaries can all be changed with the same set of commands); restarting; visualisation (xBalls and Paraview); a large self-test suite; extensive Doxygen documentation; and numerous tutorials and demos.

In addition, MercuryDPM has two major components that cannot be found in other DPM packages. Firstly, it uses an advanced contact detection method, the hierarchical grid. This algorithm has a lower complexity than the traditional linked list algorithm for polydispersed flows, which allows for the first time large simulations with wide size distributions, as shown below. Secondly, it uses coarse-graining, a novel way to extract continuum fields from discrete particle systems. Coarse-graining ensures by definition that the resulting continuum fields conserve mass, momentum and energy, a crucial requirement in continuum modelling. The approach is flexible and the latest version can model both bulk and mixtures, boundaries and interfaces, time-dependent, steady and static situations. 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. We illustrate these tools and a selection of other MercuryDPM features via various applications.

Visit http://mercurydpm.org for more information about MercuryDPM; training and consultancy is available via our spin-off company MercuryLab (http://mercurylab.org).

Figure: (left) Contact detection via the hierarchical grid: Large/small particles are in separate grids and cross-checked. (right) For highly polydisperse packings (size-ratio>10:1), a speed-up of 200x is achieved compared to single-grid algorithms.
Large-scale DEM-CFD method for a gas-solid flow in pharmaceutical engineering

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Keywords
Eulerian-Lagrangian method, coarse grain model, fluidized bed

Abstract
Large-scale gas-solid systems, such as fluidized bed, pneumatic conveyors and die-filling are often encountered in pharmaceutical processes. To understand the complex phenomena related to the gas-solid flows, numerical simulation is frequently employed. The DEM-CFD method, where discrete element method (DEM) and computational fluid dynamics (CFD) are coupled, is a standard method for the numerical simulations of gas-solid flow. In previous studies, adequacy of the DEM-CFD method has been validated. Although the DEM-CFD method is established, it has a critical problem from a viewpoint of restriction of calculated particles. In order to overcome this problem, the coarse graining DEM, where a coarse grain particle represents a crowd of original particles, is developed. Accuracy and efficiency of the coarse graining DEM have been revealed in a simple gas-solid flow system. In the present study, the coarse graining DEM is shown to simulate large-scale pharmaceutical gas-solid flow systems. In order to prove the applicability of the coarse graining DEM, the validation tests are performed in typical pharmaceutical processes, such as fluidization with inserted tubes and powder flow into a confined space. The validation results indicate that the macroscopic behavior of particles and gases well agree between the simulation and experimental results. Consequently, we conclude that coarse graining DEM is applicable to simulate large-scale pharmaceutical gas-solid flow systems.
Energy transfer and dispersion relation in granular materials from the perspective of Fourier transform

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Keywords
granular materials, discrete element method; wave propagation

Abstract
In this study, we investigated the dynamic response of granular materials from the perspective of Fourier transform. The frequency components of the stress wave were analyzed. The exponential relationship between particle acceleration (contact force) and the excitation frequency was derived to illustrate the mechanism of the effect of excitation energy on particle contact force. Then according to the average wave velocity in the granular assemblies, the dispersion relation was derived. Finally, by specifying a number of frequency values, the variation of the wave number with the particle microstructure (i.e. the radius ratio) is analyzed. Our research reveals the energy propagation process through the contact between particles within granular materials. Our research results can be a reference for material design using granular materials for energy collection, energy absorbing etc.
Numerical modelling of cone penetration test using Boundary-spheropolygong element method

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Keywords
Boundary-spheropolygong element method, cone penetration, particle breakage, energy-based replaceable particle

Abstract
The two-dimensional boundary-spheropolygong element method (BSEM) is applied for simulating the cone penetration test (CPT). This study aims to investigate the sub-particle stress under the compression of the cone and the effect of particle breakage on the tip resistance. BSEM combines the boundary element method (BEM) and the spheropolygong-based discrete element method (SDEM). The interaction between particles is simulated via the SDEM, and the sub-particle stress is calculated by BEM. In this study, the DEM model is generated with irregular particles using a Voronoi diagram. The breakage of the particles is governed by sub-particles stress and Mohr-Coulomb criterion. The replacing scheme for broken particles uses an innovative energy-based algorithm, which could effectively capture the geometrical features of the broken particle. This scheme also minimizes the change of mass and void ratio after the replacement. The tip resistance is simulated for both breakable and unbreakable DEM model to clarify the influence of the particle fragmentation during the penetration process. The spatial pattern of breakage events and sub-particle stress near the cone are also investigated. The results show a good agreement with existing numerical results. It further reveals the fundamental mechanism for CPT and the induced breakage during the penetration.
Investigating the non-uniqueness of critical solid fraction considering boundary conditions and strain rate effects

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Keywords
strain rate dependency, jamming transition, force chain

Abstract
Jamming is a broad concept that is related to a variety of phenomena in our daily life. It also refers to an important physical phenomenon that distinguishes solid phase from liquid phase, which has been profoundly investigated in recent years. It has been observed in the literature that the critical solid fraction ($\phi_J$) which marks the jamming transition in the jamming diagram is not unique but can be influenced by a number of factors including strain rate and boundary conditions. So far, none of the existing researches have given satisfactory explanations to the physical origin of the non-uniqueness of $\phi_J$. In this study, the non-uniqueness of $\phi_J$ was examined through Discrete Element Method (DEM) simulations. Isotropic compressions at different loading rates were performed on samples composed of frictionless spherical particles bounded by periodic boundaries and rigid-wall boundaries. Specifically, for each boundary condition, samples at a given solid fraction are generated and compressed isotropically at different loading rates until they reach a jammed state. The critical solid fraction (jamming density) is determined based on two critical principles, i.e., the coordination number $Z=4$ and percolation analysis proposed by Bi et al. (2011). The relationships between the confining pressure $P$, the coordination number $Z$, critical solid fraction $\phi_J$ and loading rates are analyzed. The results of different boundary conditions are compared. In the rigid-wall boundary condition, there exists a power law relationship between $\phi_J$ and loading rates. While in the periodic boundary condition, although the $\phi_J$ value varies with loading rates, no clear relationship between $\phi_J$ and strain rate can be observed. Special attentions are paid to the generation process of the major force chain. A new parameter which is defined as the ratio between the number of particles contacting the boundary in the major force chain and the total number of particles in the major force chain is proposed to evaluate the stability of the major force chain. This new parameter can also help explain the difference of the force chain generation processes and strain-rate dependency of $\phi_J$ between the different boundary conditions.
DEM simulation of different types of railway ballast under shear and compression

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Keywords DEM simulation, Railway ballast, Model validation, Particle contact modelling

Abstract For the validation of a DEM model several topics have to be addressed. Particle shape representation, contact modelling and parametrisation using principal experiments are the key influence factors for prediction quality. Regarding the simulation of railway ballast, in the literature there exist many works focussing on particle shape modelling while using simple contact laws, e.g. Cundall’s linear spring model or the simplified Hertz-Mindlin law. This contribution aims to follow a balanced approach. Particle shape modelling is kept simple: clumps composed of two or three spheres will be used. A more advanced contact model, the Conical Damage Model (CDM) [2], is applied, which incorporates additional physical effects, such as edge breakage or yielding. For the parametrisation two different load cases are considered: uniaxial compression tests and direct shear tests. Due to the simple shape representation the resulting DEM model is computationally efficient.

The authors followed the described approach in [3] and [4]. In [3], uniaxial compression tests and direct shear tests taken from literature, [1], were considered. In [4], own uniaxial compression and direct shear tests were conducted for two different types of railway ballast. The experimental results are openly available at zenodo.org (https://doi.org/10.5281/zenodo.1423742).

Thus, the available experimental results cover three different types of railway ballast, at different initial porosities and at different applied stresses. The conducted DEM simulations will be summarised and analysed. In all cases the same behaviour is seen: For the simple clump shapes, combined with the simplified Hertz-Mindlin law, it is not possible to find a set of parameters such that simulation and experiments are in good accordance. On the contrary, when the CDM model is used, the model can be successfully parametrised, such that simulation and experimental data agree well for both compression and direct shear test. From these results the authors conclude that the CDM model seems to be well suited for the simulation of railway ballast.

This contribution concludes with an outlook on future work, regarding DEM model validation.

REFERENCES
A Hybrid approach to include fluid contribution to conductive heat transfer in dense granular systems

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Keywords Granular Heat Transfer, Conduction, Multi-scale, CFD, DEM, Granular Bed

Abstract Heat transfer in a granular medium is an important mechanism in many industrial applications. For some applications conduction is the dominant mode of heat transfer. There are many proposed models to describe particle scale conduction both between particles (particle-particle) and also walls (particle-wall). Within these conduction models are several distinct modes: conduction through physical contact [1], conduction through surface roughness [2], and conduction through the stagnant gas film surrounding each particle often called particle-fluid-particle or particle-fluid-wall conduction [3]. For materials with low thermal conductivity, the gas film conduction through interstitial gases is the dominant mode of heat transfer [4]. While gas film models have been well developed in literature [3,4], the applicability of these models to dense systems is doubtful given that these models are derived from an isolated, binary particle collision. In this work we adopt a multi-scale approach to investigate the contribution of interstitial gases to overall heat transfer in a randomly packed bed using CFD with both the particles and fluid fully resolved in the mesh. Based on the results we propose a new dimensionless variable which we call the proximity number which describes the relative closeness of neighbouring particles within some screening distance. The proximity number is shown to provide a good correlation between the packing structure and the relative contribution of the fluid to the overall heat transfer. When combined with the particle-wall gas film model [4], the proximity number approach is shown to closely match the net heat flux and temporal temperature evolution of the resolved CFD simulations for both adiabatic and heated wall boundary conditions. Using this hybrid approach provides the opportunity to include the fluid effects in a particle based DEM calculation without the need to explicitly include the surrounding fluid thereby reducing the computational effort required to accurately represent these systems. This computational advantage becomes important when dealing with large particulate systems where the particle dynamics dominates the system behaviour and the ability to model the fluid effects without explicitly modelling the fluid phase makes the problems tractable without being computational prohibitive. For the representative packed beds in this study, we show that the computational time is reduced from days for the resolved CFD approach to minutes using the hybrid proximity approach with negligible difference in the predicted net heat flux.

REFERENCES

51: Discrete element simulation of wire-mesh retaining systems: An insight into the mechanical behaviour

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Keywords
wire-mesh, discrete element, soil-structure interaction, anchored flexible facing

Abstract
The use and application of wire-mesh retaining systems have experienced a significant growth in the last decades combining their high resistance capacity with the low environmental and visual impact. However, the design techniques still be very simplified and based on field experience because of the complexities in their modelling and a lack of field performance data about their mechanical behaviour. These structures are classically designed using a limit equilibrium approach under strong assumptions on the system behaviour. The interaction between the mesh and the retained material is poorly schematized and the mesh is often considered as a constant and uniform pressure along the slope.

Advanced numerical methods can help to enhance the understanding of mesh systems permitting the analysis of specific aspects which are non-trivial to measure experimentally. The discrete element method (DEM) has proved to be very efficient in simulating rockfall barriers permitting investigations in large deformation conditions and to handle local ruptures. Recently, the same approach has been extended to wire-mesh retaining systems.

In the present study, the interaction between a mesh system and a granular soil is simulated in order to highlight the potential of a micromechanical approach. The mesh is represented as a connection of distinct cylindrical elements with specific tensile behaviour directly derived from experimental tests. Instead the soil is schematized using spherical particles of different sizes. Representing the mesh as a discontinuous structure, permits to consider a more realistic interaction at the soil-mesh interface. Furthermore, it allows to evaluate the influence of the constraint system and the possible interactions between different mesh elements (e.g. cables, connections, etc.). Another important feature of this approach is the possibility to characterize the mechanism of progressive activation of the mesh response with the displacement of the system.

The final aim of this study is to provide detailed information on the mechanical behaviour of wire-mesh systems which can be used as guidelines in the optimization of the design methodologies.
Overview of GranOO, a versatile opensource DEM code

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Keywords opensource, dem, c++, python, development

Abstract In this presentation, the free and open-source DEM code named "Granular Object Oriented code" (GranOO) will be introduced. GranOO is a robust and versatile workbench able to build 3D dynamic simulations.

The design of GranOO promotes versatility. This is perfectly adapted to conduct non conventional DEM simulations for research activities. In fact, GranOO is not a software. GranOO is a collection of C++ libraries and tools that help users for building a specific DEM simulation. Python bindings have been recently released. This modular architecture helps users to build their own simulations by plugin specific treatments in any order.

GranOO mainly focuses on the simulation of pseudo-continuum brittle elastic media such as concretes, rocks or ceramics. It embeds thermo-mechanical original approaches closed to Lattice Element Model (LEM) based on the cohesive beam model [1] and virial stress computation [2]. In addition, GranOO offers state-of-art detection collision algorithm with arbitrary convex shapes.

Influences of operating parameters on the fluidized bed coal gasification process: A coarse-grained CFD-DEM study

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Keywords
Bubbling fluidized bed; Coal gasification; Back-mixing; Solids mixing; Coarse-grained CFD-DEM

Abstract
A comprehensive coarse-grained computational fluid dynamics and discrete element method (CFD-DEM) is developed for modeling the fluidized bed gasifier. Based on the model validations against experimental measurements, a series of simulations are conducted to investigate the effects of different operating parameters on the coal gasification in a bubbling fluidized bed. This study offers new insights into the effects of gas-solid mixing on the gasification reaction. The results show the non-uniform spatial distributions of the gasification rate in both the horizontal and vertical directions, which reflects the preferential distribution of fuel particles. It is found that the gas back-mixing plays an important role in controlling of the pyrolysis gas combustion, which is undesired for producing gasification products. The results show that the sand particle size has the most remarkable effect on the gas back-mixing. Though the uniformity of the fuel particle distribution is not a key factor influencing the average product yields, the horizontal fuel particle mixing is found to be the main cause of the fluctuations of the gasification rate. Fundamentally, it is demonstrated that the fluctuations of the horizontal fuel mixing are mainly dominated by the bubble behaviors.
A LBM–DEM Coupled Approach for Fast Simulation of Particle-Fluid Two-Phase Flows

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Keywords
LBM, DEM, Discrete particle simulation, Particle-fluid flows, Computational multiphase flow

Abstract
A coupled Lattice Boltzmann Method and Discrete Element Method (LBM–DEM) approach is usually a kind of direct numerical simulation (DNS) algorithms for modelling particle-fluid two-phase flows, in which the size of fluid grid is generally one magnitude smaller than particle diameter and force acting on particles directly calculated by integrating both viscous force and pressure gradient force on the particle surface. However, DNS algorithm is still formidable to simulate the hydrodynamics of an industrial fluidized bed due to huge computational cost. In this work, we present a fast discrete particle simulation algorithm for LBM-DEM modelling of particle-fluid two-phase flows at particle scale. The proposed LBM-DEM coupled approach (the size of fluid grid is one magnitude larger than particle diameter) describes the flow and transport behaviors by the LBM, tracks the motion of particles by the DEM, and utilizes the energy-minimization multi-scale (EMMS) drag for correcting the interaction between gas and solid particles to improve the simulation accuracy. Fast fluidization in a riser is successfully simulated and the results are in good agreement with experimental data. The numerical results show that the proposed LBM-DEM method can be a powerful tool for exploring lab-scale gas-solid systems.
55: **Investigation of dynamic mooring forces and motion responses of moored floating body using MPS-DEM coupling method**

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**Keywords**
MPS; DEM; FSI; moored floating body

**Abstract**

The interaction between the free surface and the moored floating body with restriction of the mooring rope is a typical strongly nonlinear FSI problem. The wave provides the driving force and the mooring rope gives the restrictive condition. In order to simplify the interactions between the wave, the floating body and the rope, hypothesis were usually proposed as the mooring rope was very thin and the mass of which could be neglected. Based on this theory, the interaction between the mooring rope and the wave is ignored no matter the rope is slack or stretched during calculation. However, in reality, the mooring rope is usually made to be heavy to decrease the influence of wave impact and to limit the motion of floating structure.

In this paper, the hypothesis is canceled, and the interactions among the wave, the mooring rope and the floating body are all considered. To solve this complex problem, a fully Lagrangian coupled method has been developed to analyze the motion response of the moored floating body under wave impact. The Moving Particle Semi-implicit (MPS) method has been applied to model the fluid domain, while the Discrete Element Method (DEM) with a parallel bond model is used to represent the floating body and the mooring rope. An FSI model is established by coupling the MPS and DEM method.

A bending cantilever beam case is carried out to validate the DEM model for deformable mass. The results show that the present DEM method can calculate the forces and the deformation of the flexible structure correctly. Furthermore, the dynamic mooring forces and the motion responses of a moored floating body under wave impact are calculated using the coupled method. The motions and deformation of the floating body and the mooring rope are shown in time series, and the influence of different mooring systems on the floating body is discussed.
Application of DEM in geogrid-soil interaction

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Keywords DEM, Geosynthetics, Geogrid–soil interaction, Load transfer, Visualization

Abstract Due to the economic and ecologic advantages of geogrids, this kind of geosynthetic material has been widely used in practice to reinforce various soil structures. Geogrid reinforcing effects are achieved via the interaction of geogrids with the surrounding soil. In order to improve the understanding of geogrid–soil interaction, discrete element modeling was carried out in this study.

In the numerical modeling of unbonded soil particles, a new iterative approach was suggested for the determination of reasonable 2D porosities in DEM studies. In the DEM investigations of geogrids, a piecewise linear model was developed to characterize the nonlinear tensile behavior of geogrids.

Based on the developed models of soil and geogrids, the geogrid–soil interaction was investigated under different experimental loading conditions. In the numerical compound tensile tests, the frictional interaction between one geogrid tensile member and soil was visualized by the force development and soil particle rotations in the specimen. Based on the discrete element modeling of geogrid pullout tests, the bearing resistance achieved by the geogrid transverse members was obtained. The numerically obtained normal stress distribution in the geogrid plane was found to vary with increasing clamp displacement but on average in agreement with the prescribed normal stress. Moreover, the DEM investigation results also illustrated the influences of rigid and flexible top boundaries on the geogrid pullout behavior. In the DEM investigations of biaxial compression tests, the compound stress–strain behavior of geogrid reinforced specimen was significantly improved with increasing number of geogrid longitudinal and transverse members. The geogrid reinforcement mechanisms were visualized by the kinematic behavior and load transfer behavior of unreinforced and reinforced specimens.

Besides the DEM investigations under each single experimental load, the developed DEM models were applied in the numerical modeling of real geogrid reinforced soil structures under combined loading conditions. The geogrid reinforcing effects in such practical loading conditions were visualized by the responses of soil and geogrids.

The DEM simulation results of this study demonstrate that PFC²D can be used as a practical tool to investigate the complex interaction between geogrid and soil. The visualization results provide researchers detailed insights into the geogrid–soil interaction and an improved understanding of geogrid reinforcement mechanisms at a microscopic scale under different loading conditions.
Numerical Investigation of Wire Icing Mechanism Using Particle Method

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Keywords

Wire icing, Heat transfer, Phase change, Moving particle semi-implicit method

Abstract

Wire icing by frozen rain in winter is harmful which would heavily increase the load of wires and even break down the power line and tower. Mechanism study of wire icing using numerical method is helpful to understand the phenomena and find out ways to reduce the hazard. A typical particle-based method, an improved moving particle semi-implicit (MPS) method was proposed to reproduce the process of heat transfer with phase change. The improved MPS method includes a heat transfer model to calculate the liquid/solid temperature field, and a phase transformation model to track the phase interface. The cases of droplet’s impacting on a cold plane surface/cylindrical wire, and the accumulation and solidification of multi-droplets on rigid surface were calculated and investigated. The results are consistent with the numerical and experimental data in previous researches. The validated models and methods were employed to study the mechanism of wire icing, important factors such as the temperature distribution, the solidify position and the layer stacking principle etc. were discussed.
Numerical simulations of shock waves attenuation by granular materials

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Keywords
MP-PIC, five-equation model, shock interaction with granular materials

Abstract
The dynamical behavior of granular media subjected to unsteady pressure loadings is one of the most fundamental problems in the mechanics of multiphase flows. Yet the phenomenon is not fully understood in terms of how the shock attenuation is affected by the compression of solid phase and the gas filtration. Numerical investigations ought to properly account for the momentum and energy transfer between phases. Coupling the five-equation model for the multi-species compressible gases and the MP-PIC model for the particle phase, we numerically investigate the shock propagation through a column of particles. The pressure profiles inside and downstream are obtained to access the attenuation performance of the particle columns consisting of different particle size and packing fraction. The simulations reconstruct the curves of the dynamic compression and the pattern of gas filtration, which are found to have significant influences on the attenuation performance of granular materials.
**A DEM Insight on Manipulating Friction by Rail Sanding**

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**Keywords** Rail Sanding, Particle Characterisation, Tribological Testing, Discrete Element Method

**Abstract** Rail Sanding is a common practice in the railway industry to manipulate the friction at the wheel-rail interface during both braking and traction [1]. Although sanding has been widely accepted as an effective material, in particular for contaminated conditions such as leaf films on the line, there is a lack of understanding on the influence of the sand characteristics.

In this study, a tribological testing method, called High Pressure Torsion (HPT) [2], is modelled using Discrete Element Method (DEM). The HPT method is a means of quantifying the friction between two specimens, in presence of third body materials. In this approach, the torque required to gently twist a specimen in contact with another specimen under a given normal pressure in an annulus is measured. This allows the calculation of shear stresses in the contact and therefore characterisation of the friction. Here, the specimens are made from wheel and rail materials and the third body material is a different type of sand particles.

To systematically study the mechanisms of traction enhancement of sand particles in the rail-wheel interface, a DEM model is developed which allows incorporation of different particle shape and the breakage of particles under loading (see Figure 1). The role of particle morphology, i.e. size and shape, is evaluated and compared with previous experimental studies [3]. Further work will investigate extending the range of particles properties, such as material strength and fracture energy with the ultimate aim of enhancing the current engineering guidelines.

![DEM Simulation of High Pressure Torsion (HPT) test](image)

**Figure 1:** DEM Simulation of High Pressure Torsion (HPT) test, (a) before contact, (b) after contact showing particles fragments.

A Modular and Extensible Software Architecture for Particle Dynamics

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Keywords
Particle Dynamics, Flexible Software Architecture, High Performance, Open Source

Abstract
To create a highly parallel and flexible discrete element software, expertise from different disciplines is needed. On the one hand domain specialists provide interaction models between particles. On the other hand high performance computing specialists optimize the code to achieve good performance on different hardware architectures. In particular, the software must be carefully crafted to achieve good scaling on massively parallel supercomputers. Combining all this in a flexible and extensible, widely usable software is a challenging task.

Here we outline the design decisions and concepts of a newly developed particle dynamics code MESA-PD that is implemented as part of the waLBerla multi-physics framework. Extensibility, flexibility, but also performance and scalability are primary design goals for the new software framework. In particular, our modular architecture is designed such that physical models can be modified and extended by domain scientists without understanding all details of the parallel computing functionality and the underlying complex data structures that are needed to achieve good performance on current supercomputer architectures. The code will soon be released as open source under GPLv3 within the publicly available waLBerla framework (www.walberla.net).

The architecture of MESA-PD is centered around advanced abstractions. For example, new powerful interfaces have been designed to decouple the domain partitioning from the rest of the code. This makes domain partitioning more flexible and allows to support a variety of partitioning schemes that only need to adhere to certain functionality requirements. In particular, they can now be adapted to cooperate with other simulation software in multi-physics scenarios when a coupling between different simulation software is required.

To simplify the task of implementing new particle interaction models we have separated this algorithmic functionality into separate kernels. This way they can be programmed without touching and understanding the rest of the framework. These kernels are connected to the data structures via abstractions which allows to change the data structures without changing the kernels.

As a new software engineering methodology, we also generate parts of the code. In particular, the data structures and communication routines are generated automatically. This allows an easy adaption to the special use case of an application. Also additional data can be appended to the particles and synchronized without much effort.
61: Numerical simulation of powder filling into complex shaped dies using the discrete element method

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Keywords
discrete element method, signed distance function, validation, die filling

Abstract

Die filling is a key process which determines the quality of final products in the pharmaceutical industry. In their manufacturing process, raw powders should be uniformly poured into dies because a non-uniform filling state might cause serious product defects. To achieve an appropriate filling state, it is important to understand the mechanism of powder filling. Since filling state is influenced by die shape, numerical simulation is an effective approach to investigate the mechanism of powder filling. Previous studies have revealed the essential features of powder filling into box-shaped dies. However, these simulation studies were almost limited to simple box-shaped dies rather than complexly shaped dies. Since the simulation of powder filling into complexly shaped dies requires an extremely complex algorithm, the difficult challenge is to investigate the mechanism of powder filling into complex die systems. In this study, the wall boundary model created by the signed distance function (SDF) is applied to the discrete element method (DEM) and the DEM/SDF approach is validated for complex die systems. In the SDF model, wall boundaries are modeled by a scalar field based on the SDF. First, powder flow filling into various shaped die systems is calculated by the DEM/SDF approach. Comparison between the simulation and experiments are also conducted in the validation tests. The macroscopic powder obtained from the DEM/SDF approach qualitatively corresponds to the experimental results. In addition, good agreements are confirmed for the spatial distribution of velocity and the final mass of filling particles in dies. Hence, the DEM/SDF approach is validated in complex die systems. Consequently, the adequacy of the DEM/SDF approach is demonstrated in complex die systems and the DEM/SDF approach is an effective method for particle systems with complex boundary shape like dies.
62: 2.4 billion particles DEM simulation of accretionary prism formation using an iterative dynamic load balancer.

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Keywords DEM, Dynamic load-balancing, accretionary prism, Stress chain, HPC

Abstract A parallel implementation of the Discrete Element Method (DEM) for a large parallel computer system is presented to simulate a sandbox experiment with realistic particle sizes. This numerical sandbox experiment is used to investigate the stress state in the accretionary prisms, which generate large earthquakes such as those occurring in the Nankai Trough. To save memory in the pairwise tangential forces and halve the arithmetic costs, interactions are calculated using the action-reaction law. An iterative load-balancer the flexible 2D orthogonal domain decomposition is applied to manage the load-imbalance in the execution time between MPI procs caused by the Lagrangian nature of DEM. The sub-domains of the MPI procs are iteratively updated within the framework of an iterative non-linear solver [1]. An overlapping communication technique combined with cell-ordering with space-filling curves is also applied to hide the overhead cost because of the MPI communication tasks [2]. The parallel scaling test shows good strong, and weak scalabilities up to 2.4 billion particles on the Earth Simulator and the K computer. We verify our complex parallel implementation of the code with the action-reaction law via a reproducibility test. These algorithms and code development enable us to perform the numerical sandbox experiments with a real-sale sand size which involve the horizontal shortening of a layer of sand (Fig. 1). We found that despite the nearly uniform initial conditions, macro-scale undulations of faults, which are similar to those observed in the trenches of an accretionary prism, appear. To understand the granular mechanism behind these undulations, we performed the large-scale stress chain analysis. The visualization of the stress chains from the large-scale DEM simulation reveals the existence of arcuate stress structures that may control accretionary prism formation, which is an important scientific discovery [3].


Figure 1: Snapshot of the sandbox simulation using 4096 nodes on the K computer.
Optimization of particle separation methods in Lab-on-a-Chip systems with the help of CFD and DEM coupling

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Keywords
particle separation, microfluidics, discrete-continuum coupling, Life Science

Abstract
Particle separation takes a central role in a lot of clinical examinations and analytical processes: such as isolating microorganisms from urine or other body fluids, separating blood components from one another or extracting tumor cells out of blood. With the help of a microfluidic separation device it is possible to reach response level of pathogens by accumulation, before they are analyzed. Therefore, separation is the basis for many significant applications in diagnosis, analysis or sample preparation. Simulation models have been created to examine and improve different passive separation methods by coupling the finite volume method (ANSYS Fluent) and the discrete element method (Rocky DEM./ EDEM). The research is specialized on passive solutions. Thus only forces resulting from the channel geometry, the flow and the characteristics of the particles are used. With the help of forces affecting against each other, depending on the particle properties (size, density etc.) the particle can be moved within the channel cross-section and separated.

One further advantage is that such miniaturized separation chip systems are easily capable of being integrated into the flow chain of any sample preparation and analytical procedure which opens a broad variety of applications in health care, pharmaceutical research and development and related branches.
Characterization of a steady state granular flow patterns of soybeans with various moisture content discharging from a cylindrical silo using three dimensional discrete element method (DEM) simulation

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Keywords
DEM, soybean, moisture content, orifice, silo

Abstract

This study investigated the physical parameters affecting the flow patterns of the soybeans with various moisture content (12 to 60%) at varied orifice size (20, 40, and 60 mm) in the cylindrical silo. The flow conditions to obtain a steady state discharge mass flow rate were evaluated using experiments and DEM simulations. Physical properties of soybeans such as the shape and the size, the mechanical properties, such as Poisson’s ratio and Young’s modulus, the coefficient of restitution, and the coefficient of static and rolling friction were measured and estimated. The moisture absorbed in the soybean dramatically changed all the properties. However, the key parameters to affect the flow patterns of soybeans were determined to be the size, shape, and friction coefficients. The discharge mass flow rate at different moisture content and different size of the orifice provided a critical size of the orifice. In this study, the reduced diameter of the orifice size was evaluated and found that, if \( D_{\text{red}} > 0.56 \), the flow showed a steady state. Based on the MFI, the flow pattern at 40 and 60% of the moisture content at 40 and 60 mm of the orifice size respectively showed funnel flows although these flow conditions were satisfied to maintain a steady flow. The maximum wall pressure during discharging for the funnel flows showed the location of the interlocking phenomena where the stagnant zone begins during discharging. DEM simulation were well predicted the flow patterns of the soybeans with varied moisture contents and orifice size. This study demonstrated that the experiments and the analytical approach with DEM simulation well predicts the flow behavior of the soybean at various moisture contents and it is useful for designing the hopper or the silo for a continuous food processing.
Computational costs of DEM models implemented by using OpenCL on GPU

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Keywords GPGPU computing, OpenCL, performance analysis, discrete element method.

Abstract The discrete element method (DEM) opened new vistas in modelling of materials. Concept of the DEM presents numerical methodology, providing quantitative description of granular media by considering motion and deformation behaviour of individual particles in the frame of Newtonian mechanics. Nowadays DEM is acknowledged to be an effective procedure extended to cohesive powders, fracture, fluidized environments and couplings with different multi-physics. The main disadvantage of the DEM is related to computational capabilities that are limited by a huge number of particles and a short time step required in simulations. Naturally, to solve the industrial-scale problems the massively parallel architecture of GPUs and GPGPU computing are the obvious options for significantly increasing computational capabilities.

The conducted research presents evaluation of computational performance of various DEM models implemented in OpenCL code for GPU and other shared-memory architectures. Linear contact model, Hertz contact model, time history dependent friction model, the external forces, torques and the bonded particle model are considered for quantitative comparison of the computational costs. Contact search is performed by memory saving infinite grid method. The fifth order Gear predictor-corrector algorithm is used for accurate time integration, which requires more than one GPU kernel for implementation. The performance of the developed OpenCL code is evaluated solving applications of gravity packing, hopper discharge and fracture of concrete. The performance measured on NVIDIA® Tesla™ P100 GPU is compared with that attained by running the same OpenCL code on Intel®Xeon™ E5-2630 CPU and Intel®Core™ i7-6700.

Performed analysis reveals that parallel computation of forces on thread per particle basis requires small amount of GPU memory and can be performed very efficiently. Evaluation of the tangential component of the contact force with the time history dependent friction model is very expensive in terms of memory and computing time, because the length of the tangential displacement of each contact between neighbouring particles should be stored for unknown number of time steps. Neighbours of particles change in time, which requires complex handling of contact lists of variable size. Thus, computation of tangential components of the contact force increases computing time up to 38.1% of the time required for DEM model evaluating only the normal contact force. Computation of torques is less expensive and adds up to 3.8% of the execution time of the DEM model evaluating only the normal contact force. As expected, the complex bonded particle model requires the largest amount of computational resources if frequent contact search is required for accuracy reasons. It increases the computing time up to 19.4% of the time required for the DEM model of granular flows, assuming the linear dependency of the computing time on the number of particles. It can be concluded that DEM models, performing operations and storing data on bonds or contacts between neighbouring particles, consume the largest amount of computational resources, because contacts might change in time and require inefficient manipulation of data arrays.
Two scale modeling of granular materials based on micromorphic continuum and discrete particle models

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Keywords
granular materials, micromorphic continuum, discrete particle model, FEM, DEM

Abstract
This study proposes a two scale method for granular materials based on micromorphic continuum in which a material point is viewed as a deformable volume composed of a granular assembly. The boundary value problem is solved by the Finite Element Method (FEM) at the macro scale, and the microscopic behavior of the granular assembly is modeled by the Discrete Element Method (DEM). Meanwhile the macroscopic mechanical responses of granular materials are obtained from the discrete granular assembly, which forms the two scale method modeling (FEM-DEM) for granular materials. In this method, the macroscopic stress is obtained by the average of the particle contact forces, and the boundary conditions for the granular assembly are derived by the macroscopic deformation. Numerical experiments have been conducted to investigate the deformation and failure behaviors of granular materials. The influence of the microscopic parameters for granular assembly on the macroscopic mechanical behaviors of granular materials have been discussed.
Towards a discrete element method to predict the thermo-mechanical behavior and the damage of continuous media during a drying process.

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Keywords DEM, Cohesive elements, Thermo-mechanical behavior, Damage, Drying process

Abstract This contribution is treated in the framework of CUBISM project funded by the European program INTERREG V which aims at developing in-situ pressure and humidity SAW sensors to follow the drying of refractory materials under high temperature and pressure conditions. More specifically, our goal is to model the thermo-mechanical behavior of the piezoelectric SAW substrate under such conditions. For example, in the context of a refractory concrete, the temperature can rise up to more than 400°C and the pressure can locally reach 40 bars. As a result, the sensor substrate material has to be carefully chosen to ensure its proper functioning and its durability. Due to the difficulty to test experimentally a large set of candidate materials with specific microstructures and properties, numerical predictions are envisaged to evaluate their ability to respond to severe operating conditions. Our choice is to consider the DEM which is a promising approach to simulate the multiphysics behavior of continuous media and their damage.

In the present work, our main objective is to develop a DEM-based approach enabling to predict the thermo-mechanical behavior and the damage of tested materials under above-mentioned conditions. For that purpose, we consider MULTICOR3D++ code which is developed in our laboratory to simulate the multiphysics behavior of multi-scale continuous media. Investigations are threefold.

First, we discuss the validity of the cohesive beam element to yield a suitable elastic medium. Typically, cohesive elements are introduced at the scale of the elementary contact between each pair of particles in contact to model a continuous medium. Our choice is to consider the cohesive beam element based on Euler-Bernoulli theory which proved its ability to model suitable crack patterns including in a specific process as the indentation test [1,2]. In a first step, a calibration process is set up to relate the parameters of the beam element to the elastic macroscopic ones. Validation tests are then led using several solicitations and configurations.

Second, a model of linear thermal expansion based on the free dilatation of each beam element is introduced in our numerical model [3]. For comparison purposes, effective coefficients of thermal expansion as well as strain and stress fields are determined and compared to Finite Elements results for several material configurations. Thermal-induced damage is also introduced using two modes of failure : the crack propagation and the interfacial debonding. The first one is modeled using the Removed Discrete Element Failure criterion introduced by André et al. [4] and the second one by the Discrete Damage Zone Model [2].

Finally, we aim at developing a mass transfer model coupled to the heat transfer by conduction. Such an approach will enable us to take into account all effects related to the residual humidity in the substrate. At the current state of our investigations, a model of heat conduction has been introduced and validated in the context of transitory and stationary regimes in homogeneous and heterogenous media. We are currently working on a mass transfer model based on a coupling between Fick’s and Fourier’s laws. This approach will be directly coupled to the mechanical state of the material via a controled shrinkage of each beam element.

REFERENCES
68: On an efficient contact detection algorithm for elliptical and ellipsoidal particles

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Keywords
Ellipsoidal Particles, Contact Detection Algorithm, Efficiency, Stability, Discrete Element Method

Abstract
The talk will focus on the description of a new algorithm to search for contact points between elliptical and ellipsoidal particles. Contact detection between two solid particles is in general a challenging task in the case of non-spherical particles. Efficiently computing the information about the contact point and the normal direction between two particles is crucial when dealing with a very large number of particles in discrete element simulations.

Existing contact detection algorithms for ellipsoidal particles can be categorized into three classes, namely the Intersection methods, the Geometric Potential methods, and the Common Normal methods. The algorithms of the Intersection and Geometric Potential methods reduce to finding the roots of a fourth-order and sixth-order polynomials for 2D and 3D problems, respectively. The Common Normal algorithms involve the solution of a nonlinear system of equations. The computational cost associated with these methods can therefore become non-negligible, especially when simulations involve thousands of particles. In some cases, stability and uniqueness of the solution can also be an issue. Therefore, faster and more robust methods to estimate contact points between ellipsoidal particles could significantly improve the Discrete Element Method.

The present talk will describe a novel approach that relies on the transformation mapping one of the two ellipsoids into a sphere. The derivation follows the common normal concept and leads, for a pair of elliptical or ellipsoidal particles, to solving a system of one or two nonlinear equations, respectively. The problem is also supplemented by an inequality constraint that ensures the uniqueness of the solution. Furthermore, the mapping allows one to construct an effective initial guess to the root of the contact point equation. The performance of the algorithm will be analyzed and illustrated on sequences of randomly generated pairs of elliptical and ellipsoidal particles. In particular, it will be shown that its computational cost is significantly lower than that of existing algorithms, and without a trade-off to its stability.
Modelling of Ballasted Tracks: Discrete–Continuum Approach

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Keywords
Railways, Track, Subgrade, Ballast, Modeling

Abstract
The increasing demand for fast heavy haul services with greater axle loads, as well as high speed commuter trains poses a critical challenge for the stability of tracks built on the problematic ground. The mechanisms of ballast degradation and deformation, the understanding of interaction between discrete ballast aggregates and subgrade media require further insight to improve the existing design guidelines for future high speed commuter and heavier freight trains. This paper presents study on the load-deformation responses the ballasted rail track subjected to cyclic loading using a novel large-scale track process simulation apparatus (TPSA) and a coupled discrete-finite different modelling approaches (coupled DEM-FDM). Experimental studies are carried out to investigate the deformation and degradation responses of ballast subject to cyclic train loading under a given frequency of $f=15$ Hz. A rigorous coupled model between the discrete element method (DEM) and the finite difference method (FDM) is introduced considering the ballast breakage and influences of the subgrade stiffness. In the coupled discrete-continuum method, the ballast layer is modelled by discrete element method and the subgrade domain is modelled by continuum method. Interface elements are introduced to transmit the interacting forces and displacements between the adjoining material media, in which the DEM transfers contact forces to the FDM, and then the FDM transfers displacements (i.e. velocities) back to the DEM. The coupled model is validated by comparing the predicted deformations of ballast with those measured in the laboratory. Contact force distributions, stress contours and corresponding broken bonds (i.e. particle breakage) are captured. This coupled DEM-FDM model is also used to analyse the load-deformation of a fully instrumented track in Singleton, Australia, and the numerical predictions are compared with the field data. These findings are imperative for a more insightful understanding of the micro-mechanical behavior of ballast from the perspective of microstructure characteristics of discrete particle assemblies.
Investigation of particle segregation in tableting process using DEM

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Keywords
Discrete Element Method; Die filling; Segregation;

Abstract
In various pharmaceutical manufacturing processes, a tablet production consists of die filling, compaction and ejection steps. In a rotary tableting machine, the raw materials in the feeder are filled into rotating dies and then are compression molded. During the filling step, raw materials should be uniformly poured in the die to achieve an appropriate filling state for compression molded. Non-uniform filling state in dies is frequently occurred in tablet production, which might decrease production efficiency. To control filling state in dies, therefore, filling mechanism should be well-understood. However, filling mechanism is generally affected by various factors such as the apparatus of filling systems, operation conditions and physical properties of raw materials. There has been still little knowledge about filling mechanism in dies.

Among these parameters, this study focused on the physical properties of raw materials, specially, size distribution of raw powders. The objective of this study was to investigate the effect of size distribution of raw powders on the segregation in the rotary tableting machine. To observe and investigate the segregation during powder filling, powder filling in dies of the rotary tableting machine was calculated by the discrete element method (DEM) simulations. To calculate the behavior of fine particles with wide size distribution, the feeder area in our simulation model was limited to only small area near to dies although the apparatus of the actual feeder in the rotary tableting machine was large and complex because of continuous supply of raw materials. In addition, to simplify the simulation conditions, this study assumed particles had two different sizes although the actual raw materials had a wide distribution. Simulation results showed that the amount of filling particles in dies had a certain variation and the volume fractions in two different size of particles might affect the variation. Experimental filling tests also showed the same trend obtained from simulation results. These results suggested that the variation strongly depended on the particle size distribution of granules.
Yielding transition depends on the driving conditions: A local rheology relation across boundary-driven, gravity-driven, and fluid-driven dense and dilute granular flows

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Keywords
dry granular flows, wet granular flows, yielding transition, kinetic theory

Abstract
Dry, wet, dense, and dilute granular flows have been previously considered fundamentally different and thus described by distinct, and in many cases incompatible, rheologies. We have carried out discrete element method-based simulations of granular flows for a variety of geometries and driving mechanisms, which cover the entire range of the particle-fluid-density ratio, Stokes number, and particle volume fraction [1]: (i) two-dimensional sediment transport driven by a large variety of Newtonian fluids (including oil, water, and air), (ii) rapid gravity-driven flows in ambient static air of varying viscosity, (iii) two-dimensional uniformly sheared viscous suspensions in density-matched fluid of varying viscosity, (iv) two-dimensional dry uniform shear flows, (v) three-dimensional rotating drum flows lubricated by a density-matched fluid, and (vi) a three-dimensional dry rotating drum flow. For all simulated conditions, except for sediment transport and gravity-driven flows close to the flow threshold, we find that the Mohr-Coulomb friction coefficient $\mu$ scales with the square root of the local Péclet number $\sqrt{\text{Pe}} = \dot{\gamma} d / \sqrt{T}$ provided that the particle diameter $d$ exceeds the particle mean free path. Despite the appearance of the granular temperature $T$, this scaling is probably not related to granular kinetic theory as the scaling coefficient depends only on the tangential friction coefficient but not on the normal restitution coefficient (the exact opposite of what kinetic theory predicts [2, 3]). Instead, we believe it originates from a competition between macroscopic shearing (rate $\dot{\gamma}$) and thermal diffusion (rate $\propto \sqrt{T}/d$). With decreasing $\text{Pe}$ and granular temperature gradient $M = d \nabla T / T$, the scaling breaks down as the system becomes increasingly isotropic, allowing the mechanical stabilization of the flow. This leads to a yield condition with a variable yield stress ratio characterized by $M$, which can be much smaller than its value for homogeneous flows.

DEM simulation of particles in a bucket elevator considering the effect of air flow

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Keywords
bucket elevators, discharge trajectory, particle size, DEM, coupled gas

Abstract
Bucket elevator is a frequently-used lifting equipment in bulk cargo handling. It completes the solids’ loading, lifting and discharging processes by dragging buckets with flexible members in a circuit within an enclosed casing. At present, air flow in the elevator caused by the high-speed movement of buckets are often neglected in the most researches of the bucket elevator discharging, as well as its influence on the discharging trajectory of particles. In this paper, a designed TD belt bucket elevator is taken as the research object. Firstly, the air flow distribution in the bucket elevator caused by buckets of 2m/s lifting speed is solved by CFD dynamic mesh simulation. Secondly, the air flow distribution result is transformed into the force information of particles by CFD-DEM one-way coupling. Lastly the discharging trajectory of particles at various scales considering the influence of air flow is depicted in the DEM simulation. The simulation results show that the air flow generated by the buckets’ relatively high-speed movement in the bucket elevator reduces the overall material discharging efficiency, in this research the efficiency declined by 11.31% compared with that neglecting the air flow. The biggest impact is on small size particles ranging from 0.5 mm to 1 mm, with a 10.38% - 40.60% decrease in discharging efficiency. For particles with middle size ranging from 2 mm to 4 mm, the discharging efficiency of particles is declined by 2.48% - 3.55%, while the discharging process of particles with size larger than 8 mm is not significantly affected. By using DEM-CFD one-way coupling, a more accurate discharging state of bucket elevator can be described, which provides a reference for optimizing the design parameters such as the distance between the bucket tips and the casing, and the spatial arrangement of the discharging outlet.
Numerical simulation of particle breakage in a telescopic roller and its structure optimization

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Keywords

telescopic roller, particle breakage, discrete element, bonding model, structural optimization

Abstract

Coal often breaks down during transportation due to impact, collision, friction, etc., resulting in the lump coal turn into small pieces, reducing its economic value. Telescopic rollers are a common mechanism to reduce breakage, but there is a lack of a reliable means to evaluate its effectiveness. Discrete element method which can study both macroscopic flow parameters and individual particle properties is an effective method to simulate bulk material transportation. In this paper, Hertz-Mindlin with bonding contact theory is used for establishing the coal particle breakage model. Based on the energy theory of rock fragmentation, bonding parameters is determined by virtual calibration. According to the influence of the structural parameters which have been studied on the particle flow and the fracture problem, structural optimization suggestions for the telescopic roller system can be proposed. As a result, the optimized telescopic roller system can effectively reduce the fragmentation of the lump coal during the blanking process and reduce the transportation loss.
Coupled CFD-DEM modelling of mechanical consequences of suffusion on granular soils

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Keywords
granular soils, suffusion, DEM, CFD, shear strength, degradation

Abstract
During the effect of severe seepage flow under heavy rainfall, fine particles in granular soils are prone to erode, such as piping and suffusion, posing potential risks of degradation of soils and dysfunction of infrastructures (e.g. foundations, embankments and dikes). This paper presents a macro-micro investigation on suffusion and its mechanical consequences in internally unstable soils using the coupled computational fluid dynamics (CFD) and discrete element method (DEM) method. The progressive loss of fine particles caused by the upward seepage flow is studied. The fines content, volumetric strain and void ratio are monitored to identify the changes of macroscopic states of the soil skeleton. In addition, the microstructural evolution of the heterogeneous distribution of particles, the clogging-unclogging events, the evolution of force chain network are detected during the migration of fine particles. A series of triaxial compression tests are performed to assess the mechanical consequences of suffusion, i.e. the variations of shear strength and the inter-particle contact properties. Parametric studies indicate suffusion could either increase or decrease the shear strength, depending on the fines content, relative density, and hydraulic conditions imposed. The corresponding variations in particle contacts, fabric anisotropy and critical states are elaborated to interpret the changes of different shear strength due to suffusion. The distribution of local porosity is also investigated using a Voronoi tessellation method in the pore scale, to quantify the evolution of void structures. These findings may provide the insight for in-depth understanding of mechanical response of granular soils under suffusion effect, which is of paramount importance in the safety assessment of urban infrastructures under water infiltration.
75: Investigation of different tablet press feed frames using DEM

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Keywords tablet press, feed frame, granular flow, residence time analysis

Abstract Feed frames of pharmaceutical tablet presses are a crucial step in the manufacturing process. They transport the powder from a mixer to a rotating die plate, in which it is compressed to tablets. Feed frames are influencing the tablets mass and homogeneity. A homogeneous distribution of the active pharmaceutical ingredient in the tablets is the most fundamental parameter in the tablet quality. Feed frames are used in batch as well as in continuous processes.

The present work uses the discrete element method (DEM) to simulate three different feed frames operated with different rotational speeds. Free flowing as well as cohesive powders are investigated. Therefore different force models, namely the linear spring dashpot as well as a macro elastic-plastic adhesive model, are applied. These simulations are used for gaining process understanding as well as comparing the behaviour of different materials. The commercial DEM software XPS is used for the simulations. Since the software is GPU-based it allows for simulating particle numbers in the range of many millions.

Analysis focuses on distributions of the residence time and the distance travelled by the particles, as well as on segregation and on the quality of the tablet. The results show the influence of the different parameters on the product quality.
76: Full-scale numerical calculation of ballasted tracks with the Discrete Element Method

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Keywords Geomechanics, Railway ballast, Railway track stability

Abstract Rail transport, both for people and goods, is becoming increasingly significant all over the world, which is reflected in the great growth of conventional and high-speed train lines. Most of these infrastructures are built with railway ballast, a granular material whose main function is to resist vertical and horizontal loads and to face climatic actions.

The growing popularity of these infrastructures has led to the development of numerical models to evaluate their performance. Among a wide range of numerical methods, the Discrete Element Method (DEM) was found to be effective for evaluating the performance of granular materials. This approach considers their discontinuous nature and has proven to be a useful tool to determine the dynamic behaviour of groups of particles. Moreover, the DEM is also used to compute the behaviour of continuum materials. In this work, rails and bearing plates are characterised in the calculations using this methodology, called the bonded DEM [1, 2]. It is a modification of the classical DEM which assumes that bonds exist between particles, resisting their separation.

The code used is developed within DEMPack, a specific software tool for modelling physical problems using the DEM. Currently, DEMPack allows the use of two different types of geometry: spheres with rolling friction and clusters of spheres. A previous analysis showed that spheres are more effective for studying the macroscopic behaviour of the ballast layer, while clusters are necessary for small-scale tests involving highly compacted particles since their results are greatly influenced by particles and contacts distribution.

![Figure 1. Velocity of ballast stones when the train is travelling through the section.](image)

After calibrating the code, full-scale tests were performed applying the load of a high-speed train on a railway track section in different situations. Considering the amount of material (about 130,000 particles) and that the aim is to evaluate the deflection of the rails, the calculations are carried out using spheres.

The numerical results correctly capture the effect on the deflection of the rails. It can be concluded that the DEM increases the possibilities for analysing innovative solutions since real case-scenarios can be studied with enough accuracy and feasible time.

References


77: ADEM Simulation for Compaction Process

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Keywords Advanced Distinct Element Method, Simulation, Powder compaction, deformation

Abstract A new simulation approach using Advanced Distinct Element Method (ADEM) was proposed in order to predict the compaction behavior and the characteristics of the green body. Powder compaction process is widely used in ceramics, food and pharmaceutical industries to produce compacted products. The internal micro structure of green body should be uniform because non-uniform structure causes cracking after compaction or occurrence of coarse defects during sintering. Powders are generally aggregated by granulation or spray drying in order to fill powders uniformly and densely. The structure of green body depends on the rearrangement of powders during compaction, which is caused by the deformation and breakage of aggregates. It is desirable to predict aggregate behavior during compaction and characteristics of green body from aggregate characteristics.

However, the relationship between the characteristics of each aggregate and the compaction behavior has not clarified sufficiently. Although numerical simulation using Distinct Element Method (DEM) is widely used to analyze the compaction behavior of particles, DEM cannot simulate deformation and breakage of aggregates. In this context, the aim of this work is to develop a simulation model for analysis of the aggregate behaviors during compaction process. ADEM, which can analyze deformation and breakage behaviors of aggregates by connecting primary particles with joint springs was used.

Both the experiment using polyvinyl alcohol (PVA) beads aggregates and the simulation using ADEM were performed. Fig.1 shows the aggregates used in the experiment and the simulation. ADEM parameters which represent characteristics of aggregates were determined by fitting to the experimental load-displacement curve of single particle compression test. The validity of the simulation model was checked by the results of the uniaxial test of a particle bed. Fig.2 shows the cross section of the particle bed during compaction in the simulation. It is suggested that when an aggregate breaks down, the fragments fill voids between aggregates, and green body becomes dense.

Fig.1 (a) PVA aggregates for the experiment (b) ADEM aggregates in the simulation

Fig.2 Visualization of breakage behavior
78: Super-quadric Element Based on GPU Parallel and Its Application in a Horizontal Rotating Drum

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Keywords
discrete element method, super-quadric particle, GPU parallel, rotating drum

Abstract
Parallel computing of large-scale discrete element method was developed for spherical particles. However, in natural or industrial applications, the granular systems commonly comprise non-spherical grains. Super-quadric elements based on continuous function representation can be used to describe the geometric shape of irregular particles accurately, and accurately calculate the contact force between elements using the non-linear Newton's method. Considering the complexity of the contact detection between non-spherical particles and the large-scale computational requirements, a CUDA-GPU parallel algorithm is developed for super-quadric elements. Based on the parallel calculation of spherical particles, the rough contact list of the bounding box and the accurate contact list of the Newton’s method are established using the kernel function. Meanwhile, the parallel computing model and the memory access mode are optimized to improve the computational efficiency. To examine the reliability of the parallel algorithm, the flow process of non-spherical particles is simulated by discrete element method and compared with the experimental results. Furthermore, Lacey mixing index is used to explore the effects of particle shapes on the mixing and motion of the granular system in a horizontal rotating drum. The results indicate that the flow regime seems to be primarily determined by the rotating speed, and the influence of the particle shape on the flow regime is of secondary importance. Meanwhile, flow is continuous for spherical particles, while the characteristics of non-particles are mostly intermittent flow.
Keywords
discrete element method, material calibration, complete workflow

Abstract
In the design and optimization of industrial processes handling granular material, numerical simulations with the Discrete Element Method are an established tool. However, on the path from the process to the simulation and back to the result, such as optimized design or improved product quality, simulation engineers encounter various challenges: choice of parameters, definition of boundary conditions or configuration of complex physical models. It is our goal to build general, yet flexible workflows useful to engineers in many application areas.

The bulk behavior of granular materials is governed by particle-scale parameters which can hardly be measured directly. We present a workflow that solves this problem using an optimization approach: Through repeated simulations of small-scale experiments, our novel tool CFDEM(R)dalilama obtains the set of parameters that best reproduces the bulk behavior measured in the experiments. This is demonstrated using experimental data of GranuTools' GranuDrum (rotating drum) and GranuFlow (silo flow) experiments and matching simulations for a metal powder. We further present a showcase of a DEM simulation application using calibrated parameters obtained by our approach.
Geotechnical and environmental engineering with coupled CFD-DEM

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Keywords Coupled CFD-DEM, multiphase flows, geotechnics, environmental engineering

Abstract Many geotechnical processes in the field of hydraulic engineering are strongly influenced by phenomena that take place at interfaces, as for example the interface between soil and water or the interface between air and water in the presence of soil. The visible effects are triggered by actions at a micro-scale, which makes unresolved coupled CFD-DEM the perfect simulation tool for such applications: while DEM can be used to resolve the soil as particles, CFD is applied for the depiction of a single or multiple fluid phases.

The authors present three different application examples:

- The first one deals with the investigation of the two excavation methods grab and suction dredging. A single-fluid-phase coupled solver (cfdemSolverPiso) was used, and the results could directly be compared against experiments. The experiments were conducted at the Institute of Geotechnical Engineering and Construction Management at TUHH.

- In the second one the water-air interface within the soil is considered. In this case a two-fluid phase coupled solver came into application. In this field we selected two topics:
  - First, we investigated on the shape of the interface between water and air that forms within a dam which separates areas with different water levels. This interface is termed phreatic line, and according to the literature it solely depends on the difference of the water levels for homogeneous dams. The simulation results were compared to a relation derived by Casagrande [1] (cf., Fig. 1).
  - The second topic was the investigation of the impact of the water level on the stability of dams. Here we conducted a feasibility study, the outcome is displayed in Fig. 2.

- The same solver is used for the third application case, in which a flume experiment is reproduced numerically: A fixed plate was placed in a steady cross flow and plastic released upstream of the plate. The evolution of the plastic accumulation profiles was recorded under slowly increasing plastic load. Experiment parameters were the flow velocity, draft of the plate (varying the plate Froude number) as well as three different types of plastic particles. The accumulation of oil in front of barriers and parallels to the phenomena of plastic accumulation were reviewed (cf., Fig. 3).

Figure 1. Phreatic line within a dike, comparison between simulation result and analytical solution.

Figure 2. For water level 1 (upper image) the dam remains stable while it fails for the higher water level 2 (lower image).

Figure 3. Example of the accumulation of plastic particles at the barrier.

Dem simulation of flow pattern and pressure distribution in a model grain silo with annular segment attached to the wall

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Keywords
grain silo, flow obstruction, granular flow, load estimation, load asymmetry

Abstract
A study was conducted to numerically simulate the effect of internal inserts in a form of an annular segment attached to the wall of cylindrical container. Series of the DEM simulations were performed with an assembly of 200 000 spherical particles with random uniform distribution of diameters in range 3.74 – 3.84 mm, filling 0.16 m in diameter and 0.48 m high cylindrical container. Obstruction was full or half ring attached to the wall at height to diameter ratio of 0.62 and width of 6 mean particle diameters. Simulations were performed using axial and non-axial (eccentricity ratio of 0.66) placement of discharge gate in a flat bottom.

Development of dead zones at the discharge initiation and their further evolution were analyzed as influenced by the attachment of insert and centricity of discharge gate. Pressure maps in height versus circumferential angle coordinates were generated showing details of pressure distribution in both static and dynamic conditions. With half annular insert attached to the wall commencement of discharge resulted in a ramp up of bending moments to the highest values of 0.65 Nm. This value is slightly higher than 0.6 Nm found in the case of non-axial discharge, thus should be considered dangerous for construction. In static state, distribution of normal pressure is fairly homogeneous, except the narrow zone below the insert, where the wall pressure is lower. At the commencement of discharge, zone of lowered pressure below an insert widens, while in the same time an area of elevated pressure above the insert is formed. This area of increased pressure is reflected on the other side of the silo wall (side without an insert), but is shifted upwards and blurred. This phenomenon results in increased bending moments in simulations with non-symmetric inserts.

Based on performed simulations it has been proposed that dangerous asymmetry of silo wall loads generated by eccentric discharge may be minimized or eliminated by placement of proper insert above the floor.
A primary factor affecting the quality of the product obtained by hot isostatic pressing is the homogeneity of the metal powder in the dies. Since metal powders consist of particles of different shapes and sizes, a desirable goal during filling of dies, therefore, is to achieve homogeneous distribution of the particles as much as possible. Inhomogeneous distribution of the particles can lead to segregation of the particles which in turn results in inhomogeneities of the microstructure, thermomechanical properties, and possibly a final engineering material product of reduced quality. In addition to segregation, another important factor is the presence of “cavities” in the dies that can also influence the quality of the HIP’d product. Therefore, minimization of segregation and reduction of cavities by optimizing the die design are very important. Many factors have been reported in the literature as having an important influence in the quality of the die-filling mixture. These include the powder characteristics (particle size, particle size variation, density, shape, particle surface properties, and initial packing), die features (die shape, location of the funnels for powder feeding, number of funnels/nozzles), and operating conditions (speed, temperature, presence of air, suction). In addition, in industrial settings, the dies used to contain the metallic powder mixtures are often intentionally subjected to a prescribed vibration to try to increase the final density of the mixture, reduce cavities and to improve the overall quality of the finished product. However, vibrations of die containers can result in undesirable segregation of the final powder mixture and may not completely eliminate cavities. In this work, computational simulations using the discrete element method (DEM) are carried out to study the mixing and degrees of segregation of binary mixtures along with the formation of cavities in a stepped cylindrical die subjected to harmonic vertical vibrations. The analyses involved spherical particles of two sizes mixed at different mass proportions. The study provided key insights into the role that vibration parameters such as frequency and amplitude play on the degree of segregation of the final mixture and the size of the cavities. In this presentation, a summary of our findings is presented.
A mixed experimental/numerical Euler-Lagrangian study of pneumatic conveying of biomass particles

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Keywords biomass, pneumatic conveying, DEM, Euler-Lagrange-coupling, pipe bend

Abstract Pneumatic conveying is a familiar method of transporting particulate materials. This process is well understood for usual materials which are free flowing. Biomass often differ from those materials because of their properties such as shape and density and their distributions, their heterogeneous structure (e.g. an inner soft material and an outer hard material) and their adhesive character to name just a few. In general, one may state that biomass often show all possible kinds of material properties because of their natural source. Nevertheless, the usage of biomass is a growing field in the energy sector as well as in the chemical industry, which motivates us to investigate pneumatic conveying of biomass in more detail.

We investigate experimentally the pneumatic conveying of biomass particles (e.g. Miscanthus, straw) in an approx. 25 m long pipe. The pipe has two 90 degrees’ bends, an inner diameter of 100 mm and is completely optical accessible. Our special interest lies on the two phase fluid mechanics close to the bends and on the influence of the very different material properties of the biomass such as density, particles, (deformable) particle shape (characterized by e.g. aspect ratio). In order to quantify the fluid mechanical behavior of such flows we measure and present data for the axial pressure drop, velocity profiles measured through Laser Doppler velocimetry and videos from a High-Speed-Camera (for various flow scenarios).

In order to gain further physical understanding of the fluid mechanics we compare the obtained experimental data with numerical data from our models. Therefor we employ a Euler-Lagrangian setup with a four-way-coupling, which is a well-known method even for pneumatic conveying (see e.g. [1],[2]). The main advantage of this method compared to e.g. multi fluid methods is, that one can directly account for the particle orientation (see e.g. [3]), which will be necessary because of the partially high aspect ratios of the biomass in use. The discrete element method (DEM)-based model for the collision dynamics allows us to present numerical data for different particle models like polyhedron, cluster and simple spheres (the radius given through an equivalent diameter). We compare the influence of the different particle models on pressure drop, local particle and particle velocity distribution and extend our earlier investigation [4].

84: Measuring granular flow properties to calibrate DEM simulations

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Keywords
Simulation calibrations, rotating drum, compaction, GranuDrum, GranuPack

Abstract
Tuning the microscopic parameters (coefficients of friction, coefficients of restitution, cohesive forces, ...) for granular material simulation is a difficult task, in particular when dealing with real powders made of grains having complex characteristics. Moreover, in many simulation techniques, the input parameters are not rigorously linked with physical parameters. Measurements can be performed at the scale of the grains with AFM techniques for example to obtain a microscopic characterization. Even if this bottom-up method makes sense conceptually, it is often practically impossible to use this approach in applications. We propose a top-bottom method based on a macroscopic characterization workflow composed of three measurements: the packing fraction dynamics (GranuPack), the cohesiveness (GranuDrum) and the ability of the powder to create electrostatic charges during a flow (GranuCharge). These measurements are performed in well-known geometries (tubes or rotating drum) and can be easily simulated. Therefore, the experimental results can be compared with the simulations to make a validation of the selected parameters. After a description of the measurement workflow, case studies are presented.
85: Methods for Saving of DEM Simulation Results

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Keywords
Discrete Element Method, Data Saving, Spatio-Temporal Data, Data Compression

Abstract
There are two main challenges related to the saving of DEM simulation results. The first problem is an extremely high volume of generated spatio-temporal data which is caused due to the simulation of large particle collectives. The second problem is the possible information loss. By the conventional saving methods, a constant saving time step is directly specified a priori by the user without exact knowledge of process dynamics. This often leads to the loss of important information especially in the scenes with heterogeneous spatial or temporal dynamics.

In this contribution, an advanced approach for the saving of DEM simulation results is proposed. In order to reduce the volume of saved data, the combination of lossy and lossless compression methods is used. Lossless compression methods are applied for exact data reconstruction for specified time points. These methods are used to compress parts of time-dependent data which are required to restart the simulation process. Contrary to this, application of lossy compression methods leads to loss of data according to the tolerance specified by the user. The top-down time-ratio compression algorithm and DEFLATE compression method are used in the proposed approach as lossy and lossless methods accordingly. For data serialization, Google Protocol Buffers mechanism is used. RAM and HDD caching are performed to provide fast data access and to organize intermediate storage of obtained results.

To estimate the efficiency of the developed approach, the different types of problems like mixing, agglomerate breakage, bunker flow, etc. have been analysed. The results show that the application of the proposed method allows one to significantly reduce the volume of saved data and to avoid the loss of important information.
86: A parallel GPU-based micromechanical simulation model for submerged geotechnical problems

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Keywords
DEM-LBM, GPU parallel computation, offshore foundations, soil resistance to driving

Abstract

Driven steel piles are commonly used as deep foundations for a wide range of engineering structures, particularly in the offshore branch. They are also an interesting example among the broad spectrum of geotechnical applications where the fluid-solid interaction at the pore-scale can play a major role for the macromechanical behaviour of the whole system.

In the context of the geotechnical practice for offshore wind-farm structures, both the industrial design and the actual dimensions of the large piles used as foundations in the seabed are often driven by factors such as the soil resistance to driving (SRD), which are still not well understood and often estimated based on mere empirical correlations or overly simplified one-dimensional models. In particular, the role of the micromechanical effects during the installation process (e.g. local dilatancy or contractancy) and their consequences on the pore pressure levels at the pile-tip and on the effective resistance to driving, are generally either disregarded or at most assumed to be covered by the simplified engineering “black-box” solutions.

Here, we propose a general framework to address such local aspects of a geotechnical application involving fluid-saturated soils while retaining the focus on the micro-scale phenomena. We advocate for an approach that combines the relative simplicity of the Discrete Element Method (DEM) for the solid mechanics with the capabilities of the Lattice Boltzmann Method (LBM) for the fluid dynamics. In this sense, we aim to compile some useful techniques and practical recommendations for an efficient GPU-based implementation of a micromechanical LBM-DEM simulation tool.
87: Numerical Simulation of Brittle Material Breakage with Dilated Polyhedral Discrete Element Method

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Keywords
dilated polyhedron; discrete element method; breakage of brittle materials

Abstract
A bond and fracture model is developed to simulate the fracture and fragmentation with an explicit algorithm in the dilated polyhedral discrete element method (DP-DEM) in this study. The Hertzian model is adopted in the contact model between the dilated polyhedral elements which is generated with the Minkowski sum theory. In the bond model, the bond points are initialized on the corresponding bond face of the interface between elements. The strain between two bonded points is calculated by the division of the distance of these two bonded points and the characteristic length, and thus the stress can be determined according to the elastic matrix. The bond force on each bond point is evaluated by stress and average area that every bond point represents on the bond face. The dynamic relaxation (DR) approach is employed to establish an explicit integration algorithm. A hybrid fracture model, considering the fracture energy and the unified damage, is developed to detect the fracture of the bond point. In the simulation of Brazilian test, parameters in the fracture model are analyzed to study the sensibility of this model.
88: DEM-CFD model for solid-liquid-gas flows with complex wall boundaries

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Keywords
DEM-CFD, Solid-liquid-gas flow, Volume Penalisation, Surface wetting

Abstract

Solid-liquid-gas three-phase flows are encountered in many industrial processes, e.g. stirred tank mixing, wet granulation and powder coating. In such processes, the mixture of particles and fluid is mechanically agitated via complex wall boundaries such as impellers and screws. The resultant flow can be extremely complex due to the particle-wall, fluid-wall, particle-particle and particle-fluid interactions as well as the interfacial interactions such as surface tension and surface wetting. It is of increasing importance to develop numerical models for better understanding of flows and optimisation of processes.

In the present work, a novel meso-scopic DEM-CFD model combined with both the Volume Penalisation (VP) and Immersed Free Surface (IFS) models is developed to take into account the aforementioned complex interactions. Several case studies are performed to show the validity of the model developed.
A DEM simulation of particle interaction in the standing wave acoustic field

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Keywords
particle interaction, standing wave, acoustic field, DEM

Abstract

Acoustic field can be applied to promote the interaction between the fine particles (PM$_{2.5}$) suspended in the flue gas, leading to particle collision and agglomeration, which has potential application for the abatement of PM$_{2.5}$. However, the dynamic behavior of particle interaction in the acoustic field is still not well understood, thereby severely restricting the development of practical acoustic particle agglomeration devices. In this study, a numerical model for interaction between two neighboring particles in the standing wave acoustic field is developed using the Discrete Element Method (DEM). The effects of important particle interaction mechanisms, including orthokinetic interaction, acoustic wake effect and mutual scattering effect, as well as the collision forces are taken into account. The predicted results by the DEM simulation are compared with the experimental data to validate the model. The time required for particle collision as well as the consequences of collision events, such as agglomeration and separation, under different operational parameters (acoustic intensity, frequency, particle properties, etc.) are investigated.
Simulation model of particle nucleus growth in rolling granulation

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Keywords Rolling granulation, Growth stage, Advanced Distinct Element Method, Simulation.

Abstract The rolling granulation method is a method of making raw material powder into granules which are required size by using a binder in a container such as pan-type. In this granulation method, the operation is simple and granules can be obtained in large quantities at relatively low cost. However, since there are many operation factors (rotational speed of the granulator, particle diameter of raw material powder) that have affected the granulation performance, it is difficult to comprehend the relationship between the operation conditions and the physical properties of the granules. Therefore, there is a problem that it takes a lot of time to optimize and scale up. In order to solve these problems, approach for prediction of granulation phenomena is required. In recent years, Distinct Element Method(DEM) is used as one of the approaching.

The mechanism of rolling granulation can be classified into three stages as follows.

(1) Nucleation stage (2) Growth stage (3) Completion stage

In this study, attention was focused on the growth stage of (2) which seems to be the most important for predicting particle size of granules among these three stage. In the growth stage, the particle nucleus is consolidated by rolling and the binder is extruded from the inside of the particle nucleus to the particle surface. After that, it is known that granules grow by adhering to the surrounding drying particles. However, changes over time in particle diameter of granules is not reproduced in DEM. Therefore, we attempted to develop a model in which the particle nucleus grows by involving the surrounding drying particles. On the other hand, it is conceivable that fracture by rolling occur in the growth stage. Therefore, we used Advanced Distinct Element Method (ADEM) which can express the behavior of fracture. The particle nucleus was represented by ADEM particle and drying particles was represented by DEM particles. When drying particles adhere to ADEM particle which assumes particle nucleus, it was set so that the drying particles were incorporated by the particle nucleus. This made it possible to express the process of growing the particles size of granules(Fig.1).

Fig.1 Snapshots of simulation result: growth of granules in time series
A new method for experimental validation of DEM simulation results of poly-dispersed granular flows

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Keywords
DEM, Poly-dispersed, Experimental validation

Abstract
Discrete element method (DEM) has been successfully applied to simulate granular flows in a wide variety of configurations. There are numerous experimentally validated simulations for mono-dispersed systems in the literature. In practice, however, most of the granular systems consist of poly-dispersed assemblies of particles. Few studies have considered the effect of polydispersity, and yet fewer have experimentally validated the results. In this study, a new experimental method is presented to confirm the results of an in-house developed GPU-based DEM solver capable of simulation of poly-dispersed systems. Silo discharge is chosen as the case study in which discharge time, flow pattern and more importantly the outlet composition’s variation with time have been experimentally evaluated and validated with numerical results. The outlet composition, which is the ratio of fine to coarse particles in the exit stream, is an essential measure of segregation within the silo which can be only predicted numerically correctly if the interaction between fine and coarse particles are modeled precisely. Measuring this parameter is not possible with common experimental methods in silo discharge study such as high speed photographing or high-frequency weight measurement of the bed. A new apparatus has been developed which can measure this parameter. This device is a compartmented turning wheel that rotates with a motor. It gathers the outlet of the silo into different compartments. Due to practical limitations, the design and the function of the apparatus are not ideal. The most important non-ideality is varying rotational speed which is consequence of sudden addition of a large mass onto the wheel. Back mixing, distribution of particles with same resident time in different compartments, is another important problem. These non-idealities must be compensated by the mean of some post-processing code so that comparable results are obtained from both experiment and simulation.
93: Evaluating the effect of fine particles in a silo using DEM

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Keywords

DEM, Silo discharge, Bi-dispersed

Abstract

Discharge time is the most critical factor in the design of a silo. It is a function of different parameters including bed geometry, outlet size, and particle size. While discharge time can be regulated by the bottom angle and outlet size of the silo, due to practical limitations, it may not be an option in some cases. On the one hand, while silos with sharp bottom angles provide faster discharge rate, their constructions and setup are costlier. In contrast, flat end or low bottom angle silos are easier and cheaper to be built at the cost of limited discharge rate. On the other hand, regulation of the discharge rate with altering geometry is not applicable for existing silos. Another solution is to add finer particles to the silo which facilitates flow by filling the gaps between main large particles and smoothen the flow of discrete particles. These finer particles are added to the main particles stream during the filling process and will be screened and separated from the outlet stream. The behavior of the silo in the presence of these finer particles must be anticipated by means of numerical simulation as they can both accelerate or decelerate the discharge process depends on their size ratio and fraction to the whole volume of particles. Discrete element method (DEM) is the best option for simulation of such flows as it can effectively predict the complex behaviors of particle mixtures with wide size distribution such as segregation, dead zones, and channeling. The problem with DEM simulation is that the total number of particles become eventually very large after addition of very fine particles which prolongs simulation runtime. To overcome this limitation, an in-house, GPU-based, massively parallelized DEM code is developed which can handle simulation of a large number of particles in an affordable time length.
DEM parameter calibration for a semi-2D hopper-silo in a large design space using discharge paths

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Keywords DEM Calibration, Design Space, Hopper/Silo, discharge performance

Abstract In design of bulk handling equipment for industrial applications the use of DEM to model system behaviour is increasingly used to improve equipment performance. Calibration of these DEM models using experimental data is a necessary step for reliable performance prediction. In many cases a single geometry is used for calibration. This limits its use in prediction of system behaviour for other geometries in the design space.

The objective of this study is to calibrate a DEM model over the entire design space of a hopper-silo. This enables the use of a DEM model to predict the performance of any hopper-silo geometry located in the design space.

Experimental data is obtained from a semi 2D hopper-silo geometry for which the hopper angle $\alpha$ and the size of the discharge opening $W_o$ can be adjusted. The material used in this study is gravel with a $W_o$ of 9mm. Discharge data is obtained through load cell measurements of the experimental setup, and are recorded for hopper angles from 20 to 90 degrees and discharge openings from 50 to 200 mm. The DEM model is calibrated to the discharge paths observed in the experiments including start and stop behaviour. Small outlet diameters and large are included to allow arching due to interlocking or wedging to occur. Furthermore this wide range DoE allows detailed observation of both mass and coreflow patterns.

The DEM model is calibrated aiming to capture the steady state and transient phases of the discharge data. Friction parameters are used to minimise the difference between discharge path in experiments and simulations. The results will show in detail to what extent a single parameter set or a mapping of parameters is capable of predicting the discharge of a silo in the entire design space.

Figure 1 Definition of hopper angle $\alpha$ and discharge opening $W_o$

Figure 2 Discharge data for $\alpha = 20$ deg. and $W_o = 50, 75, 100, 150, 200$
95: Isotropic compaction of highly deformable particles

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Keywords NSCD, FEM/DEM, large deformation, hyper elasticity

Abstract Based on the Non Smooth Contact Dynamics (NSCD) framework [1], we study the behavior of highly deformable particles under isotropic compaction. This method is the extension of the Contact Dynamics approach [2] to the modeling of collection of deformable particles, managed by classical Finite Elements. Particle deformation is managed by an incompressible Neo-Hookean law, while the contacts are handled by a unilateral condition (no regularization) and a dry Coulomb friction law. The transition between rigid to soft particle behavior is nicely captured using the ratio between the Young modulus of the particles (E) and applied pressure (P) on samples composed of 2000 disks (see Fig. 1). The description of the dense granular arrangements is performed in terms of solid fraction, coordination number, contact force distribution, contact orientations as a function of P/E.

Figure 1. Screenshots for samples under a ratio (a) P/E=1.0E-4 (barely deformable) and, (b) P/E=2.5E-1 (highly deformable). The color intensity displays the horizontal component of the right Cauchy-Green strain tensor.


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Keywords
Non-Spherical, Polyhedra, Particle Geometry, Hybrid Parallelisation, Steelmaking, Blast Furnace

Abstract
This paper presents a polyhedral particle discrete element method (DEM) model for the charging of TATA Steel blast furnaces. The blast furnace is responsible for the majority of the energy usage within an integrated steelworks. Flow distribution within the furnace, and therefore its performance, is highly dependent on the distribution of its burden material. The burden materials consist of iron ore pellets, lump ore, sinter, coke, and flux. All of which have a distinctly different shape and size. The non-spherical model is used to investigate how particle shape affects the depositing of material onto the top layer of the furnace’s burden. Polyhedra have been chosen as they best represent the angular and irregular shape of the burden material. Parallelisation is addressed in order to simulate the number of polyhedral particles required for a blast furnace simulation. By implementing both shared and distributed memory parallelisms into the code, it is able to simulate a suitable number of non-spherical particles.
97: Discrete Element Numerical Analysis of Triaxial Unloading Test of Mining Limestone

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Keywords
mining unloading, limestone, triaxial test, discrete element simulation

Abstract
Coal mining causes disturbance and redistribution of original rock stress field in overlying rock strata, which is a typical unloading mechanical process. Unloading rock mass will show different mechanical properties and failure characteristics from conventional loading rock mass. Firstly, conventional triaxial tests of the actual limestone samples are performed. Secondly, a model of the same size PFC³D numerical simulation limestone is established, and the discrete element numerical triaxial test is carried out. The stress-strain curves of the numerical specimen are consistent with those of the triaxial tests in laboratory by adjusting the mesoscopic parameters such as contact modulus, friction coefficient, particle stiffness ratio and normal contact strength. Finally, numerical tests of limestone under different initial confining pressures, different unloading rates and different unloading stress levels are carried out to study the mechanical properties and meso-failure characteristics of limestone under different unloading stress paths. The simulation results show that the peak strength and principal stress difference of limestone increase linearly with the increase of confining pressure. The ultimate bearing strength increases linearly with the increase of the initial confining pressure of the unloading, decreases linearly with the increase of the confining pressure unloading rate, and increases with the increase of the stress level during unloading. The failure characteristics of limestone under unloading conditions are mainly shear-shear composite failure. As the initial confining pressure and unloading rate increase, the penetration of the main crack increases at the peak intensity. With the increase of unloading stress level, the crack distribution at the peak intensity is more discrete, and the limestone damage is more severe.
98: On the shear viscosity of fluid-particle system of elliptical porous particles

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Keywords
rheological properties, multiphase flow, porous structure

Abstract

In view of the significance of non-spherical and permeable particles in fluidized bed reactors in industrial processes, it is essential to understand and quantify the rheological properties of multiphase flow in these processes. Many studies have been conducted to understand the interaction between fluid and solid impermeable particles, which ultimately aim at the development of rheological formulas of complex multiphase flow. However, in practice, porous and permeable particles, such as catalyst and absorbent, are frequently encountered in chemical processes. The porous structure of these particles may affect the interaction between particles and fluid, and thus affects the rheological properties of suspensions. In this study, we investigate the shear viscosity of dilute suspensions containing elliptical porous particles with different axis ratios at low Reynolds number by use of a modified lattice Boltzmann model. Volume-average macroscopic governing equations are used to describe the fluid flow around and inside the elliptical porous particle. The effects of porous structure of elliptical particles with different axis ratios on viscosities and flow field are investigated in detail. Our results demonstrate that the shear viscosity of dilute suspension containing elliptical porous particles increases linearly with solid volume fraction at various permeability for particles with different axis ratios. Moreover, a simple empirical expression is imposed for intrinsic viscosity as a function of permeability.
Keywords Granular avalanche, liquid induced cohesion, rotary drum, Discrete Element Method

Abstract Landslides are devastating geophysical phenomena, resulting in losses of life and financial damages in various mountainous regions. Yet, their flow dynamics and stability are still poorly understood, due to the complex nature of granular flows. In this work, a rotary drum partially filled with wet granular matter is used to produce avalanches and to mimic the flow of landslides. The core objective is to gain more knowledge on the physics behind landslides, by measuring the effect of parameters such as the viscosity and particle size on the avalanche dynamics.

A numerical model, based on the Discrete Element Method (DEM), is used to simulate wet granular avalanches. In this model, contact forces are simulated using the Hertz-Mindlin model [1], with a constant directional torque model to account for rolling resistance. Soulé [2] and Nase [3] models are used to account for capillary and viscous forces between the particles, respectively. In the simulations, the influence of particle size and liquid viscosity on the angle of repose, velocity profile and granular temperature, i.e. the averaged fluctuation in particle velocity, is explored.

It is observed that avalanche amplitude increases with particle size, but appears independent of liquid viscosity, while the avalanche frequency and flow layer velocity decrease with liquid viscosity, as shown in Figure 1. This indicates that particles tend to clump together more as viscosity increases, causing the granular flow to behave as a bulk. Additionally, it is found that the ability of viscous forces to reduce the avalanche frequency decreases with particle size.

Figure 1. Avalanche frequency and flow layer velocity as function of viscosity, for various particle radii. Magenta points indicate dry conditions.

Modeling of the magnetic forces acting on locked particles using DEM and FEM

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Keywords
Discrete Element Method, Finite Element Method, Magnetic Separation, Locked particle;

Abstract
In powder manufacturing, metal impurities such as iron powder should be appropriately removed to protect the quality and safety of the final product. This operation is usually performed by magnetic separation, whose efficiency requires the understanding of the particle behavior in the magnetic field. Whereas numerical simulations were proven effective to describe the behavior of completely liberated particles, they have not shown any satisfying result for locked particles.

The objective of this study was to model the magnetic force acting on locked particles and to highlight the differences between liberated and locked particles. For this purpose, finite element method (FEM) simulations were coupled with discrete element method (DEM) simulations. To simplify the analysis, this study assumed that locked particles were composed of two minerals with different magnetic permeability. The magnetic field analysis by FEM revealed that the magnetic force acting on locked particles depends mostly on their orientation, whereas the magnetic force acting on liberated particles was invariable. The magnetic anisotropy of locked particles was modeled as a function of 3-axis magnetization. In addition, the magnetic field around locked particles was modeled based on superposition of magnetic dipole.

In the simulation, two parameters were investigated, namely fraction of magnetic material in the particle and particle orientation. Simulation results highlighted that both parameters affected the behavior of locked particles. Comparative experiments conducted to support the simulation confirmed qualitatively what observed in the simulation. Furthermore, experimental results highlighted that the liberated particles formed a stable and long magnetic particle chain in the magnetic field, while locked particles formed an unstable and short magnetic particle chain.
101: Particle Dynamic Simulations of Heat Transfer in a Bladed Mixer: Conduction vs. Convection

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Keywords
Heat transfer, bladed mixer, DEM

Abstract
Drying of active pharmaceutical ingredients (APIs) is an important step in the production of pharmaceuticals that controls the moisture content of the drug crystals. Despite its widespread implementation, agitated drying remains a challenging manufacturing step for the pharmaceutical industry. Simultaneous transient changes in heat transfer, mass transfer, and physicochemical properties occur during drying, making it a complicated process to understand and optimize. To this end, in this work we decouple the problem and focus on better understanding the heat transfer component of agitated drying. We make use of the discrete element method (DEM) to examine both heat transfer and flow of granular material in a bladed mixer geometry by varying the thermal conductivity of the particles and the agitation rate. Based on the processing and material conditions, we capture two important modes of heat transfer: conduction and dry granular convection. The first mode involves heat exchange through physical contacts between particles, while the other one describes heat transfer due to movement of particles. We observe that these modes of heat transfer can be expressed via two relevant time scales. The first time scale is a conductive time scale that describes the time needed for a single particle in contact with a heated surface to attain the temperature of said surface. The second time scale is a mixing time scale that defines the rate at which thermal energy is distributed throughout the bulk material. By looking at the relative significance of these competing time scales, we witness and characterize different regimes for heat transfer. Furthermore, we carry out nondimensionalization of the system and obtain an equation that enables predicting heating time for a bed given a conductivity and agitation rate within the range of studied values. Developing such fundamental understanding of heat transfer in a bladed mixer provides an insight into how the performance of agitated filter dryers and their scale-up can be optimized.
LBM-DEM simulation of shear flow-induced erosion of cohesive granular media

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Keywords
LBM, DEM, erosion, cohesive, granular, shear, flow, GPU

Abstract
Quantifying the resistance against erosion of cohesive soils is crucial to prevent the earthen hydraulic structure (e.g. earth-dams, levees and dikes) from erosion induced failures. Several testing devices have been developed during the last decades in order to estimate the soil’s erodibility, i.e. the erosion rate coefficient and the critical fluid shear stress based on the assumption of a linear excess shear-stress erosion law. The most commonly used devices are the Jet Erosion Test (JET) and the Hole Erosion Test (HET). However, to ultimately estimate soils’ erodibility, their interpretations rest on a set of over-simplified assumptions and empirical correlations.

Based on this background, we adapt here a micro-scale simulation approach in order to analyse the erosion phenomena at the scale of a representative elementary volume (REV) of the tested material, aiming to find a link between micro parameters (e.g. the cohesive bond strength, particle diameter) and macro parameters (e.g. the erosion rate coefficient and the critical fluid shear stress). The approach consists in coupling the Lattice Boltzmann Method (LBM) and the Discrete Element Method (DEM) for modeling the fluid phase and the granular materials, respectively. The frictional DEM scheme was extended with specific models for intergranular cohesion and time-dependent subcritical damage.

In practical terms, the fully resolved two-dimensional LBM-DEM code was drastically accelerated using a GPU-based approach and now allows to mimic the overall erosional phenomena at a reasonable computational cost with a reasonable number of particles (thousands to tens of thousands).

The particular configuration of the present study is the erosion of a cohesive granular material stressed at its upper surface by a shear driven (Couette) fluid flow. From the results of a preliminary parametric study, we found that a power law relating the erosion rate to the excess shear stress seems more suitable than a simple linear law to estimate the erodibility of the cohesive material. Furthermore, a comprehensive parametric is now being carried out to clarify the dependence of the erosion rate coefficient and critical fluid shear stress with respect to the cohesive bond strength and particle size.
Implementation of JKR contact model in LIGGGHTS

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²Fulbright University, Ho Chi Minh City, Vietnam

Keywords
JKR model, LIGGGHTS, adhesion, contact force

Abstract
The JKR contact model usually used for auto-adhesive interactions between silt sized particles, was implemented and further developed in the Open Source Software LIGGGHTS for the simulation of a cemented sandstone material. In the first stage of development, the original JKR model has been successfully implemented and verified with theoretical solutions. The computational algorithms and procedures in LIGGGHTS were modified to take into account the calculation of negative overlaps when inter-particle contacts are maintained by the adhesive forces. Contact behavior between two spheres was simulated and the calculated errors between the simulation results and the theoretical solutions less than 2,6e-7%. In general, the errors are higher during contact unloading and at the contact break point. The results show that the total negative overlap depends on the interface energy value $\Gamma$. For higher values of $\Gamma$, the critical overlap values are larger indicating that the connections between particles under tension become stronger. Triaxial tests were simulated using the default Hertz contact model in LIGGGHTS and compared with newly implemented JKR model to demonstrate the effect of contact bonding on the material behavior. In the next stage of development, the contact bond model will be modified such that bonding is formed only once as in the natural intact sandstone and Discrete Element Method model will be coupled with multiphase flow solver using OPEN FOAM for the simulation of oil flows in sandstone reservoir.
Modelling of sintering effects in macro porous structures with discrete element method (DEM)

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Keywords: sintering, macro porous structures, crack formation, ceramics, thermal barrier coatings

Abstract: A novel concept for thermal barrier coatings is based on highly porous structures with three-dimensionally highly-ordered macro pores, also called inverse photonic crystals. In experiments they show crack formation, delamination and opening of the structure after being exposed to 1200 °C, due to sintering effects. However, for an application as a TBC, the material requires to be stable at high temperatures, i.e. maintain its macroscopic photonic and structural properties. A study using discrete element method (DEM) is done to evaluate the structural changes of these 3D macro porous structures according to the temperature.

The used DEM contact model, which is based on previous work from sintering science and has been applied in literature by several authors, describes densification between particles due to sintering effects and thereby the overall behavior of the structure according to initial cracks and delamination.

Simulation case studies show differences in material transport within the structure leading to the formation of defects, e.g. initial cracks on the surface (Fig. 1) and within the structure at the struts. Besides this shrinkage, deformation of pore shapes occur as well as shrinkage of the whole structure in vertical direction. The influence of different parameters like initial relative density or macro pore arrangement is investigated and compared with results of experiments to reach a deeper understanding of the process.

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Projektnummer 192346071 – SFB 986
105: Shear strength of material with size-shape correlated particles

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Keywords Polydispersity, Particle-scale, Particle-shape

Abstract Coarse materials like rock-fill and coarse mine waste must be scalped or scaled for shear strength testing in the laboratory as the size of commercial equipment is not big enough to test the full-scale material. Samples of coarse material prepared for testing differ from their prototypes in the characteristic sizes of the particles and/or the form of the PSD. The representativeness of the shear strength parameter determined in the laboratory on scaled samples is questionable, nevertheless they are typically used for geotechnical design without additional consideration.

The particle shapes in a natural mine waste of colluvial sediments derived from eroded ancient sedimentary rocks from the Pilbara region of Australia was analyzed and a correlation between shape and size was identified. The fragments have a particle shape ranging from slabs to sub-equant blocks with a tendency larger particles to be flatter and platy. Therefore, material scaling for shear strength determinations inevitably alters not only the size of particles and proportion of sizes, but the characteristic shapes of the material particles as it implies substituting larger (slabs) particles by smaller (sub-equant) particles.

Simulations with a Discrete Element Method (DEM) reveal that the changes in the shear strength observed when altering the PSD are not due to the change in particle sizes. Instead, these changes in shear strength result from the variation of the particle shapes induced by the alteration of the PSD. This suggests that particle shape is a higher order factor than particle sizes and PSD shape on the shear strength of granular materials.

In the simulation, the particles were 2D rounded cap rectangles (RCR). Samples with a varied particle size distribution from uniform to very polydispersity were analyzed with and without correlation (Discs case) size/particle elongation. The samples were biaxial sheared and the mechanical behavior compared.

This finding highlights the importance of particle shape quantification in soil classification and its consideration in activities such as sampling, sub-sampling, and scaling of coarse materials for geotechnical testing.

Fig: Close-up views of samples at the end of isotropic compression for different size polydispersity. (a) Discs series. (b) RCRs series. Grey particles represent floating particles (i.e. with 0 or 1 contact).
Three-dimensional DEM method analysis of projectile obliquely impacting into granular media

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Keywords
granular medium, three-dimensional, elastic-plastic, penetration, oblique impact

Abstract
The dynamic process of particle media being impacted is essentially a multi-body collision problem with nonlinear multi-scale phase features. The penetration dynamics of a projectile obliquely impacting a bed comprising of smaller granular particles has been studied in three-dimensions using the elastic-plastic discrete element method. Scaling of the penetration depth and trajectory of projectile are compared with experimental observations for different impact velocities and angles. Drag force experienced by the projectile obeys the generalized force law developed by our group, which is conductive to understanding the drag force in the recent experimental data.
108: Mechanics and statistics of sea ice loads on marine structures - a FEM-DEM study

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Keywords FEM-DEM, ice loads, buckling, force chains, marine structures

Abstract This paper presents our recent research that uses combined finite-discrete element method simulations to study the failure process of sea ice against an inclined structure. The complexity of the deterministic failure process requires the use of statistical methods in the analysis of the output data. The simulations are sensitive to initial conditions, with a similar sensitivity likely applying on ice-structure interaction processes in nature, in which the load measurements always show high scatter. In more detail, the paper focuses on the statistics of the peak ice load values on the structure and on the mechanics behind the peak ice load values.

We first demonstrate that the simulations yield ice load statistics that compare fairly well with those based on full-scale observations. Then we present a fairly simple buckling model that captures the physical phenomena in the simulations: Despite the high scatter in the peak ice load values, the buckling model normalizes the peak load observations. The buckling model, thus, connects the peak ice load observations to force chains, known to have an important role in the ice-structure interaction process, and quantifies the effect of the force chains. Our results demonstrate how discrete element modeling offers a platform for in-depth analysis of very complex engineering problems. We are unaware of any other modeling method, which would yield the findings we present in this paper.

Peak ice load event on an ice-structure interaction simulation: the peak load occurring at an instance with L=132.7 m of ice being pushed against the structure buckles. The buckled configuration with L=132.9 m of pushed ice is also shown in the figure.
Simulation of composite failure under impact loading using discrete element model

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Keywords: Composite, impact, failure, delamination, strain-energy, discrete element

Abstract: Composites are gaining wider use in applications such as aircraft structures, wind turbine blades and armour plating of army tanks which may undergo impact loading. Unlike metals, the failure of composites upon impact is complex due to the heterogeneous nature of the material and phenomena associated with fibre pull-out, ply-fracture and delamination. Furthermore, failure modes vary with impact velocity ranging from barely visible impact damage (BVID) with severe delamination under low velocity to extreme fracture under high velocity [1]. Simulation of these failures in a composite is challenging owing to the dynamic nature of impact loading which makes the problem computationally intensive. In addition, a great amount of modelling detail is required to address the heterogeneity of the composite, interface behaviour, and failure conditions [2,3].

The discrete element method (DEM) can, in general, model material domain discontinuity during failure and inertial effects during impact loads. However, with the conventional pairwise interaction between the discrete elements, it is difficult to model the transversely isotropic behaviour of the composite in three dimensions. We use a novel multibody potential to account for the transversely isotropic properties of the composite. The interaction force is derived from the strain energy. A stress-based failure criterion is employed. Figure 1 shows the failure path of the composite ply reinforced with glass fibres along 45°. Through these simulations, we study the modes and propagation of failure at the various rates of impact loading on a composite.

References:
110: Modelling highly dynamic fragmentation of particles using the bonded-cells method

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Keywords

particle breakage, impact, bonded cell method, dynamic

Abstract

Many industrial granular processes involve desired or undesired fragmentation of grains. However, despite experimental measurements and numerical modelling approaches, the mechanisms of single grain fragmentation and its effects on the behaviour of granular materials are still poorly understood. In this work, we investigate the fracture and fragmentation of a single grain due to a single impact, using three dimensional DEM simulations by means of the Contact Dynamics method. The grains are assumed to be perfectly rigid but modelled as an assembly of glued polyhedral Voronoi cells. The strength of the glue represents the internal cohesion of the grain along normal and tangential directions. The numerical method allows us to calculate the forces and torques at the interface zones between cells. The inter-cell joints can open either in tension (mode 1) or by slippage (mode 2) when the fracture strength is reached and a certain amount of energy is absorbed by the relative fragments movement. A series of simulations for a range of different values of parameters (number of cells, fracture strength, impact velocity) were performed in order to test the energetic aspects of the dynamic fragmentation of grains.
Particle grinding inside rotating drums: method and parametric study

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Keywords
grinding, particle breakage, rotating drums, mills, granular flow

Abstract

Rotating drums are often used in industrial applications in which the main objective is reducing the particle size of the material (i.e. particle breakage). Because of the lack of understanding of the phenomena that take place in such processes, the system parameters are based on empirical laws. Experimentally, it is difficult to measure rheological and mechanical properties under such dynamic conditions. DEM simulations allow one to model the granular flow even under dynamic conditions and to track of the interactions between the particles. Moreover, by means of the Bonded Cell Method, the particle fragmentation can be also taken into account. In this work, we report on the simulations of grinding of granular materials inside rotating drums using Contact Dynamics. A parametric study of the influence of some operational parameters such as rotational velocity and the filling degree was performed for the grinding efficiency, indirectly characterized from the evolution of particle size and specific surface evolution.


113: An Enthalpy Based Discrete Thermal Modelling Framework for Particulate Systems with Phase Change Materials

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Swansea University, Swansea, United Kingdom

Keywords
Phase Change Materials, Enthalpy Based method, Discrete Thermal Modelling

Abstract
Many particulate systems may be subject to phase change when the temperature changes. Such phase change materials (PCM) have been extensively used in many applications, particularly in energy storage in various forms. The current work aims to develop an enthalpy based discrete thermal formulation that can take both thermal conductivity and phase change into consideration. The computational aspect of the formulation will be fully discussed and described. The resulting algorithm is simple and effective.

In addition, the equivalent thermal properties of bulk particle materials with phase change will also be derived based on the combination of a multi-scale modelling scheme and the classic one-phase Stenfan melting problem. The numerical results will be compared with experimental results to validate the development.
Tests and extensions of the mu(I) granular rheology

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Keywords
Granular rheology

Abstract
The last 15 years have seen major progress in the description on how grains flow. The framework of the mu(I) rheology, where the effective friction of the system solely depends on the inertial number of the flow, has proven successful in this modelling. It is now extended in several ways and challenged by non-local effects. Here we precisely report recent extensions of the granular rheology, where other parameters are varied, e.g. grain stiffness, shape or activity, and show how they affect the constitutive laws. We also discuss further tests where the geometry of the system is changed and where the hysteretical behaviour of the flow around arrest is studied.

Related publications

115: Strength and fracture of porous, granular and cellular materials by peridynamic simulations

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Keywords
Peridynamics, Failure, Cemented granular materials, Porous materials, Cellular solids

Abstract
Heterogeneous materials are involved in numerous natural phenomena and industrial applications. Therefore, it is crucial to understand how macroscopic mechanical properties of such materials emerge from underlying micro-structure. To address this topic, numerical simulation approaches are valuable tools, especially when discretization scale is smaller than micro-structure scale. In such a way, the influence of structural parameters can be extensively studied.

Among available numerical methods, bond-based peridynamics is a non-local approach which relies on breakable elastic bonds between distant material points within a neighborhood of finite size. As peridynamics is a nonlocal approach, the influence of local mesh anisotropy on crack patterns is significantly reduced, compared with local approaches like lattice elements method.

In present study, the bond-based peridynamic approach was implemented in 2D and parallelized by message exchange (MPI). The scalability of the calculation tool and the mesh convergence were tested. Finally, three cases are studied: 1) the probability of rupture of porous materials; 2) the evolution of the mechanical properties of a cohesive granular medium for different cementitious matrix contents; 3) the evolution of the damage in various phases of a cellular material as a function of cell wall/interface toughness ratio.
Numerical investigation of highly deformable particle systems

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Keywords
Granular materials, soft particles, finite element method, contact dynamics method

Abstract
Granular materials composed of soft particles which can undergo large deformations are ubiquitous in pharmaceutical, food, cosmetic industries as well as in biological systems. The large deformations of the particles strongly affect the mechanical behavior of the system compared to hard particle granular materials which are more often considered in research on granular materials.

In this work, we investigated and analyzed the rheological behavior of a model system of deformable neo-hookean particles subjected to uniaxial compressions by means of numerical approaches. The effect of both friction and bulk modulus of the particles on the mechanical properties of the systems are clarified, including systems with packing fractions close to 100%.

The simulation [Fig.1] relies on coupling the Finite Element Method and the Contact Dynamic Method, taking into account the high deformability of particles and interactions between them using the software LMGC90 [1].

References

Coupled CFD-DEM modeling of debris flow over erodible natural terrain

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Keywords
Coupled CFD-DEM, debris flow, erodible natural terrain, solid-fluid interaction

Abstract
Debris flow consists of debris solids and interstitial fluids where the interactions between fluids and solids unpin key behavior of the flow, including transportation, impact and deposition. When a debris flow hits and travels over a natural terrain, its flow kinematics and mobility may further be complicated by the mass exchanges between the flow and the channel bed via entrainment and deposition. In this study, we present a unified computational framework to simulate a debris flow over a natural erodible terrain, based on coupled computational fluid dynamics and discrete element method (CFD/DEM). In this approach, we consider a debris flow as a mixture of a continuous viscous fluid phase including fine sediments and a discrete phase consisting of gap-graded frictional particles. In simulating the topology of a natural terrain, erodible channel beds are considered with bonded particles whose mobilization is governed by an erosion criterion. The proposed computational framework enables us to capture the complicated four-way interactions during a typical debris flow among the natural terrain, erodible beds, slurry and debris particles for rigorous modeling of debris flows. The interplays among inter-phase interactions in a debris flow, bed erosion and debris flow mobility, as well as their underlying mechanisms are carefully examined. We further employ the Yu Tung Road debris flow (Hong Kong) as a benchmark case, and compare our numerical predictions with available data and previous studies. We further discuss the capability of coupled CFD-DEM in simulating flexible barriers for debris flow mitigation. The study offers a promising new methodology towards physically based, quantitative modeling and analysis of debris flows for rigorous hazard zone mapping and mitigation.
118: The Development of Coarse Graining Strategies for Large Scale Granular Systems based on a Multi-scale Modelling Approach

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Swansea University, Swansea, United Kingdom

Keywords
Coarse graining, Multi-scale Modelling, Discrete Element Method

Abstract
Huge computational costs associated with discrete element modelling of large scale particle systems have been one of the major factors that hinder the application of DEM to industrial problems. Coarse graining and multi-scale modelling, together with high computing platforms, are promising approaches to achieving such a goal.

In the current coarse graining framework, in addition to the upscaling of particle sizes, interaction laws need to be modified/changed. These are, however, developed often in an ad-hoc manner, leading to different formulations and different solution accuracy and efficiency. One the other hand, the multi-scaling modelling has been an effective approach to representing granular matters as continuous media, in which the equivalent constitutive models of particles are derived so that a continuous based numerical methods, such as Finite Elements, can be employed to more effectively solve large scale particle problems.

This work aims to establish a multi-scale approach based coarse graining framework. In this approach, some basic conditions or principle for developing coarse graining models will be emerged from which different coarse graining can be derived.
Verlet buffer for broad-phase interaction detection in Discrete Element Method

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Keywords
DEM, Collision Detection, broad-phase, Verlet Buffer, HPC

Abstract
The Extended Discrete Element Method (XDEM) is a novel and innovative numerical simulation technique that extends the dynamics of granular materials or particles as described through the classical discrete element method (DEM) by additional properties such as the thermodynamic state, stress/strain for each particle. Such DEM simulations used by industries to set up their experimental processes are complexes and heavy in computation time. Therefore, XDEM is parallelized in MPI/OpenMP in order to be able to process hundreds of millions of particles. One of the most expensive computation parts of a DEM simulation is the collision detection of particles classically divided into two steps: the broad-phase and the narrow-phase. The broad-phase uses simplified bounding volumes to perform an approximated but fast collision detection. It returns a list of particle pairs that could interact. The narrow-phase is applied to the result of the broad-phase and returns the exact list of colliding particles.

In this work, we apply a Verlet buffer method to (X)DEM simulations regardless of which broad-phase algorithm is used. We rely on the fact that such DEM simulations are temporal coherent: the neighborhood only changes slightly from the last time-step to the current time-step. We use an optimization of Verlet list to extend the list of pairs returned by the broad-phase by stretching each particle's bounding volume with an extension range (SKIN) based his own characteristics (size, velocity, ...).

In our method, the number of broad-phase to be skipped is not defined beforehand opposed to what is found in the literature, a condition based on particles displacements to ensure the validity of the broad-phase is checked at every timestep without incurring any additional costs. This guarantees identical results because the broad-phase is performed when any particle moved outside of his SKIN and the narrow-phase is executed at every time-steps anyway.

We evaluate the influence of the Verlet extension range on the performance of the execution in terms of computation time and memory consumption and demonstrate that our method allows to skip a significant number of broad-phase execution (> 95 %) improving running time up to a factor of 5 on more than 580 cores while maintaining a reasonable memory consumption.
120: Modelling and rheology of soft granular materials

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**Keywords** Material point method, Contact dynamics, Soft matter, Granular materials, MPI

**Abstract** Many materials can be described as granular materials composed of soft or ultra-soft grains. Most food products, metal powders, microgels and many suspensions are soft-grain systems. Despite their different mechanisms of deformability, depending on their composition and structure, their common feature is that they can undergo large strains without rupture. As a result, these materials can reach high packing fractions beyond random close packing through both grain rearrangements and grain shape change. Until now, because of the lack of proper numerical and experimental tools, their compaction behavior under stress, volume change behaviour under shear and microstructure have mostly remained unexplored.

In this work, we present a numerical technique to model soft granular materials in which the grains can undergo extensive shape change and large deformations. It combines an implicit formalism of the Material Point Method and the Contact Dynamics method [1-3]. In this framework, the large deformations of individual grains as well as their collective interactions are treated consistently. In order to reduce the computational cost, this method is parallelised using the Message Passing Interface (MPI) strategy. Using this approach, we investigate the uniaxial compaction of 2D packings composed of elastic grains. We consider compressibility rates ranging from fully compressible to incompressible grains. The packing deformation mechanism is a combination of both grain rearrangements and large deformations, and leads to high packing fractions beyond the jamming state. We show that the packing strength declines when the grain compressibility decreases, and the packing can deform considerably. We also investigate the evolution of the connectivity of the grains and grain deformation distributions in the packing.

**REFERENCES**


Extended Kinetic Theory for steady, inhomogeneous shearing of spheres

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\textbf{Keywords} Granular flow, phase interface, rheology, kinetic theory

\textbf{Abstract} Extended Kinetic Theory, a kinetic theory of granular gases in which the roles of velocity correlations, friction and particle stiffness are taken into account, is able to reproduce the results of Discrete Element Method (DEM) simulations of soft and hard spheres in steady, homogeneous shearing flows at volume fractions both less and greater than a critical, above which rate-independent components of the stresses develop (Berzi 2014; Berzi & Vescovi 2015; Berzi & Jenkins 2015). In steady, homogeneous shearing, the boundaries play no role. A striking advantage of kinetic theory over any other proposed model of granular flows is that it permits the derivation of boundary conditions at solid surfaces (Richman 1988; Jenkins 1992; Jenkins & Louge 1997) and phase interfaces (Jenkins & Askari 1991; Pasini & Jenkins 2005), using arguments of statistical mechanics in the energy and momentum balances. Those conditions are required when numerically solving the system of partial differential equations that govern granular flows in realistic geometries. The use of appropriate boundary conditions has permitted EKT to be successfully tested also against discrete numerical simulations of steady, inhomogeneous shearing flows of frictionless spheres between bumpy planes in the absence of gravity (Vescovi et al. 2014); and inclined, gravity-driven, free surface flows of frictional spheres over rigid, bumpy planes, with and without flat, frictional sidewalls (Gollin et al. 2017). In these flows, the solid volume fraction was always less than the critical. Here, we apply EKT to steady, inhomogeneous shearing flows in which the solid volume fraction may exceed the critical value for the development of rate-independent components of the stresses in steady, homogeneous conditions. An example is the steady, gravity-driven, free surface flow of frictional, soft spheres between flat, frictional sidewalls, when a sufficient number of particles is fed to the system. In this case, the flow takes place over an erodible bed in which the particles creep (Komatsu et al. 2001; Richard et al. 2008).

\textbf{References}
Multi-scale modeling of thermo-mechanical responses of granular materials

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Keywords
Multi-scale modeling, granular materials, thermo-mechanical problem, FEM-DEM coupling

Abstract
A hierarchical coupling of the finite element method (FEM) and the discrete element method (DEM) for modeling thermo-mechanical behaviors of granular materials is proposed. The DEM is employed to model the thermo-mechanical behaviors of a representative volume element (RVE, a granular assembly) served as a Gaussian quadrature point shared by two superimposed FEM solutions of two concurrent boundary value problems (BVPs), i.e., heat conduction and mechanical deformation. The two concurrent FEMs exchange information (e.g., temperature change and fabric variation) with one another at each Gaussian quadrature point. The proposed approach is applied to investigating the thermo-mechanical responses of dense and loose granular materials subjected to thermal-cycling-induced quasi-static biaxial cyclic compression.
Second-order concurrent computational homogenization method for saturated granular materials

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Keywords
Saturated granular materials, concurrent computational homogenization method, Generalized Hill lemma.

Abstract

A framework of second-order concurrent computational homogenization method of saturated granular materials is established. The generalized Hill’s lemma for the second-order concurrent computational homogenization method of saturated granular materials is derived. In light of the derived generalized Hill’s lemma the downscaling rule from the macroscopic scale of saturated porous gradient Cosserat continuum to the mesoscopic representative volume element (RVE) scale of saturated porous Cosserat continuum is specified so that the Hill-Mandel energy equivalence condition for the hydro-mechanical process in saturated granular material is ensured. The boundary conditions imposed on the RVE boundary are comprised of downscaled macroscopic strain measures and pore pressure, and constrained fine scale fluctuations of meso-sopic hydro-mechanical variables expressed in terms of periodic boundary conditions. A novel scheme for determining and imposing constrained periodic boundary fluctuations on the RVE of saturated discrete particle assembly is proposed. A staggered DEM/FEM solution scheme is presented and implemented for initial and boundary value problems of coupled non-linear hydro-mechanical analysis at the RVE scale of saturated discrete particle assembly. With volume averages of the DEM/FEM solutions at the RVE scale, the effective stress measures with the elasto-damage-healing-plastic modular tensor for the solid phase, the average pore pressure and Darcy’s velocity with the permeability coefficient tensor for the liquid phase, are determined and upscaled to the high scale of macroscopic saturated porous gradient Cosserat continuum. There is no need to specify the macroscopic phenomenological constitutive relationship and material failure model. A mixed FE is constructed and the corresponding nonlinear FE procedure with the u-p formulation is devised for saturated porous gradient Cosserat continuum at the macro-scale. A FEM-(DEM/FEM) nested solution scheme is devised for implementation of the proposed second-order concurrent computational homogenization method. Numerical examples and results demonstrate capabilities and performances of the proposed method in multi-scale modeling of hydro-mechanical behaviors of saturated granular material.
Effects of elastic layers on the behavior of different types of railway ballast under cyclic loading in a box test: micro-mechanical analysis using DEM

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Keywords DEM, Railway ballast, Elastic layer, Conical damage model (CDM), Settlement

Abstract Ballasted tracks are the commonly used railway track systems. They consist of a framework of rails and sleepers, which are supported on a compacted bed of ballast and sub-ballast that is laid on subgrade. Due to regular loading of the track with trains, the ballast deteriorates and track settles. Elastic layers are increasingly used for improving ballasted tracks. In order to better understand the effects of elastic layers, physical understanding at the ballast particle level is important.

In this study, Discrete Element Method (DEM) is used to investigate the effects of elastic layers on micromechanical behavior of two types of ballast, Kieselkalk and Kalzit. The elastic layers considered are under sleeper pad (USP) at the sleeper/ballast interface and under ballast mat (UBM) at the ballast/bottom interface. In the DEM model, the Conical Damage Model (CDM) is used for particle-particle contact modeling [1, 2]. The CDM model accounts for particle edge breakage, which is an important phenomenon especially at the early stages of a tamping cycle, and thus essential, when investigating the impact of elastic layers in the ballast bed. The calibrated CDM model for the two types of ballast was taken from Suhr et al. [2]. Results from DEM simulations confirm that edge breakage at the sleeper/ballast interface is reduced during cyclic loading when USP were used. On the other hand, higher particle movement throughout the ballast bed was observed when UBM were used1. It was found that both the ballast rearrangement and edge breakage are the responsible mechanisms that effect the (initial) settlement of the sleeper. Microscopic investigations provide important insights into the dominating mechanism(s) responsible for the sleeper settlement. The results are in good (qualitative) agreements with experimental observations from the literature. By considering the edge breakage in the contact model, DEM simulations can aid to gain better insights into the micro-macro phenomena occurring in railway ballast. This can help to improve the track components and track design based on simulation models considering the physical behavior of ballast.

The authors would like to acknowledge the financial support of the COMET K2 – Competence Centers for Excellent Technologies Programme of the Federal Ministry for Transport, Innovation and Technology (bmvi), the Federal Ministry for Digital, Business and Enterprise (bmdw), the Austrian Research Promotion Agency (FFG), the Province of Styria and the Styrian Business Promotion Agency (SFG). Additionally, the authors acknowledge funding of the Austrian Science Fund (FWF) for the projects P 27147-N30: Short- and Long-Term Behaviour of Solid-Like Granular Materials and ORD 85-VO: An Open Data Pilot for the validation of Discrete Element Models.

The authors would furthermore like to express their thanks to their supporting industrial and scientific project partners, namely Getzner Werkstoffe GmbH, ÖBB Infrastruktur AG, SBB Infrastruktur, voestalpine Schienen GmbH, voestalpine VAE GmbH and to the Technische Universität Graz.

References:

1Note that UBM can be useful in reducing ballast fouling, vibration isolation, stiffness adjustment in transition zones and in bridges/tunnels etc., which is not the objective of the present study.
Energy dissipation due to particle size and shape in a sheared granular mixture

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Keywords

Segregation, Particle properties, Rotating Tumbler, Discrete element method

Abstract

We study the energy dissipation in sheared granular mixtures consisting of particles with different sizes and shapes. Specifically, we generated energy dissipation spectra from DEM simulations of binary mixtures of cubical and spherical particles and of large and small particles in a slowly rotating tumbler. Mixtures of spherical particles of varying diameter have a single spectral peak while mixtures of cubical and spherical particle have two broader peaks. We developed an analytic model for these spectra by considering the particles as damped driven oscillators. The functional forms of the driving forces account for the sizes and shapes of the particles.
The mechanism and fracture processes of Baige landslide based on cohesive fracture model in discrete element method and GPU acceleration

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Keywords
Cohesive fracture model (CFM); discrete element method (DEM); GPU acceleration.

Abstract
Understanding the mechanisms of landslide failure and fracture processes is crucial for constraining the hazard chain associated with landslide events. The landslides in the upper reaches of the Jinsha River is intensive, most of which occurred in high mountain gorges. In these areas, the landslides have special characters such as short sliding distance, high sliding speed and a large scale. Using the Baige landslide as a model, this paper reconstructs the three-dimensional failure and fractures development processes during the landslide based on an investigation of the landslide area and the cohesive fracture model (CFM) in the discrete element method (DEM). The study investigates the failure mechanism during the whole process from continuum to dis-continuum of Baige landslide. The CFM gives an insight into the fracture initialization, propagation, and interaction inside the Baige landslide. Because of a large scale of the Baige landslide, GPU acceleration is applied to the simulation.
Evolving conditions in granular matters: from numerical DEM results to constitutive modelling

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Keywords Constitutive relations; phase transition; unsteady shear flows; numerical simulations

Abstract This work focuses on the behaviour of granular systems under shearing, unsteady conditions. We propose a theoretical model, based on the continuum mechanics approach, able to predict granular flows in both quasi-static and dynamic conditions. The capability of a granular assembly to behave like a solid, that is to resist applied stresses without deforming, or to flow like a fluid, depending on the macroscopic characteristics of the system, is introduced in the theory through appropriate constitutive relations. In particular, in the constitutive model, both volume fraction and granular temperature have been chosen as state variables, and the stress tensor is computed as the sum of two contributions: the quasi-static and the collisional one. The former one is determined by using an elasto-viscoplastic model including the critical state concept as a limit steady state, while the latter one is derived from the kinetic theory of granular gases. The evolution of the granular temperature, fundamentally governing the material solid-to-fluid phase transition, is obtained by imposing the kinetic fluctuating energy balance. Moreover, the smooth transition between the two regimes is provided by accounting for the softness of the particles in the two contributions of the stress tensor. Contrary to the non realistic case of rigid particles, very dense flow configurations can be attained only when soft particles are involved. In such conditions, contacts are not instantaneous but take a finite time during which a part of the energy, the elastic potential energy fraction, is stored due to the persistent deformations of the particles.

Whereas several numerical results have been obtained in the literature concerning steady, shearing granular flows, unsteady conditions have been less investigated. In order to test our model under unsteady conditions, we performed DEM numerical simulations of time evolving homogeneous shear flows. We considered an assembly of frictional, deformable spheres, under constant volume conditions. Simulations have been performed by systematically changing both the volume fraction, ranging from very dilute to very dense flows, and the shear rate. The proposed theoretical model is quantitatively compared with the results obtained from the DEM simulations in terms of time evolution of the granular temperature and main components of the stress tensor. Admissible initial conditions are imposed in order to reproduce either an initially static system or a system flowing under stationary conditions. We show that the present model is in very good agreement with the numerical simulations, under both fluid-like and solid-like conditions. In particular, it is able to reproduce different mechanical behaviours, such as purely collisional, visco-elastic or visco-elasto-plastic which derive from different initial and shearing conditions.
128: Application of coarse grain model in a die filling simulation

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Keywords
Coarse grain model, DEM-CFD method, Die filling

Abstract

Various experimental and numerical studies have been performed to demonstrate and measure the flowability of particles in die filling. Numerical simulation of the behavior of small-sized particles acting on drag force in a moving boundary is one of the challenges in the numerical study of die filling process. Small sized and low-density particles are selected for application of pharmaceutical engineering. In this work, the interaction of particle-particle and particle-fluid are taken into account. The discrete element method (DEM), a widely used numerical method in granular flow simulation, is combined with computational fluid dynamics (CFD) to deal with not only complex particle-fluid interaction but also wall-fluid interaction. For the sake of industrial die-filling, large amount of particles is necessary. In the present study, coarse grain model of the DEM is employed to examine the applicability of the large-scale DEM-CFD simulation in die-filling. The coarse grain model represents a group of original particles where total energy agrees between the coarse grain particle and the group of the original particle. In this study, verification tests are performed by comparing it with the original system to examine the applicability of the coarse grain model in a die filling system. The verification results indicate that the coarse grain model can simulate the original system. Consequently, application of the coarse grain model is shown in the die-filling system.
130: DEM simulations of granulation process in 3D rotating drum

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Keywords

granular matter, granulation, capillary bond, Discrete Element Method, rotating drum

Abstract

We study the agglomeration process of wet granular materials in a rotating drum by using 3D DEM simulations. Agglomeration of fine particles is presented in many industrial processes such as powder metallurgy, iron-making industry, food and pharmaceutical industries, as well as in natural processes. Fine granular materials are prepared and mixed in required proportions, compacted into a granularity or tablet and finally sintered to acquire sufficient mechanical strength and toughness needed for subsequent operations. We present a numerical model for the agglomeration of a single granularity in rotating drum [1, 2, 3]. The particles interact through capillary liquid bridges, which are modeled by accounting for the cohesive and viscous forces expressed analytically as a function of different parameters such as the distance between primary particles, liquid volume and viscosity, surface tension and particle sizes. The model also assumes that the liquid is transported by the primary particles modeled as agglomerates of fine particles. We find that this model is able to simulate the granulation of particles in a rotating drum in which a given amount of liquid is homogeneously re-distributed. Our simulations show that the granularity size increases exponentially with the number of drum rotations and in proportion to the amount of liquid in the pendular state. We investigate the effects of process and material parameters such as particle size distribution, mean particle size, friction coefficient between the primary particles and liquid viscosity in each agglomeration process.
Biomass Pellet Breakage: Comparing Bonded Contact Models

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Keywords DEM, Biomass, Breakage Behaviour, Bonded Particle Model, Timoshenko Beam Theory

Abstract Biomass pellets, due to their fragile nature, may fracture during transportation and storage and generate fine particles. Different biomass pellets show different breakage behavior regarding their physical properties. High strength pellets could tolerate higher forces resulting in a less brittle nature. However, the physical properties of biomass pellets have been less considered by the researchers and the breakage behavior is not fully understood yet.

The breakage behaviour and more specifically the stress-strain curves of biomass pellets during compression could be investigated experimentally or numerically. Meanwhile, the Discrete Element Method (DEM) is a proven powerful numerical method for modelling characteristics of (biomass-based) materials. In DEM, to investigate breakage of pellets, a biomass pellet particle can be created by filling the cylindrical shape of a pellet with individual particles that bond together by a suitable contact model. There are multiple contact models available to establish bonding, however since each contact model has its own specifications and parameters, results may vary depending on the contact model.

In this research, the breakage behaviour of individual biomass pellets is investigated using two different DEM contact models; 1) the bonded particle model (BPM), 2) Timoshenko beam theory model. In BPM, the cylindrical bonds between particles can resist normal and tangential movement until the maximum normal or tangential stress is reached. After that point, the bond will break. However, in Timoshenko beam theory, a cylindrical bond connects every two neighbouring particles where the bonded particles can resist compressive, tensile, and shear forces at two ends as well as bending and twisting moments up to a maximum value after which the bond will break.

Different particle packings with a various number of spheres were used in this study. Each pellet is subjected to a uniaxial compression test, Brazilian tensile test, and a 4-point bending test where the models' predictions of macroscopic properties of pellets are compared to those of the experimental results. The macroscopic properties include maximum stress at failure, strain at failure, and the bulk modulus of elasticity. The results show that both models reasonably predict the maximum stress values, however, the Timoshenko beam theory model can predict better the module of elasticity and the strain values. Therefore, the Timoshenko beam theory is recommended for further investigating the breakage behaviour of biomass pellets.
132: Numerical modeling of wet agglomerates

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Keywords
granular matter, agglomerate, Discrete Element Method, plastic strength, diametrical compression

Abstract

We study the effects of material parameters on the plastic properties and texture of wet agglomerates composed of solid particles by using molecular dynamics simulations under diametrical compression. The numerical algorithm with a capillary cohesion law in which the cohesion force is an explicit function of the gap between particles and liquid-vapor surface tension [1], and the binding liquid content is mainly accounted for a rupture distance \( d_{\text{rupt}} \) with the binding liquid assumed to be distributed homogeneously inside wet agglomerates [2, 3]. We present the method and analyze the behavior and evolution of the microstructure during diametrical compression. We find that due to the rearrangement of wet primary particles during compression, the granule shows a ductile behaviour. The compressive strength of wet agglomerates reaches a plateau before failure due to the irreversible loss of wet contacts between primary particles.
Abstract

Discrete Element Method (DEM) is a well-established and validated tool for the simulation of bulk materials. However, a lot of questions still need answering in the domain of cohesion and adhesion. Cohesive materials display a wide range of distinct and elusive properties which contribute towards their reduced flowability.

The JKR model is one of the most widely used models in this realm which takes into account surface energy density and increased particle overlap to explain cohesion. The ambiguity associated with surface energy or interfacial energy is tackled in this work by developing thorough calibration procedures which will help in fine tuning these parameters. One of the limitations of DEM is the usage of reduced Young’s Modulus to capture collision time scales for a stable simulation in manageable computational times. Reducing the Young’s Modulus in a cohesive JKR simulation usually leads to unrealistic overlaps which can be mitigated by also reducing the surface energy density.

In recent years systematic parameter calibration and validation endeavors have quite successfully tried to answer those questions on a macroscopic level. This work focuses on an analytically driven calibration protocol using draw down and angle of repose tests which can be classified as uniaxial low consolidation tests. Hence, complications due to high compaction stresses can be neglected. Cohesive DEM parameters will be calibrated using a combination set of friction coefficients, Young’s Modulus and surface energy density. The calibration protocol also aids in deciding to which extent these parameters can be reduced in order to get good agreement between simulation and experiment. Further investigations will be carried out to assess the effect of cohesion and adhesion on rolling resistance. The JKR model is used during the exercise due to its robustness, manageable computational times and a relatively wide area of application. The presented calibration procedure will allow to narrow down on a unique set of parameters for different materials.
A numerical investigation of the effect of particle shape on the friction angle at critical state

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Keywords
DEM, particle shape, railway ballast, numerical modelling

Abstract
The behaviour of a granular material depends on the shape, material properties and packing of the grains. Starting with a particle characterization, the ability to make predictions of the macroscopic behaviour of an assembly of particles without recourse to laboratory or numerical experiments would be very useful. With this ultimate goal in mind, this work is a detailed investigation of the effects on macroscopic behaviour of two key measures of particle shape: form and angularity. The form of a particle can be quantified using the Longest (L), Intermediate (I) and Shortest (S) dimensions of an equivalent scalene ellipsoid; A sum of the local volumetric deviations from the that ellipsoid as a ratio of the ellipsoid volume gives a measure of angularity.

Discrete element, periodic cell simulations of ellipsoidal and realistic particle shapes sampled from railway ballast are used to investigate mechanical behaviour in terms of void ratio and critical state friction angle. Characterization of the observed behaviour in terms of a single shape parameter is explored. It is found that deviation of particle form from that of a sphere together with increases in angularity both lead to higher angles of friction at critical state. It is argued that, to some extent, the higher critical state strength exhibited by non-spherical particles is due to form suppressing particle rotation and leading to increased interparticle sliding, a mechanism that in comparison requires more energy.
135: DEM-LBM Approach for the Simulation of Dense Granular Suspensions

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Keywords
Lattice Boltzmann Method, Discrete Element Modeling, Granular Suspensions

Abstract
Numerical simulations of dense suspensions with a high resolution of the liquid phase (below the particles scale) requires two-way coupling of particle dynamics with stepwise resolution of Navier-Stokes equations for the fluid phase. The Lattice Boltzmann Method (LBM) provides a versatile approach, which has shown its high robustness for the simulation of simple situations such as the free fall of a particle inside a fluid and for the calculation of the permeability of a packing of fixes particles [1,2]. We show here how LBM can be coupled with DEM and parametrised for the simulations of suspensions with several thousands of particles. In particular, we show the differences between the MRT and BGK models for the collision term. Then, we briefly present a parametric study of the effects of fluid properties (viscosity, density), particle properties (size, density) and boundary conditions (shear rate, confining pressure) in immersed flows. We show that our results, in terms of effective viscosities of the flow, are in excellent agreement with reported experiments in literature [3].

Exploring Discrete Element Modeling through Non-Convex Chained Polyhedral Shaped Particles

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Keywords
Modelling, particle shape, non convex particle, granular media, GPU

Abstract The Discrete Element Method (DEM) has recently been extended to a number of new applications and larger scale studies, in particular due to the computing power of the Graphic Process Units (GPUs). However, a number of applications has remained elusive often due to the limited shape representation of particles in conventional discrete element environments. For example, Yan et al. [1] considered a two-dimensional DEM using disc shaped particles, while Yang et al. [2] incorporated elastic-plastic material models into a three-dimensional DEM model using spherical particles. Often these models need to capture the lack of proper shape representation, which may lead to poor generalization of the models. In this study we explore whether there is potential to utilize non-convex chained/linked particles [4]. The capability to model angular chained/linked non-convex particles is currently limited the BlazeDEM3D-GPU framework [3, 5]. In addition, BlazeDEM3D-GPU can simulate a single DEM run on multiple GPUs, which allows for thousands of chained particles to be modelled.

References
137: Adapting and validating a breakage model to discrete elements using polyhedral particles

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Keywords
Discrete element method, particle breakage, comminution, Rocky DEM

Abstract
In several particulate systems that are object of simulation using the Discrete Element Method (DEM) breakage of particles can occur. The extent of this breakage can be significant, such as in crushers and mills, which are meant to do exactly that; or not so significant, such as when particles are subjected to handling, mixing, compaction and separation operations, where breakage is not desired. In all these cases, however, conducting DEM simulations without accounting for breakage can lead to biased results, and sometimes even useless ones.

The description of breakage in DEM is still limited and very computationally demanding. Several approaches have been proposed to mimic particle breakage. Yet, these methods disregard important rock properties and their validation is still scarcely reported. The Tavares Breakage Model, implemented in Rocky DEM 4.2 commercial platform, covers important rock behavior characteristics, such as the inherent variation of particles’ fracture energy and the influence of their size and weakening of particles due to damage accumulation. Rocky DEM also uses polyhedrons to represent particle shape, with mass and volume conservation after a breakage event.

The model has been tested in different size reduction systems. Tests in laboratory scale, such as single particle impact tests and breakage of particle in beds demonstrated very good ability to describe breakage probability and particle size distribution. Particle weakening has also been assessed by simulation of repetitive impacts, presenting good agreement between experimental and simulated values. Pilot and industrial scale crushers and mills were then simulated and compared quantitatively and qualitatively to data. The outcomes demonstrated the feasibility of adopting the Tavares Breakage Model on Rocky DEM to simulate several comminution processes.
Modeling root growth in a granular soil

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Keywords
Granular soil, root-soil interaction, DEM, force chain

Abstract
The variability of plant root architecture is generally attributed to genetic, physiological and environmental factors such as the mechanical strength of soil. However, the soil has often been modeled as a continuum, and the complex particle-scale mechanisms at the origin of root development are not easily accessible to direct measurements [1,2]. In particular, a key issue is to determine how the inhomogeneous distribution of force chains are reflected in the forces experienced by the root cap. We introduce a numerical model of a growing flexible root inside a granular assembly composed of solid particles. The particle motions are computed by stepwise integration of the equations of motion for all particles by accounting for their frictional contact interactions and the gravity and boundary forces. We use the same framework to model the root, defined as a flexible tube represented by an array of segments interconnected by linear springs and growing as a result of its continuous elongation. The general numerical model and simulations are in two dimensions as the root growth requires long-time simulations and we needed to perform a large number of independent simulations in order to be able to assess the variability of the results and the effect of system parameters. We present the particle interactions and the root model, and we investigate the mean force experienced by the root cap as a function of root flexibility, gain size, soil cohesion and particle size distribution. We show that a single dimensionless parameter combining different root and soil parameters controls the mean force. We also show that the distribution of root cap forces reflects that of interparticle forces [3].

References
Influence of lateral confinement on granular flows: comparison between two geometries

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Keywords granular flows, confinement, non-local effects

Abstract Confined granular flows are strongly influenced by the presence of sidewalls which can stabilize them [1] or modify the shear localization [2]. This can be explained by co-operative effects induced by the sidewalls whose lengths might be comparable to the confinement length. It is therefore crucial to implement accordingly, the effect of confinement in any model aiming to describe the granular flows.

Yet, from the literature it is unclear if the effect of the confinement depends or not on the geometry of the flow. Moreover, the question of the boundary conditions that have to be used at sidewalls is still far from being fully addressed [3,4].

To address these points, we compare here the properties of granular flows in two different confined geometries. The first one is a confined chute flow for which stabilization is induced by the sidewalls [1,5]. It allows attaining unexpected high flow angles [1]. The second is a confined shear cell for which it has been found that the sidewall friction can modify drastically the shear localization [2,6,7]. In both the cases, the sidewalls are flat and frictional.

We show that in both the geometries, the importance of confinement on the kinematic properties of the flow is crucial. In particularly, we show that depending on the flow regime (sheared or quasi-static) the sidewalls can behave like a granular temperature source or sink. This result indicates that the effect of the sidewalls, and consequently the boundary values, are correlated to the flow properties. In both the geometries, the sliding friction is also studied. A stress analysis also shows that, in both the geometries, the presence of sidewalls, leads to friction weakening of the flow [5,6] in the creep regions.

140: Peridynamics simulation of particle crushing
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Keywords
Particle breakage, Peridynamics, Particle size distribution, micro-cracks

Abstract
By means of Peridynamic simulations [1], we investigate the breakage mechanics of particles under the action of external forces. The particles have an internal texture composed of a distribution of cleavages (micro-cracks), representing the natural inhomogeneity of the particles. Mechanical tests were performed on 2D disks under quasi-static diametral compression for different particle sizes and distributions of microcracks [2]. The evolution of yield stress with diameter and the probability of failure in terms of Weibull distributions are investigated. A floodfill algorithm capable of determining the fragment size distribution after failure allows us to analyse the median fragment size as a function of the initial density of cleavage. We employ the same methodology to quantify the effect of the impact energy by varying either the mass or the velocity of an impactor.

References
141: Creep-like settlement of railway ballast under cyclic loading

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Keywords

Track Ballast, Modeling, DEM, Contact Dynamics, Differential Settlement

Abstract

Differential settlement of the railway ballast track that occurs on high-speed train circulation is a major challenge for maintenance as it requires frequent costly tamping operations to restore the initial ballast track. By means of the Contact Dynamics method, we model a reduced portion of the ballast track using a library of digitalized ballast grains settled in a box together with a sleeper on which different types of cyclic loading are applied. We are interested in the evolution of the settlement under normal conditions and in the presence of a defect. We consider different values of the sample width, loading intensity and frequency. We present the numerical model, based on the Contact Dynamics method. Then, we show that for all the operating parameters, the settlement follows systematically a creep-like logarithmic settlement law. While increasing the loading intensity leads to enhanced settlement rate, we find that by increasing the sample width or the loading frequency the settlement rate declines. We also analyze the microstructure in terms of coordination numbers and friction mobilisation.
Discrete Element Method (DEM) and DEM coupled to Computational Fluid Dynamics (CFD-DEM) are powerful techniques for optimization and design of particle processes. Macroscopic granular particles, the flow involving fluids and granular particles are everywhere - in industry, environment and everyday life. Sugar, sand, ores, tablets, chemicals, biomass, detergents, plastics, crops, fruits need to be harvested, produced, processed, transported and stored.

We give an overview of the state of parallelization and recent developments in the frame of the open source DEM software LIGGGHTS®. In particular, we share scalability benchmark information on a large cluster system, and present the details of the newly implemented RCB (recursive coordinate bisectioning) algorithm used for dynamics load-balancing of the simulation.
Feasibility study of semi-analytical modelling of irregular particle shape and simulation in discrete element method

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Keywords spherical harmonics, irregular particle shape, discrete element method

Abstract Particle shape plays an important role in many granular material processes thus determining particle shape is a crucial task. Modelling is an indispensable tool for proper understanding of the behaviour of particulates and discrete element method (DEM) is often used for this purpose. Numerical solutions to formulate and implement particle shape models are needed for simulation of particulate materials. However, such models frequently have limitations and can only be applied for limited type of particle shapes [1, 2].

Spherical harmonics is a powerful mathematical tool that allows to model arbitrary surfaces. Recently, the series of spherical harmonics (SH) has been applied in many fields [3, 4]. Modelling technique presented in this work allows obtaining the analytical function of SH from the experimental surface points. The accuracy of SH models depends on number of spherical harmonics used in a model.

The aim of this work is to obtain particle models with required accuracy using a small finite number of SH, where the focus is on the application of the semi-analytical SH technique to irregular shaped particles. Modelling results are compared to experimental data.

Also these models are embedded in DEM and several simulations and experiments are done in order to determine the possibilities of semi-analytical models.

Keywords
DEM, CFD-DEM, Open Source, Overview

Abstract
Discrete Element Method (DEM) and DEM coupled to Computational Fluid Dynamics (CFD-DEM) are powerful techniques for optimization and design of particle processes. Macroscopic granular particles, the flow involving fluids and granular particles are everywhere - in industry, environment and everyday life. Sugar, sand, ores, tablets, chemicals, biomass, detergents, plastics, crops, fruits need to be harvested, produced, processed, transported and stored.

We give an overview of recent developments in the frame of the open source CFD-DEM software CFDEM®coupling and the open source DEM software LIGGGHTS®. In particular, we summarize recent implementations and validation efforts regarding non-spherical shape representation (superquadrics and convex particles), modelling of solid structures with DEM, energy conservation tracking in DEM, modelling of magnetic dipole interaction and flexible fibers. We also present progress on immersed boundary / fictitious domain handling for solid body motion in coupled CFD-DEM simulations, as well as CFD-DEM models for chemical reactions, heat and mass transfer. On a more general level, we also summarize parallelization and code efficiency improvement efforts.

Progress and further plans on coupling DEM with averaging techniques ("fastDEM") to considerably speed up large-scale simulations are also outlined.

We highlight the possible applications and remaining challenges for DEM and CFD-DEM modelling in fields such as steel industry, chemical industry, pharmaceutical industry, consumer goods industry, agricultural machinery production, food production, powder metallurgy and plastics production.
Keywords
Calibration, Standard, Cohesionless, Draw Down, DEM, Parameters, Friction

Abstract
The numerical complexity of Discrete Element Method (DEM) simulations generally forces an idealisation of DEM models, making the calibration process the key to realistic simulation results. When calibrating cohesionless, free-flowing bulk materials, individual simple experiments are commonly used as reference for the calibration, such as the angle of repose in various test methods. Regardless of the experiment, the calibration is regularly performed by trial and error, systematic variation of the parameters, or using optimisation algorithms until a suitable combination of parameters is found. A problem of the calibration, which is often ignored, is the ambiguity of these parameter combinations. Thus, there are usually a variety of contact parameters that can map the same macroscopic reference value.

This paper deals in detail with the ambiguity of parameter combinations during the calibration process. It shows which standard tests can be used to generate different experimental reference values for the calibration. The results of simulations with systematic parameter variation highlight the problem of ambiguity. Subsequently it will be shown how the combination of different tests can significantly reduce the acceptable parameter combinations. A modified draw down test will be presented as a calibration test which can deliver different reference values in a single test. Hence, this calibration test allows to obtain an almost unique set of DEM parameter.

The paper will show how a unique parameter setting for sliding and rolling friction can be found for cohesionless gravel with two different particle size distributions as well as the validation of the behaviour in an additional test scenario.
Discrete Element Modeling of Abrasive Wear for Model Calibration

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Keywords
DEM, Wear, Calibration

Abstract Abrasive wear is ubiquitous in agricultural machinery. It is also one of a number of processes which occur when the surfaces of machine components are loaded together and are subjected to sliding and/or rolling motion or are subjected to sliding of moving materials. The objective of the present work is to compare the abrasive wear on a piece of machinery predicted by DEM with the experimental data collected using the ASTM-G65 standard.

For the DEM model, the Archard wear equation is used. The Archard wear equation is a simple model designed to describe sliding wear in particular. It is based on the theory of asperity contact.

We also present the details of the experimental setup along with its advantages and disadvantages.
Effect of particle shape on the shearing behavior of granular materials using a BlazeDEM-GPU code

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Keywords
Discrete element method, GPU, shearing, shape

Abstract
Identifying the mechanical properties and energy dissipation of granular materials are challenging in soil mechanics and industrial applications. The macroscopic behavior of granular materials cannot be fully predicted using theoretical and empirical methods. The numerical modelling using discrete element method (DEM) has become essential for studying the mechanics of granular materials on the mesoscopic grain-scale. This provides details of quantities that cannot be easily measured experimentally such as contact forces and contact energies, which is essential to obtain insight into various granular processes. The quality of the analysis conducted is directly dependent on the quality of the selected input DEM parameters to obtain a sufficient calibrated DEM model. Although, particle shape has been shown lately to be an essential parameter to not oversimplify, e.g. hopper discharge, it remains oversimplified using spherical particles or clumped-spheres using only two to three spherical particles, due to the high computational cost associated with more accurate representations. In addition, the number of particles is usually misrepresented, by significantly fewer particles, due to a lack of compute resources. GPU computing to compute the DEM has made significant strides to alleviate these over-simplification by unleashing unprecedented parallel compute capabilities as demonstrated by BlazeDEM-GPU code developed by Govender et al. Millions of convex and non-convex polyhedral shaped particles can be computed using Blaze-DEMGPU. In this study, the importance of particle shape for direct shear tests are highlighted. This is done by the 3-dimensional modelling of the direct shear test of railway ballast. In the one model the particles are simplified as spherical particles with rolling resistances, while the other model represents the particles as convex polyhedral shaped particles without rolling resistance. Both models are calibrated to their full extent using our developed radial basis function optimization approach. The macro-scale simulations results are compared to the macro-scale experimental results, which clearly indicate the importance of accurately representing particle shape in DEM simulations.
149: A Discrete Element Model involving the breakage of tube-shaped particles

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Abstract

The work focuses on a discrete element model involving the brittle fracture of the tube shaped particles (shells). In a nutshell, the strategy consists in modelling each shell as an assembly of sub-shapes that are joined where the shell is expected to break in case of radial compression. For that reason, the shell is composed of 24 sphero-polyhedral prisms adjoined so that the predefined discontinuities are radial plans. The adjacent prisms are connected through 4 sticked links located in each of their corners. A yield criterion is defined for the breakage in the normal-tangential space of forces. Once the micro-scale parameters are determined, the analysis continues at the scale of an oedometric test involving assemblies of these breakable shells. In addition to validating the approach, a two-scales examination is proposed.
Investigation of relationship between shape and flow characteristics of rod-shaped particles in a hopper: Experimental and numerical studies using pseudo-conservative polygonal DEM algorithm

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Keywords
Polygon, DEM, Hopper, Discharge, Non-spherical

Abstract

In this work, the discharge of numerous polygonal shaped particles in a hopper was investigated. To this end, a two-dimensional polygonal DEM model is proposed and implemented to simulate hopper operation. Lab-scale experiments were also conducted for validation. Influence of particle shape, discharge opening and vibration strength has been investigated numerically and experimentally. The results show that the discharge rate of non-spherical particles was significantly affected by the shape of particles, and inter-particle packing property was found to have stronger influence than rolling-related properties, such as roundness or moment of inertia. Although the discharge rate increased with increasing initial loading, the discharge rate saturated at over = 30 kg owing to the so called Janssen’s effect. The discharge corresponding to the change in particle shape and initial loading was in good agreement between the simulation and experimental results, at the expense of relatively high computational cost.
153: Wave propagation in sand- Discrete element modelling and PIV analysis

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Keywords Wave propagation, discrete element method, PIV analysis, Digital image correlation

Abstract The phenomenon of wave propagation through the soil is an important field of study as it forms the basis for dynamic response of the soil to vibrations. As the wave passes through the soil the properties of the waves are modified depending on the media through which it passes. The velocity of the wave changes based on the soil properties and this greatly affects the response of the structure. Presently wave propagation in soil can is being modelled using finite element software such as PLAXIS, DEEPSOIL, OPENSEES etc. All this software utilises the properties of soil layer through which the wave passes to arrive at the wave propagation velocity. The major assumption in the present finite element analysis is that the soil is considered as a continuum, but soil as such is made up of discrete particles and their overall behaviour is because of the interaction between the particles. The propagation of the waves also mainly happens through the contacts between the particles. This is the reason why the denser packing generates greater velocity. In such a condition, modelling the wave propagation through the discrete element method is a more appropriate way to study the wave propagation phenomenon. The discrete element method is a recently developed numerical tool which can model the individual particles in the soil and their interaction. In the present study, wave propagation through the soil is modelled using an opensource discrete element software LIGGGHTS. A small tank of size 30cm x 15cm x 22cm is filled with sand particles of sizes varying from 1.5mm to 3mm (Figure 1). A hammer hit on a plate placed on the top of sand is used to generate the waves. Two accelerometers are embedded at known depths to capture the wave. A high-speed camera is placed in front of the experimental box to record the propagation of the waves at a frame rate of 30000fps. The propagation velocity of the wave and the attenuation is captured using Particle image velocimetry (PIV) method using the images obtained during experiment. The experiment is modelled in discrete element method using characterised contact parameters and the wave propagation velocity obtained is compared with the one obtained from the experiments and from the accelerometers.

Figure 1: Experimental setup for small-scale experiment.
154: DEM simulation of rock particle breakage under different impact velocities

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Keywords
rock particle, impact loading, breakage, DEM

Abstract
Fragmentation of unconfined cylindrical specimens of rock due to different impact velocity has been investigated in this paper based on discrete element method (DEM) simulations. In the DEM model, the impactor and rock model is built by bonding rigid particles together and presented the actual size of the testing sample. The numerical model is first calibrated by comparing the stress-strain curves obtained from SHPB tests. Since the bond strength is an intrinsic parameter of the model and can’t be calibrated by the test, we have established a speed-dependent bond strength criterion that can serve as a guide for the parameter selection for future simulations. The energy analysis and crack propagation in the impact crushing process were studied using the well-calibrated model. The results of energy analysis show that the rock fracture has its maximum rupture energy and with the increase of velocity, the friction loss becomes the main form of energy dissipation. The crack propagation results show that the number of cracks increases with the rising of the impact velocity, and the cracks which don’t expand at low speeds will occur at high speeds, but the crack frame and the direction of expansion are roughly consistent, which also proves the fractal nature in rock fragmentation process.
Keywords
Dense granular flow, chute flow, Contact Dynamics, boundary layer.

Abstract
We present an extensive numerical study on a dense granular pile settling/flowing on an inclined plane. In such a problem, rapid flow and slow flow regimes of granular materials can co-exist. We have used an open-source, contact dynamics-based DEM software called SOLFEC to study the chute flow problem over a range of parameters. We critically examine flow characteristics of granular materials when the friction condition at the base of the chute is changed from a frictional to completely frictionless case. We observe that the velocity, packing fraction and temperature profiles are completely different in both the cases. For the frictional case, we observe a boundary layer near the bed which is about 2-3 particle diameters thick. Contrary to what is observed in the case of fluids, the thickness of this boundary layer remains nearly the same throughout the flow and is also independent of the angle of inclination. We also observe that the value of friction-coefficient between the particles and the base does not affect the thickness of this shear layer. This observation that yielding/failure occurs within the material rather than at the base is in good agreement with experimental observations.
DEM investigation of the breakage of wet flexible fiber agglomerates impacting a plane

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Keywords
Agglomerate breakage, Flexible fiber, Liquid bridge force, Discrete Element Method

Abstract
The breakage of an agglomerate of wet flexible fibers impacting a plane, which is prevalent in the biomass fuels production processes, is investigated in this work using the discrete element method (DEM). The wet flexible fibers are aggregated due to cohesive liquid-bridge forces. Agglomerate breakage with various impact conditions, initial configurations, fiber properties, and liquid bridge properties is systematically investigated. The degree of breakage is governed by the impact energy, the cohesion energy due to liquid bridges, the energy dissipation/absorption through fiber-fiber contacts and fiber deformation, and the efficiency of energy and force transmission within the agglomerate. More specifically, breakage is promoted by increasing impact velocity, decreasing agglomerate size, increasing initial compaction, increasing fiber bending modulus, increasing fiber aspect ratio, decreasing liquid surface tension, and decreasing liquid-to-solid volume ratio. Breakage is strongly dependent on the modified Weber number, i.e., the ratio of the Weber number to a dimensionless rupture distance, which is a measure of the impact energy relative to the cohesion energy.
A Combined Discrete Element Method and Evolutionary Algorithm Approach to Designing New Fit for Purpose Granular Materials

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Keywords Evolutionary Algorithms, DEM, Machine Learning, Materials Design

Abstract We apply a combination of the Discrete Element Method and Evolutionary Algorithms to develop new fit for purpose granular materials that are tailored to specific applications. These applications range from determining optimal morphologies and compositions of granular materials for maximum density, through to more complex optimisation of material properties and device design for maximum performance.

We utilize a fully dynamic linear spring Discrete Element Method (DEM) simulation that allows for the specification of the particle properties including the sizes, masses, inter-particle friction, coefficient of restitution, particle shape and their interaction with arbitrary dynamic mesh objects. Further details of our DEM technique are given in ref. [1]. In our model particle shapes are represented as superellipsoids, giving us the ability to investigate a broad range of particle shapes, smoothly transitioning through a range of surface curvatures and aspect ratios. [2].

Evolutionary algorithms employ techniques inspired by biological evolution such as reproduction, mutation, recombination, and selection to optimise a population of candidate solutions (individuals) based on a specified fitness function [3]. Figure 1 shows an example evolution of the fitness (here specified as the packing fraction) of a population of bidisperse packings of superellipsoids, where we have allowed the shape parameter and aspect ratios of each species to be varied. The evolutionary algorithm iteratively explores the parameter space, improving both the maximum and mean fitness of the population of candidate solutions, converging on final shapes that balance the relative contributions of surface curvature and aspect ratio for each species. This approach can be used to optimise any desired properties of the granular material and the properties of simulated dynamic mesh objects that the material is interacting with.

Figure 1: (Left) Image of a dense bidisperse packing of superellipsoids obtained via an evolutionary approach. (Right) Evolution of the fitness (packing fraction) over 21 generations for a population of bidisperse packings of superellipsoids.

References
DEM Modelling of Metal Powder Flow in Additive Manufacturing Systems

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Keywords Additive Manufacturing, Powder Bed, Powder Morphology, Selective Laser Melting

Abstract The Discrete Element Method is a powerful tool for studying the complex flow behavior of granular systems in modern industrial devices, allowing for precise specification of the detailed geometry of the device, the particle morphology and the interaction properties of the individual particles.

We present results of a discrete element method (DEM) model of metal powder flow in an additive manufacturing device. In powder-bed based metal additive manufacturing applications, the addition of the powder layers is the crucial first step in building up of the part in 3D and has a significant impact on final part quality. A common technique employed is to add successive layers of metal powder by raking a new layer across the existing surface. Understanding this raking process and how the properties of the powder particles (e.g. size, shape, density, interaction properties) and process parameters (e.g. height of powder layer, rake geometry, rake speed) affect the properties of the bed after raking is crucial in optimizing the performance of the system and ensuring the quality of the 3D-printed part.

Our DEM model directly incorporates the powder’s particle size distribution, particle shapes and experimental measurements of the powder flowability. Results will be presented of the raking of both Arcam Titanium powder and CSIRO Manipulated Titanium Powder, with comparisons to detailed experimental data characterizing the powder bed structure after the addition of a powder layer.

Figure 1: Discrete Element Method Simulation of the addition of a layer of metal powder via raking in a 3D printing device. Particles are coloured by velocity.


**Abstract**

This work presents a simulation of an industrial milling process with the use of an advanced breakage model. The presented model is based on the Discrete Element Methodology (DEM) [1] and focuses on demonstrating the capabilities of the model to capture the different breakage mechanisms and provide quantitative analysis. Particle breakage and subsequent size reduction is a perpetual problem across a wide range of industries including the food, chemical, mineral and pharmaceutical sectors which encompass an even wider range of processed materials [2,3]. The phenomenon of breakage includes different mechanisms, starting with abrasion (or degradation, weakening, damage) by repeated low energy stressing events and resulting to final body breakage. This is an important subject that range from materials handling to comminution. There are many applications where undesirable degradation can take place such as cyclones, fluidized beds, centrifuges, stirred vessels; and in transport equipment, such as pneumatic, screw and hydraulic conveyors and chutes [4,5]. For instance, degradation is of relevance from materials such as coal and iron ore lumps, used in steelmaking, to fine powders that are processed in the chemical, food and pharmaceutical industries [6-8]. Another example in which degradation is actually desirable is the case of crystallization processes as it is used to provide a consistent size distribution, which would not be achieved through controlled crystal growth alone [9,10].

Research has shown that particles are often loaded using insufficient energy to cause breakage inside comminution equipment, being fractured only after repeated low-energy stressing. This has been particularly well-known for autogenous and semiautogenous mills, where rock lumps are broken by a combination of attrition and self-induced impact-fracture [11]. Breakage by repeated stressing is also the major mode of breakage for coarse particles used in the mining and mineral processing sectors. Therefore, this mode of particle fracture is likely to be of significance for applications that use crushers too. This has led to an increased demand in the simulation of particle breakage and degradation to better describe the fracture of particles subjected to repeated loading.

This work simulates a pilot-scale milling application from MEGlobal with the aim to assess the performance of the equipment and the resulting material after the end of the process. The material used is iron ore and is being processed in 3 different tests with the use of steel balls, that help towards the breakage of the particles, during the rotation of the drum. The virtual material is simulated by using single spheres and is described by specific DEM parameters to resemble the real iron ore, while the kinematics of the virtual geometry replicates the mill. Furthermore, the threshold of the material to breakage is described by a number of inputs such as, its fracture energy distribution and the minimum size that the particles can break to. Once the impact energy exceeds the maximum energy that the particle can withstand, then they break and are replaced by fragments. The size distribution of the fragments is defined by using the $t_{50}$ parameter. The presented breakage model is based on the work of Tavares, M. (2009) reflecting the latest advances in research thus provides information on the final particle size distribution, the mass loss that the particle suffers due to abrasion, the new fracture energy per particle type, as well as the required power mill. This type of analysis brings great benefits to a wide range of industries as it enables the assessment of the performance of comminution apparatus and/or other equipment where breakage is a by-product.

**Keywords** DEM, Breakage, Calibration, Abrasion

**References**

Minimization of wear in a transfer chute by geometric optimization of convex pattern surface: A DEM study

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Keywords transfer chute, material equipment interaction, wear reduction, DEM

Abstract Using bionic surface on the material equipment interface of bulk handling equipment is a promising solution for wear reduction. A bionic surface is a flat surface outfitted with a pattern of convexes that disrupt the natural sliding flow of bulk material. Previous numerical work has shown a significant reduction of wear of bionic surfaces compared to a smooth surface [1].

The aim of this paper is to find the optimal configuration of bionic surfaces in order to minimize wear in transfer chutes. Four geometric parameters were introduced to define the shape and size of these convex patterns (see Figure 1). The geometric convex patterns were evaluated with the aid of Discrete Element Method (DEM). The simulated material was iron ore with d50 of 10 mm sliding down a smooth chute transitioning into bionic surfaces of different geometric configurations. Hertz-Mindlin (no slip) model and Archard wear model were implemented to calculate the sliding wear volume. The experimental plan was based on a full factorial design, which varied the parameters of a₀, a₀:b₀, c₀ and d₀.

Simulation results show that different patterns of convexes have different influence on wear volumes and velocities of particles. The factors a₀ and d₀ of each pattern have significant influence on sliding wear, while there are insignificant interactions between geometric parameters. It is found that the existence of convex patterns makes the particles closest to the chute’s surface have the tendency to slow down, causing the remainder of the particles to slide and roll over these bottom particles instead of sliding directly over the surface, which reduces the chute’s wear.

Figure 1: Geometric Parameters determining shape of bionic surface

Bridging the gap between MD and DEM: Models for particle systems on the nano to micro scale

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Keywords MD, DEM, MDEM, CFD, enzyme, PDC, biological structures, biocatalysis

Abstract Discrete particle systems are present in many applications of biotechnology and process engineering and the physical phenomena involved therein spread over vast scales of size and time. Depending on the scale of interest, various models have been developed for discrete systems, either in the DEM framework (typically >10µm) or MD framework (typically <100nm). However, models bridging the gap between the two regimes and frameworks are rather scarce and will be addressed in this contribution. These scales are especially interesting for biological structures, such as enzymes, which can be looked at as functional particles with interesting properties concerning their interaction, agglomeration (i.e., structural formation), and reactive process properties. Such systems have received increasing interest in recent years [1] and as they are difficult to investigate experimentally in detail [2], the need for modeling techniques on this scale is driven.

To gain insight, we develop models to transfer the essential dynamics and complex interaction behavior from MD to DEM (see Fig. 1) in a modeling methodology termed by us the molecular discrete element method “MDEM”. In the regime between 100nm and 10µm diffusive effects are significant and interaction of particles is anisotropic (influenced by e.g., shape, electric charge, atomic structure). To capture this, we developed a force-based diffusion model for DEM [3] and complex data-driven interaction models derived from MD [4–6] (both atomistic and coarse-grained) simulations. The diffusion model [3] is generally applicable to any diffusive process in DEM to enforce a canonical ensemble (i.e., constant temperature) and additionally enables a straightforward coupling to CFD. The models are parameterized “bottom-up” and validated “top-down” by comparison with experimental data, which is obtained from biolayer interferometry (BLI) and dynamic light scattering (DLS). As a model system the multi-enzyme Pyruvate Dehydrogenase Complex (PDC) is used, as it features organized self-structuring processes and a highly regulated multi-enzymatic machinery dependent upon the structure.

Obtained results for PDC components show that the dynamic formation and breakup of enzymatic agglomerates can be predicted using the developed DEM diffusion model [3] jointly with complex interaction forces derived from MD. This approach requires no experimental data fitting and produces accurate scale-bridging kinetics as well as agglomerate sizes matching corresponding dynamic light scattering data [2].

We gratefully acknowledge financial support by the DFG (SPP 1934) and BMBF (031B0222).

Discrete modeling of silo discharge on flow behavior characterization

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Keywords
Granular flow, DEM, silo, velocity fluctuation

Abstract

The discharge behavior of granular material from flat-bottomed silo was investigated by performing Discrete Element Method (DEM) simulations. Regular velocity fluctuation was observed in both funnel flow and semi-mass flow regimes. The characteristics of velocity fluctuation along the vertical and horizontal directions were carefully examined. It was found that the velocity fluctuation was closely correlated with the fluctuation of particle contact force. The fluctuations were found to take the form of waves initiating from the lower center of the silo and propagating in the opposite direction of the granular flow. Quantitative characterizations of these waves including the frequency, amplitude and propagation velocity were performed.
Quantitative Simulation of Mechanical Properties of Porous Ceramic Materials by Discrete Element Method

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Keywords
porous ceramic, particulate material, fracture, crack

Abstract
In this work, the mechanical response of porous ceramic was investigated by performing discrete element method (DEM) simulations. To account for the spatial coupling effect of solid bonds under multi-contact condition, the classic Hertz contact model was modified by introducing a correct factor which reflects the influences of contact size in-between grains and the geometrical arrangement of grains. The quantitative predicting ability of the built DEM framework was then evaluated by using the partially sintered alumina ceramic as investigated system. It was demonstrated that the predicted effective Young’s modulus and fracture strength are both in quantitative agreement with experimental data. As to partially sintered alumina ceramic containing large pores, both the interaction behavior between pores and the influence of pore arrangement on effective Young’s modulus and fracture strength predicted by the theoretical analyses or finite element method were successfully captured by our DEM simulations. All these quantitative comparisons demonstrate that the built DEM framework can be used to quantitatively model the mechanical properties of porous ceramics.
Keywords
Granular flows, discrete element method (DEM)

Abstract
We investigate numerically high speed granular flows down inclines. Recent numerical works have highlighted that the presence of lateral frictional walls allows to produce novel Steady and Fully Developed (SFD) flow regimes at high angle of inclination where accelerated regimes are usually expected (Brodu et al., 2015). These SFD regimes present non-trivial features, including secondary flows with longitudinal vortices and “supported” flows characterized by a central and dense core supported by a very agitated dilute layer.

We present a review of these new regimes and provide their domain of existence in the parameter space including the mass hold-up M and the inclination angle θ. We also investigate the sensitivity of these states to the gap width W between the lateral walls and the wall friction μ_W.

We emphasize two salient outcomes. (I) First, our simulations reveal that secondary and supported flows disappear for small gap width (typically, W<20D, where D is the particle size) and low wall friction (typically, μ_W<0.5). (ii) Second, despite the diversity of the features of these regimes, the simulations bring to the light that the mass flow rate Q obeys a simple scaling law with the mass hold-up and the gap width: Q~M^{3/4}W^{1/4}.

References
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DEM and PLASTICITY Modeling of the stress-strain behavior of granular materials in the strain hardening and softening regimes

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Keywords
DEM, stress-strain, rolling resistance, bifurcation, strain localization, strain softening, plasticity

Abstract

A combined DEM and plasticity modeling of the stress-strain behavior of granular materials in the strain hardening and strain softening regimes is presented. The macroscopic plasticity model is based on micro-mechanical observations obtained from particulate simulations of the response of granular materials during biaxial loading using the Discrete Element Method (DEM). The DEM modeling was carried out using the Particle Flow Code (PFC), and homogenization techniques were used to convert discrete micro-mechanical quantities to continuum macro-mechanical parameters. In agreement with observations from laboratory testing, DEM modeling showed that deformation of granular materials is initially homogeneous followed by bifurcation causing the formation of one or two narrow shear bands where the deformations are localized. As a result of localized deformation, the load-carrying capacity of the granular assembly reduces with increasing strain and strain softening ensues. Following localization, the DEM modeling focused on the response of the granular material within the shear band, and these observations were then used to establish a continuum model of the post-failure behavior of the granular materials. A non-associated plasticity model was used for the homogeneous strain hardening regime, and the onset of strain localization is predicted using bifurcation theory. Post-localization response was based on the model smeared discontinuity, where it is assumed that elastoplastic deformation comes from the localized deformation of the material in the shear band while the material outside the shear band deforms elastically. Based on the DEM results, the deformation inside the shear band was modeled following simple shear condition. This localized deformation is then averaged over a sampling volume of the material. The thickness, orientation, and degree of principal stress rotation and non-coaxiality within the shear band, which are all needed to establish the simple shear stress-strain behavior of the shear band, were also all obtained from DEM results. The complete continuum plasticity model was shown to be capable of replicating the DEM results on the full spectrum of the stress-strain behavior of granular materials from strain hardening to failure and strain softening. Use of the model in simulating the response of RF-Hostun sand under bi-axial plane strain loading showed that the model can realistically reproduce real granular material behavior. One of the main findings from both micro and macro-mechanical modeling is the importance of shear band thickness in relation to the sampling volume in determining the magnitude of strain softening.
166: A multiple-relaxation-time LBM for modeling a free-surface flow containing floating ices

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Keywords
Ice jams; river ice dynamics; multiple-relaxation-time LBM; free-surface flow

Abstract
Floating ice blocks can cause extreme flooding, damage to structures, interference with navigation, and restrictions on hydropower operations. In this work, a mesoscale method is applied to simulate free-surface flows containing floating ice. The multiple-relaxation-time Lattice-Boltzmann model (LBM) is used to solve fluid dynamics problems due to its overall computational efficiency and its capability to deal with complex geometries and topologies. Validation test cases are presented and the results show promise to serve as a useful tool for river ice dynamics.
167: Discrete element model for a general constitutive behaviour

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Keywords Discrete element Model, Multi-body interactions, Brittle fracture

Abstract Current numerical models to predict the mechanical behaviour of materials can be classified into two approaches namely continuum models and discrete element models (DEM). While continuum models have been studied in great detail, incorporating the effect of microstructural features such as grains texture, cracks and other defects proves difficult. DEM is gaining importance because they are simple, easy to set up and allow the description of microstructural features at various length scales. DEM describe the material in terms of lumped masses interacting through constitutively prescribed forces. These interaction forces between the lumped masses do not arise from physical arguments as in molecular dynamics. Most commonly, the interactions have been taken to occur through linear springs connecting pairs of particles [1]. Such pairwise interactions are known to describe a very limited range of constitutive behaviour [2] and impose non-physical conditions on the elastic moduli [3]. There are no systematic means of a generalization of interparticle interactions in DEM to various constitutive behaviour observed in materials.

In this work, we propose an alternative approach which allows for multi-body interactions and description of more general constitutive behaviour. In our approach, the domain is discretized into lumped masses and the interaction forces are derived from the continuum strain energy density ($\phi$) function. This novel interaction force allows DEM to be generalised to describe any general constitutive behaviour, provided we choose an appropriate strain energy density function. We illustrate the applicability of the model to anisotropic elastic materials and their brittle fracture behaviour. Simulations of compact tension specimens with isotropic and orthotropic constitutive properties are presented. A simple failure criterion based on strain energy is used i.e., interaction force is set to zero when the strain energy density ($\phi$) reaches the critical value ($\phi_c$). The model indicates that the crack path (see figures) in the isotropic plate remains straight whereas it curves due to anisotropy.

Fluid grain coupling for microstructural modeling of internal erosion in granular materials

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Keywords
Micromechanics, DEM, fluid/grain coupling, suffusion

Abstract

Suffusion is the most complex internal erosion mechanisms occurring in granular materials subjected to internal fluid flows. By use of a Discrete Element Method (DEM) coupled with a Pore-scale Finite Volume (PFV) scheme, this study investigates the consequences of an internal fluid flow on granular materials at the scale of representative elementary volumes. A particular attention is given to the occurrence of grain transport for different stress states and for different flow intensities and directions. For dense widely graded granular samples, it is shown that grain transport is increased when the macroscopic flow direction is aligned with the major direction of compression. This observation is then interpreted in terms of micromechanics thanks to the definition of pore networks and force chains. The stress induced microstructure modifications are shown indeed to influence the transport distances by controlling the number of rattlers in granular materials.
170: Transient granular rheology

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Keywords
Granular media, granular rheology, rate-and-state, Discrete Element Modelling

Abstract
Geological flows often exhibit sudden motion events separated by long periods of extremely slow displacement. For example, the slow deformation of a fault can lead to earthquakes, the creeping motion of soil eventually triggers landslides, and ice-shelves also exhibit similar intermittent behaviours during their evolution. These phenomena are reminiscent of stick-slip effects which can be observed in situations where elasticity and friction are together at play. Such effects may be described using rate-and-states models, which assume that the medium can is characterised by an additional state variable whose evolution over time modifies the effective friction, and consequently the dynamic response, in the material.

However, at higher deformation rate, granular materials such as the one composing geological flows are typically described by a $\mu(I)$ rheological model, base on a bulk friction coefficient monotonically increasing with strain-rate at steady state, without any concept of internal state variable. Such rheological law may have difficulty predicting any stick-slip phenomena. More generally, the extension of the $\mu(I)$ model to very low shear-rates, non-steady flows, and transient phenomena remain challenging.

Here we start tackling these issues by considering transient effects assuming a simplified $\mu(I)$ rheological laws on a granular layer under simple shear whose applied shear rate changes over time. We develop an analytical solution for this geometry and compare it with the results of discrete element simulations, showing good agreement between the predicted and measured timescales of the transient effects. The $\mu(I)$ relationship is then extended to take into account the effects of transient phenomena on the system boundary stresses, which allows recovering a rate-and-state-like model. This effectively shows that rate-and-state models can actually be understood as emerging at the macroscopic scale from a granular system with $\mu(I)$ rheology at the smaller scale. This connection, therefore, improves the understanding of the physical basis and behaviour of both rate-and-state and $\mu(I)$ models, and may give important insights into the relevance of different constitutive laws for transient effects and instabilities in particulate materials.
A comparative study on impact breakage of synthetic rock samples and bonded particle DEM model

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Keywords
Discrete element method, Synthetic rock sample, Rock fracture

Abstract

The Discrete element method (DEM) is a well-known numerical technique for simulating flow and breakage of particles found in many fields of application including the crushing and grinding (comminution) stage in mineral processing. In this field, it has proven to be a useful tool to complement experiments and study the mechanics of particle load response under conditions in which measurement is often impractical. During experimentation, reproducibility is often a challenge due to the inherent heterogeneity of particles. Synthetic rock samples such as 3D printed sandstone offer an opportunity to produce a relatively homogeneous sample of desired shapes and consistent mechanical properties.

This work utilises DEM to study the effect of various particle shapes on their breakage properties under impact loading. A spherical steel impactor falling under gravity is simulated, akin to a short impact load cell (SILC). A comparison of results with SILC experiments conducted using synthetic rock samples under similar conditions, are found to be in good agreement. After appropriate calibration of micro-mechanical properties, the size-dependency of fracture force observed in laboratory experiments can be precisely predicted from DEM simulations. This study demonstrates that DEM bonded particles are a useful analogue for real world impact breakage experiments, providing complementary insights on the dynamics of rock fracture under such loading conditions.
Optimization of secondary air inlet for circulating fluidized bed gasifier

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Keywords
Circulating fluidized bed gasifier, secondary air inlet, CPFD, optimization

Abstract

Circulating fluidized bed (CFB) gasifier is a gas-solid fluidization and reaction integrated system which can realize the bed material distribution, reaction, separation, and return back in one unit. Factors, like furnace geometry, gas-solid flow characteristics and uniformity, and reasonable organization of gasification reaction and flow, are the key issues of augmenting reaction, improving carbon conversion rate, and enhancing system energy efficiency. The CFBs gasification technology designed by Institute of Engineering Thermophysics, Chinese Academy of Sciences, has been widely applied in industry. The furnace of the unit is a cylinder with constant diameter, has only one primary air inlet at the bottom. This caused the non-uniform particle distribution - dense particle concentration in the bottom, dilute at the top, which reduces the gas-solid contact area, mixing, and prohibits the reaction rate. According to the CFB design, the secondary air injection can improve the bottom particle mixing and reduce the particle concentration. Therefore, it is a good option to introduce the secondary air inlet in the CFB gasifier system and optimize it.

In this study, a full loop three-dimensional CFB gasifier was simulated with five layers of secondary air inlets, which are located at H=0.7 m, 1.4 m, 2.1 m, 3.6 m, and 4.6 m above the bottom. At each layer, four inlets are evenly distributed around the periphery (shown in Fig. 1). The simulation was performed in the platform Barracuda. In each simulation, one layer of secondary air inlets is open while the other layers are close. The results shows that when the secondary air inlets are arranged above the particle return inlet, they have little effect on the particle distribution improvement, but when the secondary air inlets are arranged below the particle return inlet, they can help to improve the particle uniformity, and the lower the inlets are, the more uniform the particle is.
DEM simulation about the effect of the sleeper shape on the Ballast Migration

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Keywords: Ballasted layer, Ballasted migration, Sleeper shape, Discrete Element Method

Abstract: RTRI have begun numerical study by using Discrete Element Method (hereinafter “DEM”) since 2006. The authors carried out DEM simulations about the differential settlement of ballasted layers around rail joints, abrasion tests of ballast grains, the efficiency of ballast tamping and so on. The ballast migration around high cant track is common problem of high speed rail. So the authors carried out a series of DEM simulations focusing on the effect of sleeper shapes.

Figure 1-a shows featured cross section of the common sleeper in Japan, called type 3H. The cross section is the kind of hexagonal shape, which has the top half as a trapezium with moderate slope and the bottom half as a trapezium with steep slope. At the same time, DEM simulations were carried out for other types of sleepers with cross section of simple trapezium as shown in Figure 1b).

Figure 2 shows the cross section of high cant track. The sleeper dances with 32Hz of frequency. The amplitude of the outer edge of the sleeper is 4mm and that of the inner edge is 1mm.

Figure 3 shows the 3D-DEM model of track with 200m cant. Two faces in the figure are the cross sections to observe the ballast grains motion. One is the cross section around the outer edge of sleeper, the other is the cross section around outer rail position.

Figure 4 shows the distributions of ballast motion at the sleeper case of type 3H. We can find ballast grains which move over 150mm mainly on the surface of the top slope of the sleeper at both cross sections, around the outer edge of sleeper and around outer rail.

Figure 5 shows the distributions of ballast motion at the sleeper case of simple trapezium. The figure shows that there is less ballast motion between sleepers compared with the case of type 3H. We can conclude that sleeper shapes, especially the degree of side surface slope, effect on the ballast migration. It means that ballast migration can be reduced by changing the shape of sleeper.
Discrete element modelling of elastic wave propagation through granular materials for laboratory shear plate tests

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Keywords
DEM, Wave propagation, Soil mechanics, Laboratory tests

Abstract
Measurement of elastic wave signals of granular materials is important to evaluate stiffness parameters including the small-strain stiffness. Granular soils consist of many soil grains and the overall response can be described as a result of interactions between particles in contacts, which can be modelled effectively using the discrete element method (DEM). In soil mechanics research, elastic wave signals are measured using bender elements or shear plates, both composed of piezo-electric elements. Despite the growing demand for accurate measurement of elastic wave signals both in the laboratory and in-situ, there is a lack of understanding on the link between macroscopic results and the particle-scale mechanics. DEM data can provide fundamental insight.

The aim of this contribution is to discuss how well DEM simulations can capture the responses observed in soil mechanics laboratory geophysics tests considering piezo-electric shear plates. The sensitivity of the dynamic wave signal to the shear plate size is assessed to inform the design of the shear plate configuration. Secondly, the effect of particle shape on stiffness anisotropy is discussed considering both isotropic and k0 stress states. Thirdly, the effect of including finer particles on the dynamic wave signals is investigated.

The DEM simulations in this contribution were performed using a modified version of the granular LAMMPS software where equivalent conditions with laboratory experiments using shear plates were considered. A simplified Hertz-Mindlin contact model was adopted. To assess the effect of particle shape on the stiffness anisotropy, spherical particles were rigidly clumped, and the simulation results were compared with laboratory geophysics tests using natural sands.
**175: DEM numerical studies on the efficiency of the continuous operating tribo-electric separator**

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**Keywords**
Tribo-electric separation, discrete element method, numerical simulations, coal

**Abstract**
Tribo-electric separation have gained importance as a dry separator for mineral and coal beneficiation. The different grade component of coal powder can be beneficiated, classified and segregated with the help of tribo-electric separator for the use in varying purposes. A batch-mode tribo-electric separator was being used in CSIR-Institute of Minerals & Materials Technology for separating pure coal particles from gangue quartz and kaolinite particles. The separator need to be paused after operation for certain time to clean the particles stuck on the electrode plates. Need of installing two belts covering each electrode was realized. The belts designed in such a way that it bring downs the particles that were about to stick to the electrodes plates, and later cleaned by scrappers to get collected in collection bins. The modification allows the separator to operate in continuous mode. The feasibility of installing these belts along with the optimum design and operating conditions were studies with the help of DEM simulations. The bi-modal frequency distribution of coal and quartz in collection bins was observed. The rationale for the same is attributed to the fact that the initial angle and velocities of the particles entering the electric field region were not same for all the particles. The non-uniform probabilistic opportunities for the particles to attach with the respective belt resulted in two groups of particles; (a) particles attached to belt followed by their collection in the bins with the help of scrapper, (b) particles moving in a trajectory governed by external forces and directly entering into the bin. The second group of particles which were initially inclined in the direction opposite to which they were forced to move, followed a trajectory and collected in a bin which was unexpected to collect the particles. The phenomena resulted in the bi-modal distribution giving another peak of particulate collection.
Keywords

signed distance function; coarse graining dem; liquid bridge force

Abstract

Recently discrete element method (DEM) is often employed in simulations for various powder processes. There are lots of powder processes in pharmaceutical engineering, for example, fluidization, mixing, kneading, milling and die-filling. In the calculations for these processes, not only modeling regarding arbitrary shape wall boundary, liquid bridge force and solid-fluid interaction but also efficient calculation technique is required in the DEM simulations. In order to apply the DEM to the pharmaceutical systems, innovatively original models are developed in my group. Signed distance functions (SDF) [1] makes it possible to create arbitrary shape wall boundary efficiently by a simple algorithm. Toroidal approximation based liquid bridge model [2] can give flexible setting in liquid volume and contact angle. Coarse graining DEM [3] can reduce number of calculated particles drastically because of the scaling law, and hence large-scale DEM simulations can be performed efficiently on a single PC. Through verification and/or validation tests, these models has been shown to be useful in pharmaceutical systems such as a fluidized bed, granulation in a twin screw kneader and powder die-filling. Hence, the original models are shown to be indispensable for DEM simulations in pharmaceutical engineering.

References


Tillage effect on soil structure - predicting fragmentation properties

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Keywords

Particle breakage, Soil fragmentation, Discrete element, Aggregates

Abstract

Soil fragmentation is crucial for crop establishment, since the size reduction of larger aggregates improves the conditions to germination and emergence of seedlings. But it may jeopardizes soil environmental functions (e.g., carbon storage). Thus, cultivation activities must be optimized so that they promote only the necessary soil fragmentation. Although we have a good idea of adequate aggregate size distributions, our knowledge to design and obtain a desired soil fragmentation by tillage is still incomplete. Part of this is due to the limitation of current numerical models in predicting dynamic changes in soil structure, limiting the development of tillage tools. Therefore we focused on developing a discrete element model of a soil composed by aggregates with different sizes. Then we implemented a Python function to measure the variation of aggregate size distribution and to quantify the number and location of aggregate ruptures along the soil profile during tillage. From the first we calculated fractal fragmentation, and from the second we quantified the number and positions of cohesive breaks along soil width and depth. A soil bin with 0.70 m depth, 1.2 m width and 1 m length was modelled with three soil layers of 0.25 m depth each. The upper layer was composed by aggregates with diameter of 0.055 m, the intermediate layer with aggregates of 0.06 m and the bottom layer with aggregate diameters of 0.065 m. The aggregate density and particle bond strength were calibrated to reproduce the same aggregate tensile strength of a reference soil. Two tillage tools were used to promote soil fragmentation: a conventional furrow opener (CFO) used in sugar cane planting and a rotary hoe combined to a furrow opener (RCFO) also for sugar cane planting, but designed to reduce the area of soil disturbance. The horizontal displacement rate of CFO was set to 2 m/s and the rotation of RCFO was set to 135 rpm with horizontal displacement rate of 2 m/s. Results accounting for particle size distribution within the entire soil bin showed that tillage with CFO increased the fractal fragmentation from 0.51 in the initial soil condition to 0.99. RCFO also increased fractal fragmentation from a initial value of 0.42 to 0.94 after tillage. However, the disturbed area promoted by RCFO was half the disturbed area promoted by CFO. Within the width -0.1 and 0.1 m around the tool centre, CFO promoted 44% of the total cohesive breaks while RCFO promoted 69%. The smaller number of breaks promoted by RCFO out of the disturbance area suggests greater assertiveness in promoting aggregate rupture at desired locations. Along soil depth, the number of breaks promoted by CFO was approximately constant from soil level up to the tip of the subsoiler at 0.65 m. However, RCFO presented two distinguished break distribution, one referent to rotary hoe, from soil surface to 0.5 m, and other referent to subsoiler tip at 0.6 m. In both, the number of breaks were smaller then those promoted by CFO. Thus, the model and the implemented function quantified in detail the effects of each tool on the soil structure. As future development it is necessary to calibrate and validate the fragmentation parameters with empirical data.
DEM simulations and continuum modeling of size-segregation in bedload sediment transport.

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Keywords

size-segregation, bedload, DEM simulations, continuum modeling, inertial number

Abstract

Bedload sediment transport corresponds to the fluid-induced transport of sediment particles by rolling, sliding and/or saltating in the near bed region. It has major consequences for public safety, water resources and environmental sustainability. In mountain streams, steep slopes drive intense transport of a wide range of grain sizes implying grain size sorting or segregation, which makes prediction of sediment fluxes much more complicated than in mono-disperse systems.

In this work, insights on vertical size-segregation are obtained by studying the infiltration of fine particles into a bed formed of large spherical particles. Numerical experiments of two-size particle mixture have been performed using a coupled Eulerian-Lagrangian fluid-discrete element model developed at Irstea (Maurin et al. 2015, 2016). It is composed of a 3D discrete element model (based on the open source code YADE), describing each individual particle, coupled with a one dimensional Reynolds Averaged Navier Stokes model (Chauchat 2018). A 3D domain inclined at 10% slope (angle of 5.71°) consisting of an initial number of layers of 4 mm spherical particles deposited on top of a 6 mm particle bed, was submitted to a turbulent shear boundary layer flow. After a transient phase the hydrodynamic model reaches a steady state.

From the DEM simulations, the inertial number has been identified as the driving mechanism for segregation. In addition, the small particles have been observed to infiltrate as a layer of constant thickness which indicates that the bottom of the layer is a key position concerning the dynamics of segregation.

The problem has then been studied in the framework of a continuum model with the advection-diffusion model for segregation of Thornton et al. (2006). Based on the DEM simulations, a new form of the segregation flux is proposed giving remarkably good results when comparing both approaches. An analytical study of the segregation model with diffusion allowed us to demonstrate that the diffusion coefficient should have the same dependence to the inertial number than the segregation flux to predict the dynamics observed with the DEM simulations.
Fluid-particle interaction in granular material using coupled 3D LBM-DEM

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Keywords
Granular material, LBM, DEM, Fluid-particle interaction, LBM-DEM

Abstract
Fluid-solid particle coupling is a common phenomenon in natural and engineering problems. The combined numerical algorithm based on lattice Boltzmann method (LBM) and discrete element method (DEM) is used to simulate this process. The LBM-DEM coupling routines are presented, and a coupling engine in three dimensions is developed based on two open source computer codes: Palabos for the LBM and Yade for DEM. Two sets of tests are performed. A classic example of single sphere settling in fluid under gravity is used to validate the coupling engine, and the results agree well with the laboratory tests by Ten Cate et al. [1]. A ratio of 1/6 between the lattice size and the diameter of the spherical particle is suggested to obtain acceptable accuracy and computational cost. The second simulation shows the capability of the developed engine for complex coupling problems, in which the piping erosion process of saturated granular material is modeled and simulated, and some insights of the mesoscopic erosion mechanism is obtained. According to the simulation and analysis of the whole process of submerged granular collapse, it is suggested that the process is divided into four stages: start → rapidly collapse → decelerated sliding → standstill, and that the particle aggregate is partitioned into four zones: flowing particles, sliding particles, shearing particles and still particles. Both lay a foundation for getting insights into submerged granular disasters. The results of this study illustrate the outstanding capabilities of the LBM-DEM coupling method for mesoscopic mechanism exploration and engineering design improvement.

Reference:
Enhanced modelling capabilities of the discrete element method with deformable particles

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Keywords deformable particles, micro-macro relationships, Poisson’s ratio, elastic wave propagation

Abstract An original concept of the discrete element method accounting for deformability of cylindrical or spherical particles will be presented. The deformability of the particles in the new method, called the deformable discrete element method (DDEM) is taken into account in a simplified way which does not increase the computational cost of the DEM too much.

It is assumed that the particle deformation is composed of the global and local deformation modes. The global deformation mode is evaluated assuming a uniform strain in the particle induced by the volume-averaged stress derived in terms of the contact forces acting on the particle. The particle strains are obtained via the inverse constitutive relationship from the averaged particle stress. The linear elastic material model is assumed for the particle global deformation mode. The deformed shape (global deformation) of the particle is obtained by an integration of the particle strain. The local deformation modes are assumed at contact zones, and they are represented by the overlaps of the globally deformed particles. The normal contact forces are determined as functions of the overlaps.

It has been shown that the proposed method enhances the modelling capabilities of the discrete element method. Deformability of particle yields a nonlocal contact model, it leads to the formation of new contacts, it changes the distribution of contact forces in the particle assembly and affects the macroscopic response of the particulate material, in particular it allows to extend the range of the Poisson’s ratio which can be reproduced in the DEM, which is important, for instance in problems of wave propagation.

The performance of the DDEM will be demonstrated by simulations of the uniaxial compression of a cohesive material modelled with bonded particles. These simulations have been used to determine the relationships between the macroscopic effective elastic moduli and microscopic parameters of the new DEM. The DDEM model will be used to simulate elastic wave propagation. It will be shown that the new method allows us to reproduce better the ratio of compressional to shear wave speed.

Acknowledgement:
This work has been financed from the funds of Polish National Science Centre (NCN) awarded by the decision number DEC-2015/19/B/ST8/03983.
Micromechanical assessment of the installation and formation of Continuous Helical Displacement piles in sand

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Keywords
Continuous Helical Displacement piles

Abstract

Continuous Helical Displacement (CHD) piles are a form of low displacement cast insitu pile developed in the UK by Rodger Bullivant Ltd, which uses a bullet shaped auger head rotated in to the soil to a desired depth, before concrete is pumped in under pressure as the tool is reversed out producing a helical shaped concrete displacement pile. Due to the nature in which they are installed, the CHD piles show behaviour akin to both displacement and non-displacement piles. CHD piles have been shown to perform relatively well in terms of its load settlement behaviour, which is assumed to be attributed to the soil displacement around the tool during installation. It is still unknown how exactly this installation method affects the soil surrounding the final pile formation. Using the 3D discrete element method (DEM), an approach to modelling the complete installation and formation of the CHD pile on a soil sample has been developed. This allows the micromechanical assessment of features undetectable through physical testing methods alone. The local density changes and particle displacement that can be captured using DEM show how the installation of the CHD bullet causes soil disturbance through cavity expansion and contraction, and further expansion when the CHD bullet is extracted, and the pile is cast in its place.
182: Numerical simulation on the dynamic penetration of a light-weight gravity installed anchor in clay

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Keywords
plate anchor; booster; offshore engineering; dynamic penetration; numerical simulation

Abstract
A light-weight gravity installed plate anchor (L-GIPLA) is proposed and designed to fulfil the requirement for the deep water oil/gas and offshore wind power development. The newly developed L-GIPLAs are comprised of two triangular or peltate flukes to bear uplift resistance and two trapezoidal shanks. The padeye, which is used to connect the mooring line, is located at the tip of the shank. The anchor is designed with the ability of high capacity-to-weight ratio and diving property during keying. The dynamic installation of the anchor is achieved with the aid of a booster, which is connected at the anchor tail to increase the anchor kinetic and gravitational energy during installation. After installation, the booster can be retrieved and reused for the next anchor installation. Numerical analyses based on the computational fluid dynamics (CFD) approach were carried out to examine the penetration depth of the L-GIPLA in the lightly over-consolidated (LOC) clay. The effects of the anchor shape, impact velocity, strain-rate parameter and interface friction on the anchor penetration depth were investigated. Finally, an energy-based empirical equation was put forward for the sake of quickly estimation of the anchor penetration depth.
Numerical simulation on dynamic penetration of a light-weight gravity installed anchor in sand

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Keywords

plate anchor; booster; offshore engineering; dynamic penetration; numerical simulation

Abstract

To examine the dynamic penetration depth of an innovative light-weight gravity installed plate anchor (L-GIPLA) in sand, this study carried out numerical analyses based on the Coupled Eulerian Lagrangian (CEL) approach. L-GIPLA is proposed and designed to fulfil the requirement for the deep water oil/gas and offshore wind power development. The newly developed L-GIPLA is comprised of two triangular/peltate flukes to bear uplift resistance and two trapezoidal shanks. The padeye, which is used to connect the mooring line, is located at the tip of the shank. The anchor is designed with the ability of high capacity-to-weight ratio and diving property during keying. The dynamic installation of the anchor is achieved with the aid of a booster, which is connected at the anchor tail to increase the anchor kinetic and gravitational energy during installation. After installation, the booster can be retrieved and reused for the next anchor installation. The effects of the sand density, impact velocity, interface friction and the anchor shape on the anchor penetration depth were investigated. Finally, an energy-based empirical equation was put forward for the sake of quickly estimation of the anchor penetration depth. The numerical results indicated that the newly developed L-GIPLA provides a promising alternative for the offshore anchoring systems.
184: Analysing Earth Pressure Build-Up Behind Integral Bridge Abutments Using DEM

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Keywords
Integral Bridge, Earth Pressure, DEM

Abstract

Integral bridges do not have joints and bearings. In conventional bridges there is damage of the joints due to de-icing salts and accumulation of debris between the joints. This means a significant amount of maintenance has to be carried out on those bridges. In integral bridges the abutment is rigidly connected to the deck. As the deck expands and contracts with temperature changes, the abutment is subjected to a cyclic movement. This movement leads to settlement of the backfill soil adjacent to the abutment and build-up of earth pressure. Currently there is no guidance in the Eurocodes on the earth pressure build up and the developing settlement throughs behind integral bridges. There are two UK guides on integral bridges which include expressions for the earth pressure applied to the bridge abutments for use in engineering design.

Some insight into soil behaviour has been obtained using physical centrifuge models and settlement tests. This study aims to further advance understanding using discrete element method (DEM) simulations.

A DEM model was created using PFC2D. It is based on the centrifuge tests that were carried out by Lehane (2011). 300,000 non-contacting particles were generated inside a box. A particle size distribution (PSD) similar to Dunkirk sand was used. The particles were subjected to a scaled gravitational load, as in a centrifuge test and allowed to come into an equilibrium state. Subsequently, they were subjected to the cyclic movement of the abutment. In order to simulate the cyclic movement, one of the boxes walls was hinged and moved at a specified strain rate.

The settlement trough observed from the DEM simulations is in line with experimental observations. This study shows how DEM can be used to critically assess the stress paths used in laboratory experiments to study soil behaviour adjacent to integral bridges.
Microstructure and internal stresses of assemblies of crushable grains under compaction

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Keywords bonded cell method, brittle, fragmentation, Voronoï tessellation, microstructure

Abstract By means of the Contact Dynamics method, we simulate and analyze the microstructural process taking place during the compaction of crushable granular materials. This numerical study is performed using the approach known as Bonded Cell Method (BCM) [1,2], in which grains are considered as assemblies of polyhedral cells held together by an adhesive contact law. The loss of adhesive interactions is assumed to be irreversible and the cell-cell interfaces (fissures) are considered purely frictional. Different packings of crushable grains were built and subjected to uniaxial compression with different values of inter-cell strength (see Fig. 1). These tests allowed us to measure the fragments size and shape evolution as function of the vertical strain as well as to estimate the mean stresses perceived by each particle in the assembly. In particular, our observations revealed that (1) grain crushing produces a well-defined power-law distribution of fragments sizes, (2) the aspect ratio of fragments tends to a self-similar distribution (the silver ratio), and (3) fragmentation produces a generalized homogenization of stresses inside the particles restraining further crushing and deformation.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Snapshots of a sample under uniaxial compression at (a) the beginning of the test (intact configuration) and (b) after being applied an axial strain of 15\%.}
\end{figure}

Heat Transfer in Vibrated Granular Beds

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Keywords
Heat transfer, Vibrated granular beds

Abstract

The vibrated granular bed is an example of a highly non-linear, dynamical system which exhibits pattern formation and represents a good scientific model for understanding granular systems in general. Although various aspects of vibrated granular bed systems, such as mixing behaviors and pattern formation, have been investigated extensively both experimentally and computationally, it appears that studies of heat transfer and the potential of such granular systems to be operated as dryers have been limited to date. In this study, the Discrete Element Method (DEM) was coupled with a particle-particle heat conduction model for computational studies of heat transfer in vibrated granular bed systems. Depending on the vibration conditions applied, a hexagonal, stripes or cellular pattern was observed in the vibrated granular bed and the efficacy with which heat could be transferred from the vibrating base to the granular materials in the presence of different patterns was investigated. A parametric analysis was conducted to evaluate the effect of material properties such as thermal conductivity of the granular materials on heat transfer behaviors. Enduring particle-particle contacts were important for efficient heat transfer via particle-particle conduction throughout the bed of granular materials. On the other hand, vigorous vibrations of the base that imparted pseudo-thermal energy to the granular materials and led to good mixing of the bed facilitated heat transfer via particle convection. The simulation results were analyzed for possible relations between temperature distributions and granular temperature distributions.
Wear Mechanism of Coal-rock Transporting Equipment in Fully Mechanized Coal Face Based on the DEM-MBD

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Keywords
DEM-MBD, scraper conveyor, wear mechanism

Abstract
Scraper conveyor is the key transporting equipment in fully mechanized mining face. It undertakes the important task of transporting coal and rock. The wear problem caused by long-term transportation has become its main failure form. It is difficult to carry out underground test of scraper conveyor as the bad working conditions, difficulties of data acquisition and high risk. With the help of simulation, the research ideas for wear analysis of the scraper conveyor are provided. In this study, the transport process of scraper conveyor was simulated and analyzed by the combination of discrete element method and multi-body dynamic analysis method. The wear mechanism of scraper conveyor during transportation was revealed by studying the factors influencing wear, the distribution of wear area and tracking the change of coal particle positions when wear occurred. It is found that by coupling the discrete element method with the multi-body dynamics, the particle motion can be combined with the motion and force transfer of the equipment, which can reflect the wear of scraper conveyor more truly and provide a theoretical basis for its wear prediction.
Abstract
Considering a granular bed sheared by a turbulent fluid flow, bedload transport is defined as the particles transported in the vicinity of the bed, and for which the turbulent fluid coherent structures have a limited effect. Despite a century of applied research on the subject, bedload transport is still very poorly predicted in engineering applications. This limitation has led to fundamental work on the subject, considering idealized configurations in particular using spherical particles. In order to attempt to bridge the gap between fundamental and applied research, we study the influence of the particle shape in turbulent bedload transport. Using a fluid-discrete element model, we perform numerical simulations varying repeatedly the shape of particles made of spheres assembled together. This allows us to study the effect of the particle entanglement on the transport, and the interplay between the modification of the granular behavior and the fluid coupling.
Modelling of Granular Flow on Micro- and Macroscopic Scales with Calibration Using Experimental and Numerical Setups

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Keywords DEM, macroscopic modeling, calibration, flow properties, silo discharge, powders, granules

Abstract

1. Introduction Granular flow often shows complex correlations, whereby small differences in the granular composition can lead to significant different flow behavior. Therefore, obtaining valid parameters by calibration for each granular system is inevitable if high accuracy is necessary. In this contribution, calibration processes and their resulting precision and range of validity are discussed, while using different numerical approaches: The Discrete Element Method (DEM) and a macroscopic model based on Finite Volume discretization.

2. Methods Within the DEM framework, firstly introduced by [1], the motion of each particle is calculated based on interactions with contact partners and other applied forces. Contact forces are calculated by contact models, which consider material deformation and surface specific parameters like the Young’s modulus, particle friction coefficients and surface energy [2–4]. The macroscopic model is based on [5], whereby granular flow can be modeled in two regimes, namely dense and dilute systems. The spatial resolution is large in contrast to particle sizes. The calibration includes parameters like bulk viscosity, bulk energy dissipation, granular thermal conductivity and packing fraction relations [5, 6].

3. Contents of this contribution Firstly, the calibration of DEM parameters for a powder is described. This is achieved by numerical and experimental shear, rolling, nanoindentation and free fall tests [7]. After the parameters are obtained, DEM simulations are used to extract further information for the calibration of the macroscopic model. By extracting velocity profiles and shear stresses for different normal stress levels from the DEM shear cell (Fig. 1), the macroscopic model parameters are adjusted accordingly (Fig. 2). The obtained results are demonstrated with hopper discharge.

References

Cross-Scale Validation and Evaluation of Wurster Coating Processes

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Keywords CFD-DEM, Wurster coater, Validation, Scale-up, Heat and mass transfer

Abstract The Wurster process is commonly used to modify the release rate or the taste of granulated beads in the pharmaceutical industry. Hereby, beads are coated with one or multiple functional films that control the release of drug substances or mask a specific taste. The coating process takes place in the Wurster tube, in which the particles are transported centrally upwards followed by a subsequent downwards movement outside the tube. Thus, the particle flow resembles a torus-shaped recirculation pattern.

The inlet temperature of the fluidization air is adjusted such that the drying process of the sprayed particle occurs at a sufficient rate and that the correct film forming temperature is reached. The thermal effects are quite complex, and a thermal equilibrium inside the Wurster coater is reached only some time after start-up. Several combinations of operating conditions can lead to similar outcome in terms of this thermal equilibrium. However, experimental investigations show large deviations in the performance of the final product, i.e. the dissolution behavior of the API.

Due to the complexity of the process, recent numerical investigations were limited to simplifications regarding geometry, batch size or spray modeling (see e.g. Askarishahi et al. [1] and Pietsch et al. [2]).

In our work a fully integrated CFD-DEM environment is presented. The commercial code XPS (eXtended Particle System) is used for the DEM simulation and is coupled to AVL-FIRE™ for the CFD simulation. State-of-the-art models for momentum, heat and mass exchange between continuous and discrete phase are integrated in a fully coupled manner. Most importantly, a direct comparison of two different scales (i.e. lab scale Glatt GPCG-2 and production scale Glatt GPCG-30/60) Wurster coating processes is presented. Large scale experiments are performed to validate the numerical investigated operating points.


Comparing two Continuous Tablet Coating Process Scales Using CFD – DEM Simulation

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Keywords CFD-DEM, heat transfer, mass transfer, tablet coating

Abstract An important trend in the pharmaceutical industry is to move manufacturing processes from traditional batch to continuous process operation. This may allow for higher throughput rates, as well as more flexibility at the production site, a decrease of waste across the product lifecycle, and an increase in quality and safety. Tablet coating is often the last step in solid dosage form manufacturing before packaging. The reasons for tablet coating range from simple color coating, to adding protective functionality (environment, low pH of the stomach), to adding a second active pharmaceutical ingredient, or taste-masking.

Due to the rising demand for continuous production, GEA Pharma developed a semi-continuous tablet coater which can be incorporated into the ConsiGma 25 continuous line[1]. This new tablet coater operates at high rotation rates (Fr~1) and allows for short processing times, low changeover times and high throughput, while providing a good coating quality. The ConsiGma tablet coater can be equipped with two different drum sizes which are differentiated by the drum depth (160 and 320 mm). Both sizes are considered in this work.

Use of modern simulation technology can help to increase the understanding of the newly developed tablet coating processes. CFD-DEM simulations [2] allow a detailed investigation of the physical processes occurring during the coating process. CFD allows users to model the fluid phase through the tablet bed/coater geometry by tracking the velocity fields, heat and mass transfer rates and phase change (evaporation). DEM allows the tracking of the tablet movement inside the coater elucidating the tablet bed formation and mixing. This has the potential to reduce the amount of experiments needed to investigate potential failure modes without the risk of product loss. The goal is to compare the influence of the wheel width size on the coating process and the heat and mass transfer of the coater.

References:
Micromechanics of transient liquefactions in granular materials

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Keywords
DEM, micromechanics, instability, inertial transition, second-order work

Abstract

One of the fascinating features of granular materials is their ability to behave either like a solid or like a fluid depending on the loading conditions. This remarkable property results in a class of failure known as diffuse failure (or static liquefaction) mode responsible for dam failures, landslides or avalanches for instance. Because of the non-associated character of granular plasticity, standard instability criteria based on the concept of plastic limit surface fail to anticipate this type of failure and the loss of positiveness of the second-order work has to be considered instead. By taking advantage of discrete element modeling, this study investigates the micro-mechanisms responsible for transient liquefactions in granular materials at the scale of a representative elementary volume (REV) when the second-order work vanishes. It is shown that inertial transition results from the propagation of an outburst of kinetic energy consequently to the weakening of the contact network and to the deconfinement of force chains.
Abstract The current work has applied the Discrete Element Method (DEM) simulations in combination with experiments to study the effect of two different mills, an attritor and a planetary ball mill, on the transformation of \( \gamma \) alumina into \( \alpha \) alumina. Alumina exists under several allotropic forms (\( \kappa, \gamma, \delta, \theta, \alpha \)) with \( \alpha \) alumina being the thermodynamic stable phase. This can be obtained by calcination of \( \gamma \) alumina at temperature over 1200\(^{\circ}\)C[4]. \( \gamma \) alumina can be transformed in \( \alpha \) alumina either by thermal effects, raising the temperature, or by supplying mechanical energy at much lower temperatures [5, 6, 7]. Several studies reported in the literature have used high energy ball mills to induce phase transformation at room temperature but only some of them were successfully. From these researches it was highlighted that the best conditions for the conversion from the \( \gamma \) form into the \( \alpha \) form were by using conditions such as: a high bead powder ratio, large grinding media and media with high hardness [5]. In the current work, the simulations employed the open source DEM code LIGGGHTS (DCS computing, Linz, Austria) adopting the standard Hertz-Mindlin contact model to solve normal and tangential contacts. The motion of the grinding media, in both an attritor and a planetary ball mill, was modelled by DEM for a variety of conditions (speed, grinding media size). This allowed the study of additional information on the collision frequency and the impact velocity of the grinding media that was not possible from the experiments. The DEM particle information was then used for the calculation of both the average stress energy and the average specific energy, which represent the maximum energy theoretically transferable by the media to the alumina during milling. High speeds and large grinding media were selected for the milling experiments to obtain high stress energy within the mill. The material was milled for 4hr with a ball to powder ratio equals to 10 and then characterised for particle size measurements by laser diffraction, BET surface area by nitrogen absorption and X-Ray diffraction measurements. DEM simulations revealed that the planetary ball mill achieved stress energy levels two orders of magnitude higher than the attritor mill. This was in perfect agreement with the experiments that showed transformation of the alumina from \( \gamma \) to \( \alpha \) phase at room temperature only for the planetary ball mill, inferring that for the latter case the stress energy was probably high enough to overcome an activation energy barrier. In fact, in the planetary ball mill first signs of phase transformation were detected by XRD diffractograms already after 1hr of milling. In contrast, in the attritor mill the XRD diffractograms did not show any phase transformation not even after 4hr milling. The simulations pointed out that the media diameter is the most important parameter in order to maximise the energy per impact. Further, they showed that achieving a high energy per impact is more important than having a high global energy within the mill. Therefore, from these experimental results it can be hypothesised that an energetic barrier exists, and a minimum energy should be transferred to the material before inducing the transformation. This assumption was fully supported by the DEM modelling calculations of the stress energy done by simulations and it will be covered in the conference presentation, highlighting the ability of modelling to provide useful insight in complex processing systems.

References
Particle-scale analysis of soil arching during underground cavity formation using suction-tension model in DEM

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Keywords
Discrete Element Method, Arching, Cavity, Capillary forces

Abstract
Design of resilient infrastructure, including underground structures, is of prime importance in growing cities all over the world. However, in recent years, increasingly underground structures face many challenges. For example, an increased number of underground cavities have been reported, primarily due to defects in buried structures such as pipelines, box girders, etc. Such defects in underground structure can cause soil erosion if the structure lies below the groundwater table, eventually resulting in an adjacent cavity. Fluctuation of ground water level can promote cavity expansion and in due course cave-in incidents may occur. The necessity to repair the caved-in surfaces inhibits proper investigation of the underlying causes. The location of buried infrastructure plays a vital role in the cavity formation and propagation (Sato & Kuwano, 2015). Although groundwater fluctuation causes the cavity to expand, the arch formation around the cavity along with capillary forces acts to prevent it from collapsing.

Discrete element method (DEM) simulations have been performed using a modified version of granular LAMMPS software (Plimpton, 1995). Since the cavity formation is dominated by the presence of water in the soil, there are noticeable marks of soil suction and surface tension. To simulate the cavity experiments, the typical Hertz-Mindlin model was modified to introduce a ‘Suction-Tension’ model (Ji-Peng, Xia, & Hai-Sui, 2017). Since most of the cavities develop around underground structures lying beneath roads and highways, a cyclic surcharge load was applied on the top surface of the model to represent the effect of traffic loading.

Simulations were performed using both spherical and non-spherical particles in a rectangular 3D sample having a bottom opening of a certain size. Results showed that the cases without any soil suction could not sustain arching and the sample collapsed, whilst the introduction of suction-tension model held the soil structure firmly and a stable cavity with arching was formed. The cyclic loading tests revealed how the subsurface stresses are transferred around the cavity. Model cavity tests, using the spherical glass beads and silica sand of equivalent diameter to the DEM simulations, were performed to validate the simulation results and a good agreement was found between both approaches.

REFERENCES
Calibration and Validation of the Properties of Bulk Solids for Numerical/DEM Simulations of Industrial Processes

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Keywords calibration, bulk properties, DEM

Abstract In the chemical industry the majority of the relevant processes are not fluid processes but solid dominated processes. For the development of processes which are dominated by fluids, the application of Computational-Fluid-Dynamics (CFD) is nowadays more and more established in the chemical industry and becoming a standard tool as it already is in the automotive industry. In contrast to that, the application of Discrete-Element-Methods (DEM) for simulating the majority of solids dominated processes is still in an evolving stage. Although advanced commercial and open source software for DEM-simulations is available and their usage is well established, there are still challenges to face for a broader use of the DEM for developing, designing and optimizing granular processes in the chemical industry.

BASF’s point of view is that today’s main limitation is not the absence of reliable contact models but the absence of a standardized approach for calibrating bulk properties of technical relevant materials. To overcome this gap, BASF has participated in several EU-funded projects where several European universities and industrial companies collaborated. Defining a method to calibrate bulk material was one of the main project objectives.

However, using the projects’ results within industrial context requires additional effort which is related to the collection and evaluation of the findings. This step shall be the development and implementation of a calibration method in BASF. For that reason, BASF has been collaborating with experts in bulk mechanics as well as with experts in DEM modeling. Based on this collaboration an approach is presented which allows the standardized calibration of technical relevant bulk materials.

The standardized approach comprises the definition of reliable calibration experiments. For calibrating bulk materials applied in DEM simulations not only the calibration experiments are important but also the sequence to obtain a distinct parameter set. In addition, this sequence can depend on the process behind the calibration step. Furthermore, performing DEM runs for several experiments to calibrate the bulk material takes a lot of time. Each investigated bulk parameter has to be varied and compared to the experimental result until a certain agreement is achieved. To avoid this huge time and cost consuming effort, each experiment is built-up in a DEM framework. Every single experiment/simulation of this framework is mapped to a certain bulk parameter which is calibrated by the variation of itself in a simulation run. A parameter is considered to be calibrated if a certain quality criterion is achieved. These criteria are also presented and discussed. The final step is the coupling of all necessary DEM simulations required to determine the bulk parameters with a numerical optimizer.

Finally, a tool is available which allows the fully automated calibration of (non-cohesive) bulk materials. This method has been used in industrial projects, and some representative results are shown. In addition, the coarse graining of the particles and the scaling of their properties will be discussed as coarse graining is mission critical to simulate a process in technical size within an acceptable time frame.
200: Friction of wheat on corrugated steel. Experiments and Discrete Element Method modeling

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Keywords coefficient of friction, wheat, corrugated steel, dem

Abstract The friction between grains and walls of storage silo or handling equipment is an important factor in the design and operation of such structures. Characteristics of the friction can be measured in many different test devices but due to the lack of consistent theory experimental results are often not easy for interpretation. One of the simplest method to measure coefficient of friction is direct shear test. Corrugated steel walls have been in use to build grain storage bins for many years but details of deformation in grain - corrugated wall interface remain unclear.

In order to examine the critical test parameters associated with measurement of friction coefficient between wheat and corrugated wall a modified direct test apparatus was constructed and the process was modeled using Discrete Element Method (DEM). The modified device differ from the standard direct shear apparatus in the way that corrugated wall was pulled to create a shear plane as it moved within stagnant grain.

Numerical simulations were carried out using the Discrete Element Method as implemented in the EDEM software package. A wheat grain was modeled as a spheroid of volume equal to volume of the real seed. Multisphere method was used to approximate the spheroidal shape.

The coefficient of friction was found to vary as function of both, sliding speed and normal pressure. Experimental results showed that coefficient of friction increased with increasing velocity of shear and, in the studied range, decreased with an increase in the normal pressure.

Numerical simulations clearly reproduced sliding plane, typical friction force-displacement relationships were mimicked and simulations gave deeper insight into the micromechanics of the process.

An example of the simulations. Colors mark different velocities of grains in horizontal direction at steady-state flow. A scan of real wheat grain was imposed on the particles.
Keywords
FEMxDEM, multi-scale, contact law

Abstract
In the context of simulating the behavior of cohesive-frictional geomaterials under plane-strain deformation mode, we present specific advances in the development of a FEMxDEM double-scale numerical model. In this fully integrated approach, the macro-scale problem is resolved using the Finite Element Method (FEM); while at the micro-scale, a simulation using the Discrete Element Method (DEM) is performed on a periodic elementary volume, composed of a 3D spheres packing with a predetermined initial state. As the two models are used simultaneously, the later acts as a constitutive relation for the macro-scale simulation where each elementary volume, associated with an integration point, is continuously evolving with the imposed deformation. In turn, the FEM simulation is directly dependant on the state and properties of these granular arrangements representative of the behavior of the micro-structure.

In this communication, we present a damageable cohesive-frictional contact law at the level of the elementary volume for DEM simulations. Results from a number of simulations are also presented, demonstrating the mechanical behavior and localization characterization for this model under various stress paths and micro-structural arrangements.
Computationally generated rheology in non-cohesive granular Couette flows

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**Keywords**
Rheology, DEM, Couette granular flow, granular material

**Abstract**
Pharmaceutical, energy production and food processing industries have a lot of unit operations handling storage and transport of particulate solids. A fundamental but challenging question is how to control the flow state of granular materials in such operations, which leads to the study of rheology of granular materials. Rheology reflects the relation between stresses and strains in a material, which inherently determines the dynamic behaviors of granular materials. Carrying out the particle-scale dynamics simulation with DEM has the potential of providing detailed insights for exploring granular material rheological behaviors.

In our current research, we carried out DEM simulations of granular flows in a Couette cell, a prototype flow system in fluid mechanics. Through the analysis of the stress and strain information extracted from the simulations, we proposed a rheological correlation which well explains the stress-strain relation in the studied system as shown in the Figure. The developed rheological correlation can be adopted as a closure model in the continuum description of granular flows.

\[
\tau_{r\theta} = \eta \frac{dV_\theta}{d\tau}
\]

\[
\eta = \eta_1 + \eta_2 \\
\eta_1 = \frac{a}{\sqrt{T}} (1 - \phi/\phi_c)^{-1.3} \\
\eta_2 = \sqrt{T/\pi} f(\phi)
\]
A DEM modeling of biomass fast pyrolysis in a dual auger reactor

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Keywords
DEM, Biomass Pyrolysis, Dual Auger Reactor, Heat Transfer

Abstract
Biomass is a low-carbon renewable resource that has been used for thousands of years to provide heat and energy in rural areas. More efficient and clean ways of utilizing biomass such as fast pyrolysis were promoted in recent decades. Screw reactors are one of the commonly used reactors for biomass fast pyrolysis. In a screw reactor, mechanical forces are provided to the bed to enhance particle mixing and heat transfer, and achieve particulate matter transport for continuous operation. The pyrolysis process in the screw reactor configuration is a reactive granular flow system which involves particle flow, heat transfer and biomass devolatilization reactions at the same time. However, the reactor-scale evaluation of heat and mass transfer effects on the biomass fast pyrolysis is very limited.

In this research, we proposed an extended DEM method for modeling the reactive granular flow in a double screw reactor. The motion of particles is resolved with Discrete Element Method (DEM). The heat transfer model which takes into consideration heat conduction and radiation between particles was developed for predicting particle temperature evolutions. A semi-detailed biomass devolatilization kinetics is adopted in the simulation and the decomposition dynamics of the major biomass components and pyrolysis products are analyzed at different operating conditions.

Results reveal that the heat of pyrolysis needs to be considered for accurate prediction of biomass pyrolysis process in the reactor and the limitation factor in the biomass fast pyrolysis arises from external heat transfer to the biomass particles. The hemicellulose and cellulose decompositions are predicted to start around 480 K and 600 K, separately, and the predictions are in agreement with experimental studies. The yield prediction of tar vapor, non-condensable gas and char are in reasonable agreement with experimental studies considering the limitations of the model itself and the pyrolysis kinetics available in the literature.
Optimisation of ballasted tracks maintenance using DEM

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Keywords railway, track, ballast, maintenance, DEM

Abstract Maintenance of ballasted railway tracks has been heavily relying on empirical observations for decades. Railway companies are now investing in innovative approaches in order to be able to analyse and optimise the maintenance processes which are becoming stricter because of more frequent and heavier traffic. The discrete element method (DEM) is considered the most adequate approach to treat these problems because of the granular nature of ballast.

In the present study, the non-smooth contact dynamic (NSCD) approach of DEM has been used to analyse the interaction of different ballasted track maintenance tools with ballast in processes called tamping, dynamic stabilisation and crib compaction. Tamping consists in compacting the ballast under the railway sleepers after lifting them for track geometry correction (figure 1). Dynamic stabilisation consists in vibrating laterally the track to stabilise it after tamping. Crib compaction is an alternative to dynamic stabilisation which consists in compacting directly the ballast between the sleepers by applying a vertical load with vibrating plates. The DEM code called LMGC90 in which ballast is represented by polyhedra has been used to resolve different problems related to these maintenance processes.

Tamping is for example very aggressive regarding ballast. Solutions aiming at reducing ballast degradation due to tamping like ballast fluidisation using plate or needles, or tools insertion speed control, have been analysed, the latter being the most promising. Dynamic stabilisation efficiency depends on various parameters including vibration frequency, vertical load or rolling speed. These were analysed in a parametric study which pointed out the importance of rolling speed of the stabilisation equipment on the ballast density and the lateral resistance of the track which is crucial to avoid buckling of the track during high temperature variations. Although promising as an alternative to dynamic stabilisation thanks to its efficient compacting capabilities and related lateral resistance, crib compaction in its present conditions alters considerably the profile of the shoulder of the track (figure 2) hindering its compliance with the French railway network standards. Compared with dynamic stabilisation, it seems however more effective in correcting the heterogeneity of the ballast layer induced by the tamping process and a lateral resistance just 20% lower.

DEM proved finally an excellent tool to address this type of analysis and really helped improving the maintenance operations of ballasted tracks. This work is still under development. Efforts are under way to improve the accuracy of the process by introducing a multi-body module to LMGC90.
206: Numerical study on particle breakage and mechanical behavior of coral sand

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Keywords
Coral sand, particle breakage, triaxial compression test

Abstract

Breakage of particles has a significant impact on mechanical behavior of coral sand. This paper describes the numerical study on the effects of particle shape, particle size distribution, void ratio and confining stress on particle breakage and mechanical behavior of coral sand under conventional triaxial compression, using the commercial code PFC3D. A new method of using continuous triangular planes to simulate the membrane is proposed. Bond contact, allowing tension shear fracture within each coral sand particle, is adopted to explore the particle breakage. Validation of the model with consideration of the particle breakage is conducted by comparing the numerical macroscale response with the results from laboratory tests. With the validated model, macroscale behaviors of the specimen including the stress-strain relationship, volumetric strain, and state at peak strength are studied. And mesoscale behaviors at particle level including particle rotation, particle velocity, particle displacement of the specimens are investigated. Finally, the relation between mechanical behavior and evolution of particle breakage is studied. The numerical modelling of the particle breakage and mechanical behaviors of the coral sand is supposed to be useful for the future further study of the practical projects related to coral sand.
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Keywords Particulate process, Selective laser sintering, multiscale, virtual prototyping

Abstract Additive Manufacturing refers to a set of processes where a product is manufactured by depositing material. One of these techniques, which is gaining attention, is Selective Laser Sintering (SLS). Using this technology, aircraft components, medical implants, and even fashion products can be produced from particulate materials (e.g., granulated plastic, ceramic, metal). In the SLS approach, a three-dimensional object is formed by hardening selective regions of the raw material with a scanning laser. While some components of this process are well-understood at a macroscopic stress-strain level, very little is know about what is happening at the microscopic particle level. In addition, how microscopic changes affect the macroscopic domain, especially during the sintering process, cannot be reliably predicted. Therefore, the calibration of the SLS process relies on trial-and-error experiments.

In order to understand, predict, and optimize the mechanical performance of SLS, we propose a virtual prototyping (ViPr) approach, whereby the full process is simultaneously simulated at the macro- and micro- scale. Thus, we can model the whole physical system, ranging from the dynamic region where the laser impacts, to the heat-diffusion within the bulk material. This work uses the discrete particle method (DPM) to model the sintering region [1,2], while a continuum thermo-mechanical model is applied elsewhere [3]. The two models are coupled in an overlapping region using the coarse-graining technique [4], which obeys the macroscopic conservation laws of continuum mechanics. For computational efficiency, two open-source software packages are integrated into a single executable: oomph-lib as FEM solver [5], and MercuryDPM as particle solver [2]. Furthermore, goal-oriented mesh refinement will be used to determine when and where micro- and macro-model must be applied. Finally, for validation and calibration, rapid prototyping will be used to create miniature setups, which can be fully simulated.

References:
Critical time-step for DEM simulations using a Hertzian contact model and Euler integrator

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Keywords
discrete element method (DEM), time-step, Euler, velocity Verlet, integrator

Abstract

Discrete element method (DEM) simulations usually adopt an explicit, conditionally stable numerical integration scheme. The simulation time-step should be maximised to ensure simulation efficiency while ensuring the simulation remains stable at all times. A recent publication [Burns, S.J., Piirainen, P.T. & Hanley, K.J.: Critical time-step for DEM simulations of dynamic systems using a Hertzian contact model, Int. J. Numer. Meth. Engng.] has proposed a novel method to determine the critical time-step for two contacting Hertzian spheres using a velocity Verlet integrator, based on the fact that the discretised equations of motion can be analysed as a nonlinear map. In this paper, the methodology has been extended to a simpler Euler integrator. An explicit expression for the critical time-step is obtained in the absence of damping which is a function of particle shear moduli, radii, densities, Poisson’s ratio and the impact velocity of the particles. The expressions derived for critical time-step are the same for an Euler integrator as for a velocity Verlet integrator, i.e., the critical time-step does not depend on which integrator is selected. Increasing the impact velocity leads to a smaller critical time-step.
DEM analysis of residence time distribution during twin screw granulation

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Keywords
DEM, residence time distribution, twin screw granulation, wet granulation

Abstract
Twin screw granulation (TSG) became a popular wet granulation process in various industries, such as food, pharmaceutical, and fine chemicals, because of its high throughput, short resident time and reproducibility. However, there is a large parametric space in terms of screw design, formulation and operating condition, so how to maximise the production throughput while maintaining consistent quality of the final product is not a trivial task and still needs a comprehensive investigation. Different approaches, such as experimental study, population balance modelling and DEM simulations, were taken to explore the TSG by many researchers. Among these approaches, DEM simulations can not only provide macroscopic information but also microscopic insights into the complicated TSG process. Hence, in this study, DEM was employed to systematically explore the TSG process. DEM simulations were performed using conveying element, distribution element and kneading element within TSG separately. In addition, various staggering angles (30°, 60° and 90°) in the kneading element were also considered. The average particle velocity, resident time distribution, collision frequency and contact energy spectra were obtained from the DEM simulations for each individual screw element. It was shown that the powder flow behaviour depends significantly on the element type, the simulation can provide the insight of key physical features of each individual screws and can be used to optimise the TSG process.
210: A scaling approach for two-order faster CFD-DEM modelling of thermochemical behaviours in moving bed reactors

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Keywords
CFD-DEM; Scaling; Heat/mass transfer; Chemical reaction; Moving bed reactor

Abstract
Intensive heat and mass transfer between continuum fluids and discrete particulate materials plays a critical role in many chemical reactors. For example, the shaft furnace and the blast furnace in ironmaking are operated with continuous charge and discharge of solid materials, and it takes hours for the solid materials moving from the furnace top to the bottom. To understand and improve the operation of these reactors, discrete particle models are very helpful when combined with flow, heat and mass transfer, and chemical reaction models. However, due to the high computational cost with such discrete particle models, it is very challenging until now to study these slow and transient processes. Here, a scaling approach is established for the combined computational fluid dynamics (CFD) and discrete element method (DEM) modelling of moving bed reactors. The scaled model is first derived based on the governing equations of mass, momentum and energy and then applied to a moving bed reactor. The results in terms of flow, heat and mass transfer and chemical reactions with different scaling factors demonstrate that two-order acceleration can be achieved merely by the scaling approach. It is a critical step forward towards establishing virtual real-time thermochemical reactors with discrete particle models.
Abstract The implementation of the Finite Discrete Element Method (FEMDEM) in computational mechanics is becoming popular in industrial and university research sectors for problems seeking priority of accuracy over ability to process large particle numbers in granular flows. The Solidity FEMDEM code has been developed to solve solid mechanics problems. However, the accuracy of the Solidity code has never been thoroughly validated in terms of its contact mechanics and multi-body interaction behaviour, especially for the case of complex shaped bodies.

Figure 1: Comparison of the articulation of a rubber Core Loc tower as the base inclines from A to D taken at 5ms interval. Simulated tower (top) and actual experiment (bottom).

A validation study that compares laboratory experiments with simulation will be presented. The study uses complex shaped bodies such as cylindrical cogged shaped catalyst pellets and model scale breakwater armour units. The validation focuses on: (1) the mechanical response associated with single-body impacts, (2) the dynamics of multi-body interaction in body translation and rotation (Figure 1), and (3) the multi-body interactions of complex-shaped particles in pile column and their force chain mechanism for load transmission. Quantitative and qualitative assessments have been performed showing encouraging agreement between simulations and experiment results.
Lattice Boltzmann simulations of porous particulate flows

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Keywords Porosity, Permeability, Porous Particulate Flows, LBE, Volume-Averaged Macroscopic Equation

Abstract The comprehensive understanding of the particle-fluid interaction is very important for fluid-particles system, and thus many studies have been conducted for the particle-fluid system \(^1\)-\(^3\) of solid impermeable particles. In the real industrial fields such as the catalyst process in chemical engineering \(^4\), the particles usually possess the porous structure which will have effects on the fluid-particles interaction \(^5\)-\(^6\). However, there has been little open literature discussing the particle-fluid system of porous permeable particles. Therefore, the objective of the present study is to investigate the effect of the porosity and permeability on the porous particulate flows which are formulated by the volume-averaged governing equations \(^7\) in terms of intrinsic phase average velocity. The lattice Boltzmann equation model (LBE) \(^8\) is used to solve the governing equations. Firstly, we validate the LBE model by the numerical results existing in the literature for the flow around and through one porous particle. Then, the porous particles settling against gravity in a quiescent fluid, i.e., the DKT process \(^9\) for porous particles, is investigated. The effects of the porosity and Darcy number on the porous particulate flows are studied numerically in details. Also, we present the simulation results of the fluidization of 512 porous particles. Our results demonstrate the significance of the porous structure of particles for the particles dynamics behaviors.

Reference
Granular shear flows of frictionless and frictional cylinders with different particle size distributions

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Keywords
Discrete Element Method, granular flow, cylindrical particle, particle size distribution

Abstract
Granular shear flows of cylindrical particles are numerically investigated using the Discrete Element Method (DEM). The impact of particle size distribution on the flow behavior and stresses has been explored by adopting two types of particles (frictional and frictionless) in binary and Gaussian size distribution respectively. Without friction, due to the interaction of particles in the mixture, the alignment of longer particles is weakened, while the alignment of shorter particles is enhanced. The increasing volume ratio of a species of particles in a binary-sized system causes the stress to develop towards the monodispersed stress of this species. In Gaussian system the stresses are insensitive to the standard deviation of particle length distribution. In shear flows of frictional particles, the stress increases sharply with intense fluctuations when solid volume fraction reaches the jamming point, jamming point can be defined as the point with maximum stress fluctuation or maximum stress increase rate. In both binary and Gaussian size distribution systems, the critical solid volume fraction for jamming decreases with the increasing average particle aspect ratio. Meanwhile, for systems with the same average particle aspect ratio, jamming occurs at a higher solid volume fraction for the higher polydispersity. The results from this study may be useful for the development of constitutive models for the granular flows of polydispersed, non-spherical particle systems.
Effect of height of fall on coke collapse in a simplified model of blast furnace

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Keywords
Coke Collapse, Blast furnace, Heap

Abstract
The blast furnace is a key process unit in the manufacture of steel in which iron ore is chemically reduced to molten metal at high temperature. Coke and ore are fed alternately at the top of the blast furnace by means of an inclined chute rotated about its vertical axis. For each rotation, the particles fall on the sloping burden form a circular ring. Charging of this metallic ore burden over the layer of coke causes a portion of the coke layer to get dislodged from its original position. This phenomenon is known as coke collapse. We have studied the effect of height of fall on coke collapse in a blast furnace using quasi two dimensional rectangular bins (two vertical glass plate separated by a gap of 10 mm). In-order to get the desired density difference between the pouring media, stainless-steel balls of size 1.5 mm (representing the ore) and glass-beads of size 2.55 mm (representing the coke) are used as a model granular materials. The key parameter in this study is height of fall (HOF). We have performed experiment for fixed volume of pouring and size of particles (steel ball) by varying height of divider from the bottom of the bin. The images are captured using a Nikon-DX camera and analyzed using computer code to determine the position of each particle (steel ball and glass bead). The results presented here are in terms of concentration of steel balls by making bin of size 5 x 5 mm. The interface line between steel ball and glass bead is analyzed separately and plotted for all data sets. Each experiment is repeated three times to get an average data.
A micromechanical, μUNSAT, approach for wet granular soils: Toyoura sand case study

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Keywords wet granular soils, Toyoura sand, effective stress

Abstract Granular soils handled by civil engineering operations are often to be found in an intermediate state of water saturation. Following Chateau & Dormieux [1], we propose a micromechanical approach, combining analytical homogenization with Discrete Element Method simulations for a better understanding of the mechanical behavior in wet conditions, and its possible interpretation in a stress-strain-strength effective stress framework.

Analytical homogenization first leads to a micromechanical, so-called μUNSAT, expression for the stress state of wet granular soils, whereby all internal forces are accounted for, through:

- a so-called contact stress accounting for the contact forces between solid particles, being equal to the total stress in dry conditions;
- additional capillary stresses which include both the pressure difference between air and water, and the air-water surface tension. The corresponding internal forces are described within the bulk fluid volumes, within the fluid-fluid interface, as well as along the solid-fluid interfaces, through tensorial terms. The tensorial (non-spherical in general) nature of the expressions aptly describe preferential directions for those internal forces, corresponding for instance to the orientations of the wetted solid surfaces, which sustain water pressure along their normals only [2,3].

Then, a recent DEM model [4,5] allows us to present new applications of the μUNSAT approach, to the case of Toyoura sand in the pendular regime. In line with recent results on other granular materials [6,7], the combination of DEM with the μUNSAT expressions demonstrate:

- the tensorial nature of the capillary stresses;
- the stress-strength effective nature of the contact stresses, with a unique, cohesionless, failure description of dry and wet conditions;
- a limited stress-strain effective nature of the former. Similar stress-strain behaviors are actually observed along contractant loading paths and for dense samples, where energy dissipation phenomena are less marked.

217: A framework for the simulation of coupled thermal-hydraulic-mechanical processes in discrete element systems

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Keywords
yade, extensible, thermal, hydraulic, mechanical, THM, DEM, open source

Abstract
This presentation outlines the theoretical framework and practical implementation of a fully Thermal-Hydraulic-Mechanical model, ThermalEngine, in Yade (Smilauer 2015). Yade, an open source software, is combined with a thoroughly validated Pore Finite Volume (PFV) scheme (Chareyre 2012, Caulk 2019) to simulate pore-scale fluid fluxes and poroelasticity. These pore scale fluxes are reused to enable a highly efficient heat advection scheme based on conserving pore energy. Conductive heat transfer is solved explicitly in time by conserving energy and modeling heat fluxes between pores and particles with classic heat transfer models. Particles and pore fluids thermally expand or contract based on temperature changes, which enables estimates of volume changes that are superimposed on the rate of volume change used for the solution in the PFV scheme. In addition to the theoretical framework, the practical parallelization of these methods in Yade open source code is discussed. Toward application, the conduction model is analytically verified with a simple 1D case, the advection model is numerically verified with a finite element comparison, and the fully coupled thermal-hydraulic-mechanical model is experimentally/numerically validated with literature-based data. Following the validation, a brief overview of the accessibility and flexibility of the source code is presented for prospective users and applications.
Thermal-hydro-mechanical coupling simulation by using the discrete element software MatDEM

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Keywords
coupling, MatDEM, millions of elements, GPU

Abstract
Large deformation, failure and thermal-hydro-mechanical coupling are involved in many modern engineering construction, such as tunnel excavation, hydraulic fracturing and so on. Failure processes can be well simulated via discrete element method. However, DEM based multi-field coupling approaches and corresponding software still are lack. During the last seven years, we developed a three-dimensional discrete element software MatDEM. Based on innovative GPU matrix computing method, it can handle millions of elements in one computer. To address the multi-field coupling issues, the numerical simulation of heat generation and energy conservation is implemented in the software; heat conduction and thermo-mechanical coupling simulation are carried out based on the idea of finite difference; a discrete element pore density flow method is proposed to simulate fluid-solid coupling processes. The source code of examples and the simulate results are available on http://matdem.com.
Automatic training of discrete element model with specified mechanical properties

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Keywords
automatic training, conversion formulas, macro-micro, MatDEM

Abstract
Rock is represented by an assemblage of a series of bonded elements in discrete element method. Generally, the discrete element modeling relies on troublesome calibration processes to determine the correct inter-element mechanical parameters. We derived the conversion formulas of close-packed model. In the formulas, inter-element parameters can be determined according to mechanical properties of model, including Young's modulus, Poisson's ratio, tensile strength, compressive strength and coefficient of internal friction. Based on the formulas and an automatic training method, we are able to obtain a discrete element model with specified mechanical properties automatically. The method was implemented in our software MatDEM, which can handle millions of elements in one GPU. A series of examples will be shared, including landslides, microwave breaking rock, shear box test and heat-mechanical coupling of pile, etc. The MatDEM software and the code can be downloaded from the website http://matdem.com
220: Experimental Measurement of the Coefficient of Restitution of Peas

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Keywords
experiment; coefficient of restitution; peas; high-speed camera

Abstract
The unique characteristic of grains being a typical granular material determines the production efficiency of processing, storage and transportation processes.

The application of DEM simulation can optimize the equipment production by effectively solving the existing problems in terms of grains storage, transportation and processing, which in turn increase the efficiency at each level of production and thus decrease the cost of production.

In DEM simulation, the key to an effective simulation result is to ensure that the parameters of grain material properties are input accurately. Among the parameters, the coefficient of restitution of grains is important.

Taking peas as the research object, this paper presents the deficiency of using high-speed cameras in obtaining the coefficient of restitution of grains. Through improvisation, a new experiment device is designed. The coefficient of restitution of peas obtained from the experiment in using the new device. It is applied in the simulation of the transportation process. Assist the researchers to analyze the reasons for equipment damages in the warehouse and propose viable solutions.
Dust pick-up rate for upright vacuum cleaner with rotating brush on the carpet tufts investigated by 1-way CFD-DEM coupling with bonded particle models

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Keywords DEM, BPM, Upright vacuum cleaner, dust pick-up rate, CFD

Abstract As the enhancement of industries, vacuum cleaners for family use have been developed and are steadily evolving to efficiently remove large and small dust. The dust pick-up rate generally decides the performance of a vacuum cleaner. It is well known that the dust pick-up rate depends on the type of cleaner, the type of floor, the cleaning time, the physical properties of the rotating brush in the head, the traveling speed of the head and so on. However, traditional studies have been dependent entirely on experiments, and only the pick-up rate before and after the experiment has been macroscopically compared, so that the microscopic mechanism of actual dust pick-up inside the rotating head of the brush has not been elucidated. In order to clarify this mechanism, it is necessary to measure the behavior of dust particles in the head in real time, but in the experiment it is almost impossible due to the opacity of the head part and the carpet. Therefore, in this study, we investigated the dynamic behavior of dust particles in a carpet cleaner by Discrete Element Method using Bonded Particle Model. The simulation was modeled on the basis of upright-type on wool carpet with actual cleaners.

Dust pick-up rate is inevitably affected by the flow pattern between the head and the carpet, and the strength of the carpet tufts / rotating brush. In addition, numerous carpet tufts and many rotating brushes continuously create numerous collisions, i.e., multiple contacts, during cleaning. In particular, the collision of carpet tufts and rotating brushes can be considered as fiber-fiber contacts with long slender shape in modeling. For the deformation of carpet tufts and rotary brush, modeling of bending deformation is inevitable, and because the amount of deformation is large, it generally shows nonlinear-deformation. Therefore, the discrete element method based on BP Model was used to solve the problem of multiple contact and nonlinear bending deformation. In order to confirm the accuracy of the discrete element method based on BP model, the tensile, bending and torsion tests of the BP model were compared with theoretical results, and all of them were found to agree fairly well within 5% error.

The flow pattern between the head and the carpet was analyzed using CFD, and the result was analyzed by 1-way coupling by Discrete Element Method. The CFD analysis results without laden particles were coupled with the discrete element method by drag force.

In addition, the air flow acquired by CFD thrust the dust particles and the particles moves in accordance with the collision with the carpet brush / rotary brush based on Discrete Element Method. Therefore, the dynamic behavior of the dust particles inside the head can be accurately investigated, and it is possible to analyze the flow pattern in the front part and the rear part of the cleaner head. Therefore, based on these results, it is expected that further research will be conducted to improve the dust pick-up performance of the cleaner.

This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (NRF-2018R1A2B2004207)
Coupling heat conduction and fracture to model thermal shocks with DEM

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Keywords fracture, thermal shock, heat transfer, crack nucleation, crack propagation, DEM

Abstract Crack nucleation and crack propagation are ubiquitous in engineering applications and in natural processes. Thermal shocks are a good example of phenomena with complex crack patterns. The numerical simulation of thermal shocks is challenging when the goal is to explore both crack nucleation and propagation [1]. Thanks to its capability to account for topological modifications (crack growth, branching, ...), DEM is a powerful tool to tackle thermal shocks. Still, there are very few examples of DEM being used to model thermal shock or thermal cycling [2]. Here, we investigate the classical problem of a sample initially at a homogeneous temperature and quenched in a cold bath for which detailed experimental results exist [3]. The plate is discretized using a random packing of particles with elastic properties calibrated as described in [4]. The particle size used to discretize the plates governs the fracture toughness of the material and can be seen as a material internal length. DEM simulations are carried out in quasi-static conditions. We model heat transfer and thermal expansion on this discretized plate. The Griffith length, which describes the severity of the thermal shock [1] dictates the crack pattern. In accordance with FEM numerical results [1] and experimental data [3], we show that mild shocks (large Griffith length) result in none or few cracks while severe shocks (small Griffith length) lead to multiple cracks with a periodic pattern. We observe that initially a homogeneous damage arises with short cracks growing. A selective propagation phenomenon arises and some short cracks stop while other develop to longer cracks. The length and spacing of these cracks agree very well with the experimental data (see figure).

Experimental (top, [2]) and DEM results (bottom) for mild (a) and severe (b) thermal shocks.

High-stress impact-abrasion test by Discrete Element Modelling

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Keywords particle impact, abrasion, test, DEM

Abstract We present a Discrete Element Model (DEM) of the impeller-tumbler wear test which is used to study high-stress impact abrasion mechanism on steel plates with the use of granite particles as abrasive materials. A DEM calibration procedure of the granite particles is first performed to set particle-scale DEM parameters such as density and frictions. Using this calibration, simulations of impeller-tumbler wear test are realized and show a qualitatively agreement with experimental observations. Notably, tested sample edges are first abraded as in the experiments. Also, simulation results show a linear increase of the abrasion energies collected with the time on the steel plates which is in accordance with the linear time evolution of sample mass loss in experiments. A numerical parametric study is realized to better understand operating conditions of the test varying the rotating speeds of the impeller and the tumbler. In addition, the DEM model permits to investigate abrasion phenomena by local measurements in the simulation of forces magnitude, impact velocities and abrasion energy locations which are difficult to assess in experiments.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{granular_flow.png}
\caption{Granular flow inside the tumbler-impeller tester. Particles are colored by velocity norm from small in blue to high values in red.}
\end{figure}

Particle velocity (m/s)
Yade - Open Source Discrete Element Method

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Keywords
DEM, C++, Python, fluid coupling

Abstract
Yade is an extensible open-source framework for discrete numerical models, focused on Discrete Element Method. The computation parts are written in C++ using flexible object model, allowing independent implementation of new algorithms and interfaces. Python is used for rapid and concise scene construction, simulation control, postprocessing and debugging.

The development group is international and open to new contributors. Development is kindly hosted on launchpad and GitLab; they are used for source code, bug tracking and source downloads and more. Building, regression tests and packages distribution are hosted on servers of the Grenoble Geomechanics group at Laboratoire 3SR and UMS Gricad. Binary packages are distributed for Debian linux distributions and derivatives (Ubuntu), stable versions are available in the standard linux repositories.

Yade features a large variety of contacts models, various methods for non-spherical particle shapes, and structures such as wires, meshes, and membranes. A number of algorithms are included in the source code for simulating fluid flow and partial saturation. Yade also enables couplings with third party code such as Escript or OOFEM.
Examining roller screen performance to categorize iron ore green pellets to optimize pellet induration

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Keywords Discrete element method, Simulations, Mining, Roller screen, performance, pellets, optimization

Abstract Within the iron ore mining industry, roller screens (Figure 1) are used to segregate green iron ore pellets, which are weak and easy to break, to a size range of around 8-18 mm (on-size) from a raw pellet size range of between 6–20 mm in diameter (Silva et al., 2018). This is done by depositing the raw pellet stream onto a roller screen consisting of several sections of rolls with different gaps to remove undersized pellets (<8mm), segregate on-size pellets (8-14 mm) and allow oversized pellets to run off the end of the screen. The on-size pellets are hardened in an induration furnace prior to transport. The permeability of the on-size pellet bed allows ready flow of hot gases through the pellets reducing fuel consumption of the induration furnace, increased productivity and improved the quality and uniformity of hardened pellets. Oversized and undersized pellets are returned to pelletizing drums or discs for reprocessing (disc return rate). Optimizing the screening process to reduce the disc return rate and contamination of the on-sized pellet stream by oversized and undersized pellets can further increase the productivity and reduce costs of the pellet induration process. As it is cost prohibitive to experimentally examine the factors affecting roller screen performance, we use the discrete element method to extend the range of parameters examined by Silva et al. (2018), who found that reducing the gap between rolls in the section to remove undersized pellets from 8.8 mm to 7.5 mm the loss of undersized pellets is reduced significantly and the disc return rate reduced by more than half.

In this presentation we present roller screen pellet segregation performance as function of roll length, diameter, surface properties, and frequency of rotation. We examine the influence of the length of each of the three roller screen segments used to categorize undersized (< 8 mm), on-size (8-14 mm), and on-size (>14–18 mm) on the loss of on-size pellets and discs return rate. We also examine the effects of pellet properties on roller screen performance that include pellet adhesion/cohesion, shape, modulus, feed rate, particle size distribution, and strength (by monitoring impact forces). We then describe the set of parameters that may optimize screen performance by minimizing the discs return rate and contamination of on-size pellets.
A hybrid pore network - LBM method for integrating flow of immiscible phases in DEM.

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Keywords capillarity, surface tension, drainage, simulation, pore scale, hydromechanical coupling

Abstract Simulating complex hydro-mechanical couplings in large grain-fluid systems is a great challenge for the discrete element methods (DEM). For materials saturated by only one pore fluid, recent advances in pore-scale methods (in which the porosity is discretized as a network of connected pores [1]) enable the resolution of large coupled problems in three dimensions. These methods can reflect the dominant viscous terms at the particle scale without actually solving a Navier-Stokes problem [2]. The computational cost is thus reduced by orders of magnitudes, which opens up more realistic simulations - as illustrated by a few recent examples.

In this presentation the following question is examined: can the pore-scale approach be extended to multiple (two) immiscible pore fluids to simulate the so-called unsaturated materials? Numerical models of partially saturated granular materials based on the DEM have been used extensively, yet the majority of them are strongly limited to the so-called pendular regime in which the wetting phase is present in such a little amount that it only forms pendular bridges associated to pairs of particles. In the other saturation regimes one hardly avoid time consuming surface minimization techniques or even the direct resolution of a 2-phase fluid dynamics problem at the microscale to capture the geometry of phases and interfaces. The pore-scale approach of this problem aims at a drastic decrease of this computational cost. We show how the movements of the fluid phases and the fluid-solid interactions can be described by introducing relevant geometrical objects in a tetrahedrized granular domain, together with evolution laws. For a range of micro-scale processes this approach is successful and for instance, the primary drainage of a saturated sample can be reproduced accurately[3]. Unfortunately, a number of processes remain which still need significant efforts from both phenomenological and algorithmic points of view, such as bubble entrapement, coalescence of wetting phases, or viscous effects leading to mixed scenario of drainage-imbibition at the local scale.

A general framework is proposed in which the zoology of the pore-scale objects and their behavior is improved with the help of direct simulations with the Lattice-Boltzman method (LBM). Domain decomposition applied to a large granular specimen lets one identify relevant elementary units of the micro-structure made of less than a dozen particles typically. The LBM responses of these elementary units under particular boundary conditions are used to assemble a global two-phase flow problem to be solved by a pore-network solver, in a multiscale coupling. The numerical framework is evolutionary in the sense that the results it produces may help developing progressively analytical relationships between the hydrostatic properties of the elementary structures (such as the threshold values of capillary pressure for drainage/imbibition of one pore) and their geometrical parameters. Ultimately, the LBM resolution may only be required for a selection of subdomains where the process is too complex, while the evolution of the fluid phases in the most conventional subdomains would be entirely governed by analytical laws.

Network analysis of velocity fields in moving granular media

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Keywords DEM, granular media, graph, network, community detection, algorithm, simulation

Abstract Discrete element modeling provides information about the states of individual particles of granular media, such as positions, velocities, contact forces, etc. (microstate), while experiments and practical applications involve the bulk parameters. Therefore, techniques and algorithms are needed to process the DEM simulation data in order to derive the bulk behavior of granular media in the respective setups. Macroscopic behavior of granular media arises from certain coordination of individual particles giving rise to emergence of larger scale structures. An example of such structures are force chains that influence the bulk mechanical properties of granular medium and phenomena therein, such as jamming. Similarly, the nature of granular flows is influenced by emergence of particle groups moving in a coordinated manner. Collective and coordinated motion of particles influence the macroscopically observed phenomena, such as hopper discharge, avalanches at inclined surfaces and similar. Analysis of such phenomena benefits from detection of groups of particles moving in a coordinated manner, having the data (velocities and positions) of individual particles obtained by DEM simulations.

In this presentation, we propose the method for detection of particle groups involved in collective motion based on network analysis. Knowing the positions and velocities of individual particles, a “velocity similarity graph” is built, where the graph vertices represent the particles. The vertex pairs are connected by the edge if the distance $d_{ij}$ between the respective particles is small enough: $d_{ij} \lt r_i + r_j$, where $r_i$ is the $i$-th particle radius, $f_i$ is a certain selected factor. The edge weight is calculated to be inversely proportional to the difference in the respective particle velocities, i.e., the vertex pairs representing nearby particles having similar velocities are connected by edges of larger weight. It can be expected that the particle groups moving in a coordinated manner will have similar velocities, therefore, the corresponding vertices in the graph will have stronger connections among them. Having produced the velocity similarity graph, identification of particle groups becomes equivalent to the problem of identification of vertex groups that are more tightly connected to each other, known as “community detection” in graph analysis [1]. This problem is a topic of active ongoing research and a number of community detection algorithms have been created. The techniques developed for graph analysis can be therefore applied for analysis of granular media motion. A similar approach have been already applied for analysis of force chains in stressed granular matter [2,3].

Using the above approach, we analyse the flow of granular media in a rotating drum (in the Figure, the velocity fields are shown in granular media in the drum at two different time moments, as well as particle groups detected by the described method; the group boundaries are shown in black contours). The relation between the properties of groups of vertices identified in the graph and the mechanical phenomena in the underlying granular states are analysed.

Simulation of high resolution turbulent flow through accurate packed bed topology using an immersed body FEMDEM/CFD coupled method

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Keywords Combined Finite-Discrete Element Method, Turbulent flow, Packed Bed

Abstract Flow in packed beds has been studied for many years as it is of fundamental importance to many industries: chemical engineering, pharmaceuticals, metallurgical, and nuclear reactors, etc. Numerous models have been developed to simulate the flow and transport in packed beds. Hu (Hu, 1996) applied a generalized Galerkin finite element method based on moving unstructured grids and an arbitrary Lagrangian-Eulerian (ALE) technique to simulate the interaction between particle and liquid. Glowinski et al., (2001) developed a ‘fictitious domain’ method in which the whole is discretized into a fixed mesh, and a superimposed solid mesh locates the particles. However, these models are limited to simulating laminar flow and originally included only spherical/circular particles.

In this paper, we will present a new fluid-solid coupling method, the immersed body method, for simulating flow and pressure drop in packed beds. In this method, a new Reynolds Averaged Navier Stokes (RANS) turbulence model coupled with an immersed-body method is developed to model fluid-solid coupling for turbulent flows. This model couples a combined finite-discrete element (FEMDEM) solid model and a finite element fluid model with the often-used standard $k−\varepsilon$ model. A thin shell mesh surrounding the solid surface is used as a delta function to apply the interface boundary conditions for both the turbulence model and the momentum equation. In order to reduce the computational cost, a log-law wall function is used in this thin shell to resolve the flow near the boundary layer. Coupling between solids and fluids is realised using a dual mesh approach. One mesh is used across the whole solution domain on which the fluids equations are solved and the second mesh contains a finite element representation of the solid (particle packing) structures. Adaptive meshing resolves down onto the complex geometry of the particles at the level of detail necessary, hence addressing one of the main challenges—the accuracy of the flow field near the surfaces of the particles and container walls and the capture of boundary layer effects. The forces and volume fraction from the FEMDEM structure model are mapped onto the fluids mesh using Galerkin projection. A FEMDEM code, Solidity, is used to generate particle packing for fixed beds (see Figure 1). The particle Reynolds number is varied from 4000 to 32000. The results are in good agreement with the available experimental data. The methodology is applicable to the capture of possible solid particle displacements. Such two-way coupled behaviour bears a significantly higher computational expense than fixed bed systems.

Figure 1 Spherical particle packing (bottom) and axial packing density (top)


232: dp3D: a DEM code dedicated to materials science

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Keywords
materials science, DEM, sintering, compaction, composites

Abstract
Materials for engineering applications often exhibit a discrete nature. Metallic, ceramic, and polymer powders offer an obvious example. Powders are the initial form of many materials and are very frequently the unique route to process materials such as ceramics, composites, and nanostructured alloys. Even if the material exhibits a continuous nature, its processing or its operating behavior may trigger a discrete response. For example, a dense brittle ceramic may be submitted to a thermal shock that will cause nucleation and growth of multiple cracks, thus revealing some discrete microstructure. dp3D is an in-house DEM code that has been developed now for more than 15 years at SIMaP laboratory to model those engineering materials. Specific interaction laws have been implemented to tackle materials science applications. Powder compaction, with particular attention for submicronic powders and plasticity, has been investigated. High temperature processing such as sintering requires specialized interactions that are available in dp3D. In all cases, the focus is to allow the user to enter directly properties that are characteristic of the material to process (elastic properties, surface energy, yield stress, diffusion coefficients, ...) instead of calibrated stiffness or damping coefficients. Fracture of porous materials or of dense materials may also be treated. In this contribution, we review these possibilities through some examples. In particular, in the context of materials science investigations the coupling of X-ray tomography images and dp3D is considered. We also discuss the use and the development of the dp3D code.

Two examples of materials science applications with dp3D: a) Sintering of a porous electrode imaged from X-ray tomography. b) Crushing of two dissimilar spheres and the c) corresponding SEM experiment.
Particulate system simulations using FDEM

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Keywords Blockiness, shape descriptor, packing, granular

Abstract Geomaterials particulates, whether natural deposits, extracted and comminuted mineral fragments or materials used in construction such as larger aggregates, rockfill and rock blocks for armouring coastal structures, exhibit granular behaviour that is in part dependent on particle shape. If their granular behaviour is to be simulated, shape descriptors that take some account of their particle shape may be required. With the revolution in real shape capture through X-Ray CT imaging of bounding surface coordinates, 3D photography, big data processing and discrete particle modelling capability, it is timely to revisit the parametric characterisation of particle shape in the context of simulation. Popular descriptors of geological grains have historically included aspect ratio, sphericity and Krumbein’s roundness. With modern technology, digitally represented and triangular meshed particle surfaces provide an opportunity to reconsider the most effective combinations of shape descriptors for use with DEM and FEMDEM simulation.

In this work we report on the potential of a Blockiness parameter, $BLc$ (Fig. 1) currently used in characterising rock armourstone used in coast protection structures. Blockiness, $BLc$ is simply given by the percentage of the minimum bounding box volume (XYZ) that is occupied by the particle. A readily executable brute force bounding box algorithm is described that is computed ‘on the fly’ along with other shape descriptors, for each new particle added to a digital shape library of polyhedral grain shapes (Latham et al., 2008).

In this work we use the FEMDEM code, Solidity to investigate the circumstances in which a mono-size mono-shape assembly of rock pieces tends towards a higher or a lower packing density as a function of $BLc$ and the role of additional independent shape descriptors such as aspect ratio. As cubes will readily tessellate and fill space with low or zero void space, especially if vibro-compacted and if friction is low, greater frequency of face-to-face contacts and consequently greater packing density might be expected in higher Blockiness particulates. The paper will discuss packing density results for a suite of rock fragment shapes.

A guideline for quick LBM-DEM simulations

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Keywords: Fluid-particle simulation, granular collapse, LBM-DEM

Abstract: A systematic study is carried out on a fully resolved fluid-particle model which couples the Lattice Boltzmann Method (LBM) and the Discrete Element Method (DEM) using an immersed moving boundary technique to understand the roles of major numerical parameters (resolution N and relaxation time τ) in terms of accuracy, stability and efficiency. A series of benchmark cases with a wide range of Reynolds number are performed, starting from a single stationary particle to multiple moving particles. It is found that for flows with low and intermediate Reynolds numbers, 20 fluid cells per one particle diameter are necessary to achieve sufficient accuracy. For flows with high Reynolds numbers, a turbulence model shall be incorporated to capture the effects of unresolved small eddies. Besides, the LBM-DEM results are also sensitive to τ, especially when N is inadequate. A large τ value introduces additional diffusion of fluid momentum and weakens the fluid-particle coupling. By choosing a small relaxation time greater than the lower limit 0.5, a small fluid compressibility error and a strong coupling between the fluid and particles can be achieved, at the cost of higher computational effort. A guideline for quickly establishing a high-quality LBM-DEM model is provided and applied to a test case of granular collapse in water. The agreement between the simulation and the companion experiment (see Figure 1) demonstrates the capability of LBM-DEM to describe the dynamics of dense particle suspensions, which highlights its potential to study the granular physics in large-scale geophysical flows.

Figure 1 (a-c) Snapshots of the immersed granular column collapse in the experiments at time = 0.2 s, 0.3 s, and 0.4 s, respectively. The green lines depict the free-surface of the granular flow; (d-f) Comparison of the granular flow free-surface between the experiment and the LBM-DEM simulation at time = 0.2 s, 0.3 s, and 0.4 s, respectively.
ESyS-Particle and GenGeo: open source libraries for high performance DEM simulations

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Keywords Discrete Element Method, High Performance Computing, Open Source

Abstract ESyS-Particle (https://launchpad.net/esys-particle) is an open source implementation of the Discrete Element Method (DEM) designed for execution on parallel supercomputers. It comprises a computational engine written in C++ with a Python scripting interface for definition of simulations. Spatial subdomain decomposition implemented using the Message Passing Interface (MPI) standards permits very large-scale DEM simulations, depending upon available hardware resources. The regular grid topology of the subdomain decomposition ensures that the per-worker communication cost remains constant if the total model size is scaled up in line with the number of subdomains. As a result, scaling benchmarks demonstrate the weak scalability of the engine for simulations comprising up to 300 million discrete elements, utilising over 32,000 CPU cores.

ESyS-Particle is packaged with a range of common particle interaction types including linear elastic, Hertzian and viscous interactions. Kinematic objects such as planar walls or triangulated mesh surfaces can be imported into simulations for interaction with the discrete elements. One of ESyS-Particle's key features is its rotational brittle-elastic beam and frictional interaction classes, designed for accurate simulations of rock fracture, crack propagation and fragmentation. These interaction classes have undergone extensive validation and demonstrated to reproduce the bulk of phenomenology predicted by linear elastic fracture mechanics.

A bespoke data output framework permits targeted output of specific dynamical fields or attributes, as well as checkpoint-restart facilities. Post-processing tools are also provided for three-dimensional data visualisation using third-party software, as well as analysis of fracture evolution and fragmentation products. Recent versions of ESyS-Particle have incorporated coupled fluid-DEM simulation capabilities, as well as self-gravity. Coupling is implemented so as to exploit the subdomain parallelism of the DEM engine, thus permitting simulation of large-scale problems without the typical communication bottlenecks encountered when coupling existing CFD and DEM softwares via a serial interface.

GenGeo is an open source library designed for algorithmic construction of assemblies of spherical particles to be used as initial model set-ups for Discrete Element Method (DEM) simulations. At its core is a volume-filling sphere packing algorithm implemented in C++. Via a Python scripting interface, users specify a spatial volume to be filled with non-overlapping spheres and the range of sphere radii. The algorithm then iteratively identifies locations to insert spheres between already inserted spheres, constraint surfaces and volume boundaries. Once constructed, a variety of methods provide capacity to define different groups of particles via tags, bond together particles and output the geometry in a human-readable text file format.

A range of primitive volumes such as cubes, spheres and cylinders, are included with the GenGeo library, as well as methods to define more complex shapes via closed triangulated meshes. Such meshes can be constructed in Computer-Aided Drafting packages and imported into GenGeo in the Stereolithography (.STL) file format. Although maintained via the ESyS-Particle software repository (https://launchpad.net/esys-particle), GenGeo is a standalone library that may be beneficial for users of other DEM simulation software. The high-level abstraction of GenGeo's class structure makes it relatively easy to use and complete Python API documentation is available online.
236: 3D DEM modelling of drained triaxial tests using real-shaped particles

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Keywords
Particle shape, shape parameters, Toyoura sand, Hertz model, triaxial test

Abstract
A 3D DEM study of Toyoura sand specimen was carried out to simulate drained triaxial tests and to study the effects of particle shape on the macroscopic mechanical behavior. Grains of the numerical assembly in this study follow real size distributions of Toyoura sands. Particle shape was reconstructed from \(\mu\)CT images of sands, whose 3D shape parameters (aspect ratio, roundness, sphericity and convexity) were calculated and compared against published sources. The number of shapes required to converge to a stable cumulative distribution of shape parameters was also examined, implying that replication of the particles was sufficient to describe the shape characters and to represent an assembly of Toyoura sand. Drained triaxial tests were modelled in 3D with carefully chosen Hertz model parameters which are physically rational. Numerical and experimental results were compared. Modelling with particle shape can significantly enhance shear strength compared against spherical grains, but packing density is difficult to match. Besides, this study can be a good reference for calibrating parameters in a proper sequence.
A feasibility study for the effect of the amount of laundry and rotating speed of washer on washing performance of front-loading washer using DEM

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Keywords
DEM, Front-loading washer, washing performance, specific power

Abstract
Although computational analysis has been applied to a variety of industrial fields in recent years, there are just a few approaches for washing machines in home appliance field. The lack of analytical research on the washing machine results from the washing performance dependency on quite a lot of parameters, such as the geometrical/physical properties (the size, the amount and the type of laundry), the mechanical action (hitting and rubbing), water temperature, the chemical action (the amount and type of detergent) and washing time. Due to the complex factors, up to now, research on washing performance has been mainly experimental rather than analytical. However, experimental studies have limitations in understanding the behavior and washing process of the laundry inside the washing machine.

As the geometric structure and the working mechanism of washing machine is quite similar with them of ball mill, in this study, the mechanical action is analyzed by DEM, usually adopted in the computational analysis for ball mill. In order to avoid the complex effects such as water flow and chemical action by detergent, a front-loading washing machine with low water supply is targeted. Therefore, the simulation was carried out under the condition without water and detergent. As a feasibility test, we used laundry balls with spherical shape rather than real fabrics. In this study, the effect of the amount of laundry and the rotating speed of washer on the washing performance is analyzed under the above conditions.

Because it is impossible to directly express the "washing performance" indicating the degree of removal of contaminants using the DEM, washing performance is defined as specific power (the consumed power per unit mass). In addition, the specific power can be categorized into normal contact and tangential contact, corresponding to hitting and rubbing, respectively. The results show washing performance are inversely proportional to amount of laundry and rotating speed of washer

This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (NRF-2018R1A2B 2004207)
Analysis of effects of structural characteristics on grain breakage with DEM

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Keywords
Discrete Element Method, Grain breakage, Structural characteristics, Weibull statistics, Disorder

Abstract
The mechanical properties of most granular materials cannot be uniquely determined. A major cause of this indeterminacy lies in the fact that their structural characteristics are difficult to determine under the condition of varying porosity and porous textures, which tend to reduce the overall connectivity of the solid phase at random. Grain breakage is a critical aspect of mechanical properties of solid materials, especially for geomaterials. In the present study, the simulation of the single grain crushing test were performed employing Discrete Element Method (DEM), in which the grain was modeled in the form of an agglomerate of elementary balls with removable bonds. A novel method was proposed to generate numerous crushable agglomerates with various micro-structures. Variation in the grain crushing strength were depicted by the Weibull statistics. In addition, the relationship between fracture and fragmentation patterns and structural disorder was investigated to explore the cracking mechanism related to brittle porous media. These findings add to the understanding of the influence of structural disorder over the mechanical properties of granular matter.
GrainLearning: an efficient Bayesian uncertainty quantification framework for discrete element simulations of granular materials

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Keywords
Sequential Monte Carlo, Machine learning, Dirichlet process mixture, DEM

Abstract
The nonlinear, history-dependent macroscopic behavior of a granular material is rooted in the micromechanics between constituent particles and the irreversible change in the microstructure. The discrete element method (DEM) can predict the evolution of the microstructure resulting from interparticle interactions. However, micromechanical parameters at contact and particle levels are generally unknown because of the diversity of granular materials with respect to their surfaces, shapes, disorder and anisotropy.

GrainLearning, a Bayesian filtering framework specially developed for DEM simulations of granular materials can iteratively explore parameter/solution space conditioned on experimental data, and efficiently quantify and propagate posterior uncertainties. It utilizes Bayesian nonparametric density estimation to iteratively refine the proposal density, thus enabling an efficient multi-level sampling for global optima.

As an example, the probability distribution of the micromechanical parameters, conditioned on the experimental measurements of granular flow, is approximated, with rapid convergence within a few iterations. Six micromechanical parameters, i.e., contact-level Young’s modulus, restitution coefficients, interparticle friction, rolling stiffness and rolling friction, are chosen as relevant for the macroscopic behavior. The a posteriori expectation of each micromechanical parameter converges within a few iterations, leading to an excellent agreement between the experimental data and the numerical predictions. As new result, the proposed framework provides a deeper understanding of the correlations among micromechanical parameters and between the micro- and macro-parameters/quantities of interest, including their uncertainties. Therefore, the iterative Bayesian filtering framework has a great potential for quantifying parameter uncertainties and their propagation across various scales in granular materials.
A comparative study between two first order accurate meshless Lagrangian fluid solvers coupled with granular solids for GP-GPU computing

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Keywords

SPH, DEM, Finite Difference, Solid-Fluid Coupling, First order, Meshless

Abstract

A framework is presented for simulation of multi-phase system by expanding upon classical meshless Lagrangian methods (MLM). Specifically, this framework focuses on systems with granular particles suspended in a fluid continuum with coupling enforced by a force balance obtained from fully resolving fluid flow around the solids.

Beyond the obvious benefits of higher order discretizations in a computational fluid dynamics setting, in the context of solid-fluid coupling applications, accurate gradient information is required for two critical aspects of the proposed scheme: 1) Accurately resolving flow around solid surface, specifically for the case of fluid pressures around solid particles and 2) obtaining fluid-solid coupling forcing conditions by making use of surface pressures and shears. Due to the importance of accurate gradient information, it is chosen to use a first order consistent variation of smoothed particle hydrodynamics (SPH) as the reference MLM. The performance of the SPH method is compared against a first order generalised finite difference method (GFD). The discrete element method (DEM) is used to handle solid-solid interactions.

The above mentioned framework is used to explore the performance of the different MLMs at varying system scales by applying these methods to a 3D hindered particle settling problems. The systems are scaled in terms of the number of solid particles ranging from order ~1 to ~100. The number of fluid particles are also scaled independently by considering different fluid particle resolution for these systems. Different initial solid particle packing densities are investigated as well.

General purpose GPU (GP-GPU) implementations of the MLMs are compared inside the same computational framework by extending the DEM framework Blaze-DEM, with the study specifically investigating the performance of these solvers running on GTX 1080, GTX 1080 Ti and RTX 2080 Ti cards.
A probability-based model for quantification of particle crushing of granular materials based on DEM simulation data

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Keywords
Probability-based model; Particle crushing; Grading evolution; Biaxial shearing;

Abstract
The breakage behavior of granular materials under loading is essentially governed by their strengths and inter- and intra-particle stresses. To investigate the evolution of inter- and intra-particle stresses of granular materials under shearing, a series of discrete element method (DEM) simulations of biaxial tests are carried out. It is found that the probability density functions (PDF) of particle normalized maximum shear stress are independent of initial sample porosities, confining stresses and axial strains, but rely on the current sample grading. Based on these results, a probability-based model is developed to quantify particle crushing of granular materials under shearing according to a group of initial parameters, including initial sample porosity, initial sample grading, confining stress, stress ratio and particle strength parameters. The strength of the model is the incorporation of coupling effects between particle crushing and sample grading into the calculation. Here, the coupling effects mean that particle crushing is affected by the current sample grading, and the grading change is also dependent on the current particle crushing extent. The model shows qualitative agreement with published experimental data. The effects of the model parameters, including initial porosity, particle strength, initial grading, and crushing mode, on the calculated results are discussed and compared with previous studies.
Numerical Analysis of Degradation Evolution of Structural Loess under Loading and Wetting by Discrete Element Method

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Keywords
unsaturated structural loess, microscopic theory, degradation evolution, DEM

Abstract
The degradation evolution of unsaturated structural loess under loading and wetting is studied by discrete element method (DEM). Firstly, the equation of degradation parameter, which is used to describe the degradation for structural damage, is given based on particle contact and microscopic deformation. Secondly, the evolution of degradation with macro variables under different loading conditions is investigated by DEM. Finally, based on the simulation results, the equivalent plastic strain coefficient (the ratio of equivalent plastic strain to the structural yield stress) is defined to reasonably consider the influence of water content, and the equation for degradation parameter under different stress and wetting paths is established. The results show that the proposed degradation equation can well describe the degradation evolution of structural loess observed in the loading and wetting conditions.
A Three-dimensional thermal-hydro-mechanical-chemical Bond Contact Model for Methane Hydrate-bearing Sediments

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Keywords
Methane hydrate-bearing sediment, DEM, THMC bond contact model, Mechanical behavior

Abstract
Mechanical properties of methane hydrate-bearing sediments (MHBS) are complex and highly influenced by the surrounding temperature, pore pressure, and salinity. Studies of such influences are of great significance for the safe exploration of methane hydrate. In this paper, we proposed a three-dimensional (3D) bond contact model, incorporating the effects of temperature, pore pressure, and salinity. The model is then implemented in DEM code with thermal–hydro–mechanical-chemical (THMC) analysis being realized. The mechanical behavior of MHBS is investigated through DEM analysis. The analysis is carried out on a series of triaxial tests with various MH saturations and effective confining pressures. A comparison with experimental results reveal that the proposed contact model is able to capture some salient properties of MHBS, such as effects of hydrate saturation, environmental temperature and pressure. The numerical results show that: the shear strength and secant modulus increase as methane hydrate saturation or environmental pressure increase, while decrease as environmental temperature increases, which is in good agreement with the experimental observation.
Micromechanical study on the compression behaviour of sand-rubber particle mixtures considering grain-scale deformability

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Keywords
DEM, Deformable particle, Soft-rigid contact, Grain shape, Particle-scale behaviour, YADE

Abstract
Sand-rubber particle mixtures generally have favourable engineering properties such as high permeability, high endurance, appropriate strength, appropriate stiffness, and high damping characteristics. These properties have mainly been investigated by experimental testing. Only recently, numerical models have been used to study the mechanical behaviour of sand-rubber particle mixtures. The heterogeneous nature of such mixtures, the big difference between the mechanical properties of the two materials and the very specific shapes of the rubber particles lead to a behaviour that is hard to predict by continuum methods such as Finite Element Method. Nevertheless, the Discrete Element Method (DEM) is able to capture all these characteristics.

In this paper, we present simulations of systematic confined compression tests on sand-rubber particle mixtures with varying rubber content using the DEM. The sand grains are modelled by using the clump logic in order to accurately represent their shape. The rubber particles are modelled using a cohesive bond model which allows to take into account grain-scale deformability, i.e., the spheres making up the rubber particles can move relative to each other. The simulations are calibrated and validated by systematically carried out experimental tests.

Macro and micro investigations of the sand-rubber particle mixtures with different rubber contents are presented. The variation of the normal force on the wall shows that the total lateral force decreases by increasing rubber content. The micromechanical investigations include coordination number, force chains and contact orientation histogram. The numerical predictions indicate that the coordination number increases significantly with increasing rubber content since the rubber particulate deform leading to larger number of contacts. The force chain and the contact orientation histogram are presented for the sand-sand contacts, sand-rubber contacts and rubber-rubber contacts separately to find the contribution of each contact type to the loading. The results show that for a rubber content of less than 20% the samples exhibit sandy behaviour and for rubber contents larger than 60% the behaviour is very similar to the one of pure rubber particle samples.
Experimental and numerical studies of semi-confined heap structure after variable pouring conditions

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Keywords

coarse-graining, ensILED granular medium, forces network, homemade code, Janssen effect

Abstract

The classic experience of filling a container with a granular medium poured from a source point reveals the presence of the intergranular forces network by the manifestation of the Janssen effect (Janssen, 1895). Indeed, the measurement of the stress applied at the base of the container according to the bed particle height, shows that the static mechanical state of the ensiled granular medium is not comparable to a hydrostatic one which is characteristic of a fluid. The lateral deflection of gravity forces to the walls via the network of intergranular contacts, allows to explain the lowering of vertical stress (σzz) in relation to hydrostatic pressure. Moreover, the sliding threshold condition must be established at the walls to explain the "saturated" shape of the σzz profile (Ovarlez and Clément, 2005). If mechanical properties are involved to explain this apparent phenomenon understanding as a static equilibrium, the analyze of the free surface during pouring correlated to the local mechanical state allow to indicate that kinetic energy had an influence on the Janssen effect (Mandato et al. 2012; Duri et al. 2018). In order to revisit the Janssen effect, experiments and Discrete Element Method (DEM) simulations are compared to investigate the structure of an ensiled granular medium poured in a cell by a single point at different initial drop heights and flow rate (parameters which allow to control kinetic energy).

Experimental device. The granular medium consists of a population of glass beads of 1 to 2 mm diameter with a small span value (50/50 in volume). The experimental set-up, developed in Mandato et al. (2012), consists of an open glass cell container (51 x 100 x 160 mm) made of transparent glass walls. A flat and rectangular steel probe is especially designed to fit into the glass container. A small probe allows local measurements of the vertical stress in the powder bed. A large probe is used to simulate the bottom of the cell and allows a global measurement of the vertical stress, as in Janssen’s experiment (Janssen, 1895). Whatever its width, the probe is screwed on a rod that is linked to a load cell of a texture analyser (TA.XT2, Table Micro System), which is used as a force sensor. The filling is provided by a funnel and the flow rate is modulated by the output diameter. After pouring, the slope angle and the arrow of the free surface are measured by image analysis.

Numerical simulation. We develop our own homemade code in C++ using the DEM. Then we decide to develop also a code using the coarse-graining method (Weinhart and Luding, 2016) to highlight on the different fields. This last method which doesn’t give access to the compactness near the wall, is replaced by a new method using two grids in order to increase the accurate. With these three codes we can now explore all the contacts between the particles by the calculus of (i) normal and tangential forces, (ii) moment, (iii) mobility, of each particle.

Results. The variation of the initial drop height and the flow rate impacts the slope of the free surface: crater form in high kinetic energy conditions, heap form in lowest conditions and intermediary slopes between these conditions (from plate to “camel-like” form). The measured and calculated values of the arrow and of the angle of repose are in very good agreement in each case. Experiments and numerical simulation highlight the same layout of the vertical stress field (Fig. 1). In the upper part of the particle bed, there is a layer in which the stress is generally assimilated to a “quasi-hydrostatic” state. It can be seen that under this first layer, Janssen’s hypothesis that stresses are lateral uniformity is not valid: there is a strong local heterogeneity of the stress within the granular medium. It can be seen that the redirection coefficient defined by Janssen (Janssen, 1985) ratio between lateral stress and vertical stress, is not constant. The study of thickness and mean stress in each different zone of the bed versus kinetic energy during the filling stage had been realized. The static mechanical state of the particle bed is also due to this dynamical parameter and this point is usually not taking into account.

Figure 1. Illustration of the semi-confined heap: experiments and simulations a) experimental device, b) stress field obtained by coarse graining superposed on the force network, c) vertical stress field measured by a local probe.
Modelling flexible structures and deformable particles with YADE

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Keywords DEM, cohesive contact, remote interaction, grid, membrane, geosynthetic, rubber particle

Abstract YADE is a very popular open-source DEM package based on the classical discrete element method. Over the last decade it has been extended with many new features including the possibility of modelling flexible structures and deformable particles. This contribution presents some of these developments including examples and applications.

The first feature consists of a remote interaction model where particles interact without actually being in contact. The contact model is rather simple and only tensile forces are allowed. This allows the modelling of complex structures which are highly flexible such as textiles (Cheng et al. 2016) and wire meshes (Thoeni et al. 2013).

Then a general framework for modelling deformable structures using the concept of Minkowski sums is introduced. The formulation is based on three primitives (Effeindzourou et al. 2016): sphere, rounded cylinder, described as a Minkowski sum of a line segment and a sphere, and thick rounded facet (PFacet), described as a Minkowski sum of a faced and a sphere. The concept of a virtual sphere is introduced to handle all possible contacts. As such, all contacts can be handled as sphere-sphere contacts and classical contact laws can be used. The constitutive behaviour of the rounded cylinders and PFacets are based on classical beam theory. They can be connected to form complex structures. Some examples on how to model soil-inclusion problems (Thoeni et al. 2016) and composite structures (Effeindzourou et al. 2017) are shown.

Finally, different approaches for modelling deformable particles are presented. In the classical approach particles are glued together using a cohesive link. This is similar to the previously described approaches. An example on how this approach is used for the modelling of sand-rubber particle mixtures is presented (Asadi et al. 2018). Then the approach implemented in the deformation engine is discussed. In this approach, particles are actually not deformed but the deformation is realised by expanding the radius of the spherical particles as a function of the overlap, so that the volume of the material is kept constant (Haustein et al. 2017).

References:
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Effect of Gas Flow on Trajectories of Granular Flow Streams during Charging Process

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Keywords
Gas effect; Granular flow stream; Particle trajectory; CFD-DEM

Abstract
Charging and discharging processes of granular materials are widely observed throughout industries varying from pharmaceutical to mineral. The dynamic process of granular flow behaviors is complex and has been extensively studied in the literature experimentally or mathematically. However, the effect of resistance from fluid on granular flow streams is not well investigated. For example, in an ironmaking blast furnace burden distribution system, particles discharged from the top hopper will flow through a rotating chute and distribute particles to the blast furnace top burden surface. In such a process, the particle trajectory from the chute tip is very important in affecting the falling position and determining the ratio of different kinds of particle matters across the radius. The resistance for fluid could play an important role. In this work, the CFD-DEM method was employed to investigate the trajectories of granular materials under different conditions. We started with mono-sized particles and then extended to binary and continuous multi-sized systems. The results show that granular materials with varying properties in trajectory are prone to segregate spatially. It can be proved that the flow trajectory is significantly influenced by the gas flow, chute angle and material properties. Small size particles are much easier to be influenced by gas flow than large particles. At a critical condition of particle size, the gas flow significantly changes the particle trajectory, and the higher the gas velocity is, the stronger the resistant effect the gas flow has on particles. Moreover, the gas flow changes the particle stream impact area when the particles falling down to the ground surface. The CFD-DEM simulation results, which had a good agreement with the experiment data, suggest that the coupled CFD-DEM could be used to predict the granular trajectory under the gas flow.
Fluctuating stresses and the intrinsic viscosity of colloidal suspensions

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Keywords
colloids, Brownian Dynamics, viscosity, hydrodynamic interactions, suspension, solid-liquid, multiphase flow

Abstract
Brownian Dynamics is a standard tool to study colloidal suspensions in the Stokesian flow regime. The solvent is treated implicitly, as the source of both hydrodynamic friction and stochastic forces obeying the fluctuation-dissipation theorem. Even though this formalism has been used extensively, and forms the basis of many theoretical studies on colloids, we show that it does not predict the correct intrinsic viscosity. A straightforward Green-Kubo calculation of the intrinsic viscosity of a quiescent dilute solution of spherical particles yields the surprising result $[\eta] = 0$, in marked contrast to Einstein's well-known $[\eta] = 5/2$.

We propose a remedy to this problem, by introducing an extended fluctuation-dissipation theorem including Brownian stresses. Evaluating the correlations between these stresses and the Brownian forces gives rise to a further unexpected stress contribution. Using a recently developed rotational Brownian dynamics scheme, we also present a numerical rheology study confirming the validity of the proposed modifications to the Brownian formalism. We show that agreement is restored between the viscosities of quiescent and slowly sheared colloidal suspensions, for a range of body shapes, and that the linear rheology extracted from Brownian simulations now agrees with previous theories.
Abstract

Discrete element modelling (DEM) has become an important tool to understand the dynamics of particulate systems, as it provides detailed information at particle scale which is often difficult to obtain by conventional experimental techniques. DEM has also been coupled with CFD methods to model various aspects of particle-fluid flows. However, application of these methods to industrial process is largely hindered due to associated high computational cost and limited modelling capabilities. For example, particles in real processes are often featured with a wide variation in particle size and non-spherical particle shape, which requires an efficient handling of neighbor searching and representation of particle shape in the DEM solver. In addition, the complexity of fluid flows and geometrical complexity of the computational domains further make it difficult to rely on one single CFD method to handle all aspects of the particle-fluid flows. It is thus necessary to develop an efficient DEM solver and versatile coupling methods to handle different problems encountered in industrial applications. In this work, an overview of our development on GPU-based DEM and coupled CFD-DEM approaches is presented, including GPU-based DEM for large size ratio and non-spherical particles, GPU-based SPH-DEM coupling, coupling of ANSYS/Fluent with GPU-based DEM and coupling between LBM with DEM.

For GPU-based DEM, a multi-grid approach specifically designed within the GPU architecture is proposed for particle neighbor searching, which demonstrates significant gain in computational efficiency than conventional linked-cell method. For non-spherical particles, particle shape is approximated by a multi-sphere approach in which overlapping spheres are rigidly connected together. The GPU-based algorithm is able to handle variations in both particle size and shape. For particle-fluid flows with free surfaces, a general purposed SPH-DEM model that runs entirely on GPU is developed. The GPU-based DEM is also combined with a commercial software ANSYS/Fluent to make the best use of the parallel capability of GPU for DEM calculation and the general applicability of commercial software for CFD calculation. Some preliminary works has also been done to develop GPU-based LBM and its coupling with GPU-based DEM, allowing us to carry out both resolved and unresolved particles simulations. All the developed models have been carefully validated against literature results. Applications of these methods have been demonstrated through a range of simulations, including particle packing, compaction, powder spreading, fluidization, dam-breaking, gas-solid cyclone and agitated chemical reactors.
Advances in Discrete Element Modelling using the GPU based XPS Software

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Keywords
DEM, GPU, XPS

Abstract

Simulation of granular flow using the Discrete Element Method (DEM) is a crucial tool that is used in the pharmaceutical industry to gain understanding of processes. Typically, large amounts of particles are needed to accurately model real-world problems. Together with small time steps, the problem becomes very expensive in terms of computational effort.

This work presents the evolution of modern Graphics Processing Units (GPUs), and compares theoretical compute capabilities with actual gains in simulation performance we have observed using our code XPS. We model various pharmaceutical processes, considering non-spherical particles, advanced contact models with contact history, and coupled CFD-DEM problems using the commercial software AVL Fire. Finally we show how the GPU advances the DEM.
251: Particles motion mechanism of rock-fill dam under initial overtopping condition

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Keywords
rock-fill dam, particles motion mechanism, overtopping, coupled CFD-DEM, test model

Abstract
Although great efforts have been devoted to revealing the dam-break mechanisms in macroscopic scale, the study of mesoscopic particles motion of rock-fill dam is still not sufficient. This paper presents particles motion mechanism of rock-fill dam under initial overtopping condition based on the coupled Computational Fluid Dynamics and Discrete Element Method (CFD-DEM) analysis. The important fluid–particle interaction forces, as the drag force, the buoyancy force and the virtual mass force, are considered by exchanging interaction forces between the CFD and DEM computations. We study on the initial motion positions and movement modes of the dam particles under different hydraulic head of overtopping. It is found that the higher hydraulic head is, the lower initial motion position of dam particles will be in a certain range. The results of CFD-DEM analysis reflect particles motion mechanism of rock-fill dam well through test model validation.
252: The bending stress of elongated particles in shear cell

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Keywords
Shear cell, elongated particles, bending stress, breakage

Abstract
Crystal breakage is an issue of great concern to the pharmaceutical industry. Conservation of the desired Particle Size Distribution (PSD) throughout downstream processing is extremely important, as PSD changes are known to affect properties such as bulk density and flowability. Active Pharmaceutical Ingredients (APIs) are in majority organic and their crystal shape of high aspect ratio; their main breakage mechanism is fragmentation by bending stress.

Calculating the breakage of elongated particles in agitated drying systems is an active area of research, however, the phenomenon is not totally predictable. Computational methods, such as Distinct Element Modelling (DEM), have been used to simulate the flow of particle beds for various stress conditions and a range of particles aspect ratio. To elucidate the fracture phenomenon of elongated particles in agitated drying, the bending stress of individual crystals needs to be determined within a bed of particles.

In this study, a shear cell is built in DEM and it is used to mimic the normal and shear stress experienced by particles in dryers using moving parallel plates and periodic boundaries. Elongated rigid particles are modelled using overlapping spheres and they experience stress due to the shear application in the box. The bending stress of individual particles is calculated during the DEM simulation and a bending stress distribution is obtained for the given particles properties (mechanical and physical) and stresses (normal and shear).

Current work in this study consists on correlating particle properties and breakage: computationally determined bending stress distribution is combined with the known critical breakage strength of particles of interest. We believe that such correlations will be promising for the estimation of particle breakage during pharmaceutical isolation processing.

The financial contribution of the EPSRC Centre for Doctoral Training in Complex Particulate Products and Processes (CDT CP3) is gratefully acknowledged.
254 Numerical Simulation of the Direct Shear Test on Granular Materials Composed of Polygonal Crushable Particles: A DEM-XFEM Approach

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Keywords DEM, XFEM, Particle Breakage, Granular Materials, Direct Shear Test.

Abstract The strength and deformation mechanism of granular soils has long been investigated due to its importance in geotechnical structures, such as rockfill dams. Since large-scale traditional laboratory experiments on rockfill materials such as triaxial and direct shear tests are costly and laborious, nowadays many researchers are more likely to conduct numerical simulations to investigate macro- and micro-mechanical behaviour of materials. The Discrete Element Method (DEM) is one of the most promising numerical tools for modelling the granular media. Despite their popularity, most numerical implementations of DEM do not ordinarily consider particle breakage which is a disturbing phenomenon that impacts shear resistance and potentiality of compaction of granular materials. The eXtended Finite Element Method (XFEM) is a computational technique specifically designed for treating various displacement field discontinuities in materials such as cracks.

In this study, a combined DEM-XFEM novel approach has been developed to simulate the direct shear test on assemblies of polygonal crushable particles. The fracture within individual particles is modelled with XFEM, while the particle motion is simulated through DEM approach. Furthermore, the influence of various factors, including the aggregation of particles, grain shapes and vertical stress in the macro- and micro-scales is investigated by presenting different aspects of the assemblies’ responses such as coordination number, distribution of contact forces, particle stress distribution, particle rotations, particle displacement and anisotropy. Finally, the effect of particle breakage on macro- and micro-mechanical behaviour of granular materials is presented.
BlazeDEM-GPU for simulations where particle shape matters

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Keywords
Discrete Element Method, GPU, CUDA, Polyhedral Particle Shape, Convex, Non-Convex

Abstract
BlazeDEM-GPU is an open-source discrete element method (DEM) code, specifically designed for multiple graphical processing units (GPU) using single and double precision computing [1]. This is in stark contrast to the majority of commercial and open-source DEM codes that have been primarily designed for central processing processor (CPU) computing and modified after the fact for GPU computing. Consequently, these modified codes only deliver limited speedup that varies from 2 to 20 times, whereas, BlazeDEM-GPU has demonstrated to deliver up to 150 times speedup [1].

These computational improvements has allowed for the development of detailed particle shape representations that include particle angularity and detailed contact phase resolution that relies on the overlap volume to resolve contact forces. Detailed particle shapes include convex particle shape representations [1], that has recently been extended with non-convex particle shape representations [2]. The concrete benefit of BlazeDEM-GPU is not merely the computation with improved shape representations but the number that can be handled within realistic computational time frames. For example, resolving one second simulation time of one million non-convex polyhedral particle shapes overnight [3].

References


Particle-based simulation of aeolian sand transport and the concatenated dust emission

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Keywords
DEM, aeolian sand transport, dust emission, cohesive forces, granular solids

Abstract

Introduction
Dust emission has major impacts on weather and climate, ecosystem productivity, the hydrological cycle of our planet through interactions with clouds, radiation, the biosphere and atmospheric chemistry. Hence, it is crucial to represent the dust cycle in accurate weather models. Unlike sand, dust particles are not easily entrained due to the presence of cohesive forces and are emitted by the bombardment of sand particles during saltation, as shown in figure 1. In our research, we modeled this particulate system using 3-D DEM simulations (LAMMPS [2]) to better understand the particle interactions and the saltation process.

Methodology and observations
Inter-particle interaction forces are modeled using a Hertzian contact model for the visco-elastic interaction and a non-bonded van der Waals force (cutoff distance 1 μm) for the cohesive model. The monodisperse spherical particles ranging from 4 to 52 μm, were initially settled under gravity and the packing behavior was analyzed. It is evident from figure 2-b that for small particles in the presence of cohesive forces, there is a tendency for the formation of tree-like structures or large agglomerates [3]; whereas figure 2-a shows a settled bed in the absence of cohesive forces. This behavior is not observed for larger particles (figure 2-c,d). This is noticeable in the packing fraction trend, which rapidly decreases for particle size < 20 μm.

Figure 1: Dust emission mechanisms [1]

Figure 2: Packed bed with cohesion
Figure 3: Packing fraction (ϕ) vs particle size
Based on these particle interactions, preliminary dust emission mechanisms were also simulated, as could be seen in figure 4a/b. A large agglomerate particle when impacted onto a bed of cohesive particles could be seen ejecting smaller agglomerates after fragmentation.

Figure 4a: Agglomerate before impact    Figure 4b: Particle ejection after impact

Outlook
The cohesive inter-particle interaction model was implemented alongside a visco-elastic contact model to show the significance of cohesive forces among dust particles. Preliminary simulations of dust emission mechanisms were implemented using the parallelized discrete element method, in our goal to realize a computationally efficient tool for aeolian sand transport.

Acknowledgement
We would like to thank the German Research Foundation (DFG) for funding through this project #348617785.

References
257: GPU based DEM enabling new simulation and design paradigms

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Keywords
Discrete Element Method, Interactive Simulation, Just-In-Time, Design Optimization

Abstract
BlazeDEM-GPU is an open-source discrete element method (DEM) code, specifically designed for multiple graphical processing units (GPU) using single and double precision computing [1].

The significant computational improvements combined with explicit time integration is enabling new simulation paradigms, namely, interactive simulations [2][3].

Interactive simulations, as the name implies, are simulations where the user can interact and modify simulation parameters and geometries real-time. Although the simulations themselves are not necessary real-time, they are fast enough to be responsive from a user perspective. In addition, model fidelity is critically interrogated and a clear distinction between accurate quantities versus accurate trends (changes in quantities) is made. We demonstrate that, in general, a lower model fidelity can be used to obtain accurate trends, whereas accurate quantities typically requires higher fidelity models.

Needless to say, applications benefitting from the interactive simulation paradigm, can be widened when replacing real-time simulations by sensible reduced order models. Potential avenues in this regard is explored in this study.
Abstract

Plate-impact experiments are generally used to better understand the inelasticity of many brittle materials. Modeling these brittle materials impact experiments is a challenging problem because of the complexity of the involved physics and the high computational cost. Under extreme loading conditions, brittle materials fail suddenly through dynamic fracturing processes. These failure mechanisms are typically a result of nucleation, interaction and coalescence of micro-cracks present throughout the sample. In this study, the Finite-Discrete Element Method (FDEM), which merges the finite element based analysis of continua with discrete element based transient dynamics, contact detection, and contact interaction solutions, is used to simulate the response of a flyer-plate impact experiment in a Westerly granite sample that contains a randomized set of cracks. FDEM has demonstrated to be a strongly improved physical model as it can accurately reproduce the Velocity Interferometer System for Any Reflector (VISAR) plot and capture the spall region obtained from the flyer plate experiment.

These FDEM capabilities, in the context of rock mechanics, are very important for two main reasons. First, the FDEM can be further applied to many complex industrial problems such as planetary impact, rock blasting, seismic wave propagation, characterization of material failure around explosive crater formations, and the detection of hydrocarbon flow in petroleum industry, etc. Second, it can be used to validate high strain rate impact experiments and essentially, via virtual experimentation, replace these high cost experiments by very cost- and time-effective simulations.
Critical state behaviour of granular materials

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Keywords
Critical state, triaxial, consolidation, cyclic loading

Abstract
The behaviour of granular materials has been widely examined under laboratory conditions; however, the real micro-mechanics behind the observed behaviour has not been fully understood. Discrete element method (DEM) was, hence, adopted for investigating the behaviour of granular materials under the critical state soil mechanics (CSSM) framework. It was found that DEM is able to simulate stress and strain path tests (constant volume, cyclic loading, anisotropic consolidation, etc.), which are difficult to conduct in laboratory condition, and produces the qualitative response of granular materials i.e. captures important characteristic features of shearing response. The critical state (CS) data from a series of triaxial simulations formed a unique critical state line (CSL) in the classical $\epsilon$-$\log(p')$ space, regardless of consolidation and drainage conditions. The CSSM framework was also found suitable for synthesizing both monotonic and cyclic behaviour in DEM. The uniqueness of CSL was also observed for micro-mechanical quantities such as number of contacts and fabric anisotropy. The qualitative correlations between macro- and micro-parameters, which are important anchor concepts for soil modelling, were established.
261: Virtual Calibration Chambers for geotechnical in-situ tests

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Keywords
CPT, DMT, SPT, DEM, calibration chamber

Abstract
In-situ tests, including the cone penetration test (CPT), the Marchetti dilatometer (DMT) or the Standard Penetration Test (SPT) are a mainstay of geotechnical engineering. They are used to delineate soil stratigraphy, obtain soil properties, design foundations and evaluate liquefaction risk. They are fast, cheap and efficient. Their main inconvenience is that mechanical interpretation of these tests is not easy and many factors affecting test results are poorly understood. Experimental study, based on large physical calibration chambers or field tests, is cumbersome and costly.

In principle, numerical simulation may be also used to perform controlled experiments. In practice in situ testing involves large displacements, large strains, moving boundaries and -sometimes- high loading frequencies. It is not clear which numerical technology will be more appropriate for this kind of study. For granular soils, models based on the Discrete Element Method (DEM) appear attractive because 1) they are able to deal with large displacement contact problems in a dynamic setting 2) they have relatively few free material parameters to calibrate 3) they can easily incorporate grain scale properties such as crushability or grain shape that are known to affect test results.

This communication presents an overview of recent work done at UPC to study in situ tests in granular soils with DEM models. Several examples are presented to illustrate the capabilities and current limitations of the method.
Multi-scale modelling of charging/discharging of potassium carbonate particles in a thermochemical energy storage reactor

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Keywords
Thermochemical material (TCM), heat storage, solid/gas sorption

Abstract
There is a growing need for flexibility for the use of sustainable energy sources, which is caused by the natural fluctuations in the supply of these forms of energy. Compact thermal energy storage strongly contributes to the desired flexibility and energy savings while maintaining a secure supply and level of comfort. Thermochemical materials have the potential to store 5 to 10 times as much heat per volume as a storage system based on water with a relevant temperature difference. In addition, there are no heat losses when storing heat in Thermochemical Materials (TCM), which makes the application particularly suitable for long-term storage.

In this paper, the objective is to investigate the capability of salt hydrates (e.g. K2CO3) to store energy during their dissociation into anhydrous salts and water vapor when they are supplied with external heat. To achieve this a mathematical model is developed where the fluid phase is treated as a continuous phase and individual particles are tracked with a Lagrangian approach. The developed model describing solid/gas sorption processes considers heat and mass transfer characterization through conduction-diffusion equations. In the thermochemical energy storage system, a grain is the basic particle where the reaction takes place. The chemical kinetics of the grain (as function of pressure and temperature) determined from the experiments are used as an input for the model. In the proposed model, TCM particles can interact with each other while charging/discharging. At the same time, interaction with and through the surrounding gas phase is accounted by CFD. A parametric study provides suggestions to improve process performance by properly selecting materials for thermochemical energy storage. Results obtained from the model can help identify optimal materials configurations for thermochemical storage within practical constraints. This is a requirement for developing an efficient Heat Battery.
Modelling a propeller in various liquids with DEM-CFD coupled simulation method

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Keywords
DEM, CFD, MFIX, ball valve, propeller

Abstract
This study is about a task of the BME Solar Boat Team experienced in the Netherlands. The team develops and races an electric racing boat. Due to the low water level in the narrow Dutch channels, the massive upsurge of the sludge can be observed due to the movement of the propeller. After the team started to develop their own propeller, a theoretical approach to the task was also raised. Thus the aim of the interaction between the propeller and the impurities in the water, the dependence of the flow of the profiles and the particles, and the failure of the faster wear, were intended.

In the research, a coupled CFD-DEM simulation method was used, which proved to be appropriate for the task. To construct and execute simulations, the MFIX open source software was used. The ability of the method is demonstrated by the fact that complicated simulations can be simulated with low computing capacity and the fact that there have been several successful simulations for the used method. One of the test aspects was the change in the viscosity of the medium flowing in the chosen geometry, which resulted in different deposition and flow images. As an outline, various engineering-tribological applications were also presented, which greatly assist the work of design engineers, saving time and money by replacing laboratory measurements with simulations. In addition, they provide guidance on selecting the appropriate geometry or viscosity flow medium for machine elements. The method chosen has proven to be appropriate for examining the problems that arise.
264: Fabric features influencing the liquefaction resistance and post-liquefaction shear deformation of sand

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Abstract

The liquefaction resistance of sand and the generation of large but bounded shear strain during sand’s liquefaction are both affected by fabric features. The current study attempts to identify a variable to quantify the fabric evolution during post-liquefaction cyclic loading. The objective is to explain the post-liquefaction shear deformation development and to pinpoint the fabric characteristics and processes influencing the liquefaction resistance of sand. The discrete element method (DEM) is adopted to conduct undrained cyclic biaxial simulations on granular assemblies consisting of 2D circular particles. The numerical simulations can successfully reproduce the liquefaction behavior of sand, especially the generation and eventual stabilization of shear strain at zero effective stress after initial liquefaction. Based on macro and micro mechanical observations at liquefaction, a new fabric measurement, the Mean Neighboring Particle Distance (MNPD), is introduced. The MNPD captures the microstructural features of granular materials that govern deformation behavior in the liquefaction state. It is directly measurable, has clear physical meaning, and reflects the amount of rearrangement that is needed for a granular material in a ‘suspended’ liquefaction state to reach a stable load-bearing state. The new fabric quantity MNPD, along with the second order fabric tensor that quantifies anisotropy, is also shown to significantly influence the liquefaction resistance of sand, even overpowering the influence of overall density under certain conditions. These findings enhance the understanding of sand’s liquefaction behavior by establishing links between post-liquefaction shear deformation development and an intrinsic fabric metric, and between liquefaction resistance and changes in quantifiable fabric states.
265: LMGC90: an open platform dedicated to the numerical modelling of collections of mechanical systems in interaction

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Keywords
Contact, Dynamics, DEM, FEM, Open source, Software, Multi-physics

Abstract
LMGC90 is an open platform dedicated to the modelling of large collections of interacting objects (2D/3D). It aims at modelling objects of any shape with various mechanical behaviour and to take into account interaction laws as complex as necessary. Furthermore, multiple physics couplings (thermal effects, fluids, etc.) are progressively taken into account. This software was first designed to gather all the knowledge and developments around granular material, contact mechanics, the NSCD method made at LMGC, particularly those of J.J. Moreau and M. Jean. Its modular architecture was designed and adapted so that it ensures robustness while adding new features. After almost two decades of developments the platform now offers quite a lot of features. Concerning the modelling of the bulk behaviour of the bodies:
- rigid - mechanics with Newton-Euler equations (2D/3D),
- deformable - (linear/non-linear) mechanics with Finite Element Method (2D/3D),
- couplings to tackle thermal evolution, to model porous media
Concerning the other functionalities:
- several time evolution strategies like quasi-static, implicit time integrator (theta-scheme) or explicit one (verlet),
- a wide set of primitives (disk/sphere, polygon/polyhedron, polyline/triangulated surface, etc.) to describe contact,
- a wide set of implicit or explicit contact laws (Signorini-Coulomb, Cohesive Zone Model, etc.),
- a Non-Linear Gauss Seidel contact solver able to solve many different contact laws and bulk models modelling in a robust way. Enhancement to manage multiple physics couplings.
The core of the software is written in Fortran90 to provide computational efficiency while the API is in Python to make access to internal database easier and to allow weak coupling with other software. As such, GMSH tool is extensively used for pre-processing. The core of the software has several entry points allowing the binding with external libraries to enhance features and efficiency, like:
- MatLib library is used for behaviour law computation for Finite Element Models
- MUMPs library is used for the resolution of sparse linear systems
- RoboTran software can be used to access Multi-Body-System models
- SiconosNumerics library can be used to access different contact solvers (global solver such as Alart-Curnier Generalized Newton method)
- Migflow is currently an active collaboration allowing coupling with fluid mechanics
The current main field of applications are:
- Dry granular materials: mine engineering (SRK), ballast tamping (SNCF), tribology of complex systems (Messier), etc
- Concrete: fracture and multiple physics couplings (IRSN), etc
- Masonry structures (AIA, Freyssinet)
- Fluid-grains mixture (academic collaboration with UCL, GeoSciences Montpellier, ENS Lyon)
266: Development of continuum models of ellipsoidal grains

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Keywords
Continuum mechanics, constitutive modelling, ellipsoidal grains, dense granular flow

Abstract
Ellipsoidal grains show a complex microscopic behavior associate with their ability to orient and align with respect to each other and the flow.
These additional microscopic degree of freedom is an evolving property that gives rise to a complex anisotropic mechanical response.
Available continuum constitutive models of dense granular materials typically only consider grain size while ignoring grain shape, orientation and alignment and their effect on the mechanical response.
This presentation discusses the derivation of a generalization of the inertia rheology to ellipsoidal grains. The construction of the continuum model is motivated and supported by District Element Method simulations, imposed requirements on a constitutive law, as well as the representation theorem. The model consists of a constitutive law that relates the grain shape, microstructure arrangement and the flow to the developed stresses and an evolution law for the microstructure arrangement.

The macro-scale stress response vs. grain shape for frictionless grains subjected to simple shear
Investigating the effects of Cohesion and Screw Configuration in a Twin-Screw Granulator using the Discrete Element Method

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Keywords Powder, DEM, Cohesion, Wet Granulation, Twin Screw Granulation.

Abstract Wet granulation is a process used to create larger stable agglomerates (granules) from fine powders. This has many desirable outcomes such as improving flowability, compactibility, and homogeneity. Granulation is commonly employed in the food, pharmaceutical, detergent, and fertilizer industries, but despite its wide adoption it is often problematic in operation, with high recycle ratios in continuous processes and high rejection rates in batch processes.

Although tremendous efforts have been made to gain scientific insight into the granulating process, a fundamental understanding of wet granulation is still lacking due to the complexity of the mechanisms involved. With twin screw granulation becoming a popularly employed method of wet granulation, an in-depth understanding of particle enlargement in the granulating process is necessary in order to improve the quality of the final product without the need for large-scale Design-of-Experiment studies.

Despite the extensive experimental research carried out for twin screw granulators in recent years, there has been little computational work carried out. This paper employs the Discrete Element Method (DEM) to study a 25 mm diameter, GEA ConsiGma™ 1 twin screw granulator with a series of typical configurations for the kneading elements considered. The DEM simulations were conducted using the commercial code EDEM with a DEM contact model developed for cohesive solids. The contact model is based on an elasto-plastic contact with adhesion and uses hysteretic loading and unloading paths to model the elastic-plastic contact deformation. In these simulations, the adhesion is used to capture the effect of the binder liquid without the complication of modelling the liquid directly. The adhesion parameter is a function of the plastic contact overlap. The model has previously been shown to be able to predict the stress-history-dependent behaviour depicted by a flow function of the cohesive bulk material.

In this study, two important factors are investigated. Firstly simulations were performed to compare the behaviour of a cohesion-less material with a cohesive material to understand the effect of cohesion on the key results such as the residence time distribution, mass hold-up and the stress regimes on the kneading and conveying elements of a ConsiGma granulator. Secondly the effect of the changing screw configuration on the residence time distribution, local solid fraction and stresses experienced at different elements in the twin-screw granulator is assessed. The results shows the influence of these key factors which helps to determine an optimal configuration for the operation.
Integrated DEM and SPH Model of Woody Debris Interaction with River Infrastructure

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Keywords
DEM, SPH, debris, renewable energy, fluid, liquid, CFD, boundary conditions

Abstract
Hydrokinetic power generation that uses river kinetic energy is a promising source of electricity in rural Alaska. Many villages located along rivers are not accessible by road and that are unconnected to an electrical grid can benefit from the use of hydrokinetic energy generation. Hydrokinetic generator operations and maintenance becomes impossible without special protection from the numerous logs and other woody debris in the rivers. The Alaska Hydrokinetic Energy Research Center developed and performed a series of tests on a research debris diversion platform (RDDP), which was designed to protect hydrokinetic energy infrastructure on rivers. We developed an integrated DEM and SPH model, the hydrokinetic debris interaction simulator (HDIS) to simulate debris interaction with the RDDP to help optimize RDDP performance and different interaction scenarios.

HDIS is a new model that uses both DEM and SPH methods fully integrated with each other including solid-liquid interaction and periodic boundary condition to simulate a part of the river with the RDDP and debris. The RDDP and logs are constructed with spheres that can overlap. The logs interact with each other and other DEM objects. HDIS uses Hertz-Mindlin contact physics to model the interaction within DEM model. The river banks and the river floor are also represented with similar DEM sphere clusters. The RDDP is constructed with a freely rotating cylinder at the apex and two long pontoons behind it. The platform has a V-shape and resembles a sharp angle pointing against the river stream. The hydrokinetic generator is located inside the angle, thus being protected from floating debris that can damage the generator or accumulate in front of it and obstruct the stream.

Water flow is modeled using a standard SPH method. Periodic boundary conditions for SPH are constructed using “ghost” virtual SPH particles. The water stream is created by a slight angle tilt of the gravity vector from the normal representing the level change along the river.

The essential part of the HDIS model is the novel interaction method being developed between solid bodies and liquid particles. The liquid pressure field is integrated along the solid surface to calculate both forces and torques imposed from the liquid to the solids and from solids to liquid. A non-penetration boundary condition is strictly enforced by additional boundary equations that correct both liquid and solid particle velocities. The resulting model represents a segment of the river with moving liquid and floating debris that can interact with river structures. The model allows any size ratio between DEM and SPH objects.

A series of numerical tests with debris created in HDIS were run. The forces measured at RDDP during field measurements are compared with the forces calculated using the HDIS model. The trajectory of the logs derived from HDIS simulations are compared with an episode captured on video when a large log collided with the RDDP and then swung behind it. The HDIS simulation results well match the observations from field tests and can be used to simulate large debris behavior during its interaction with hydrokinetic infrastructure.
Granulation is the process of agglomerating particulate materials or powders into larger, semi-permanent aggregates called granules. It is employed in a wide range of industries including pharmaceuticals, foodstuffs and chemicals with an annual production value in excess of US $1 trillion in the United States alone. A type of granulation used extensively in the manufacture of pharmaceuticals is wet granulation (WG), which is performed through spraying a liquid binder onto particulate materials in a high-shear mixer, fluidized bed or similar apparatus, creating granules with desired properties. However, the design of equipment for WG relies heavily on empirical data and experiments due to a poor understanding of the fundamentals of granulation, resulting in expensive laboratory testing. WG is characterized by a three-step process: wetting and nucleation; consolidation and growth; and attrition and breakage. Twin-screw granulation (TSG) is a type of WG that has been gaining use in pharmaceutical production due to its scalability, simple maintenance, high product quality and easy integration with other processes. Through multiscale modelling techniques, specifically population balance modelling (PBM) alongside discrete particle modelling (DPM), we hope to elucidate on WG processes and develop further mechanistic understanding of particulate behavior during granulation -- with a focus on TSG. Moreover, as the PBM equations are complex and generally may not be solved analytically, we will explore efficient numerical solution techniques for solving them. Finally, to validate and calibrate our models, rapid prototyping will be utilized to create miniature setups which can be simulated fully at the micro-scale.
Density Segregation of the Granular Matter

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Abstract

Mixing of granular materials is notoriously difficult to predict partly due to the complicated mixing mechanisms of particles and partly their variable flow kinematics. Despite many theoretical studies in idealised configurations of chutes and rolling-mode drum, a generic macroscopic model for granular mixing has not been achieved. A continuum model is proposed for simulating density-driven segregation of particles, based on the convective-diffusive-segregating equations coupled with the rheology of dense granular flow. Notably, the model is implemented via a dynamic finite element method and an online coupling technique. It, therefore, allows to model the tempo-spatial variation of particle concentration in either steady or unsteady granular flows. Built on these fundamental physics, the model will have a very wide scope of application, not limited by the geometry, operation condition or properties of the material. Its performance will be demonstrated in the talk focused on a rotating drum.
272: Using DEM simulation to eliminate diamond breakage in a shape shorting machine.

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Keywords
Particle Breakage, Diamond, Shape Sorting

Abstract
We recently had an urgent requirement to adapt our shape sorting machine to be able to capture 3D models of a large number of individual diamonds. Handling diamonds comes with the additional constraint to minimise diamond damage (cracking) and prevent particle breakage.

Having identified the area in our shape sorting machine with the highest possibility of damaging diamonds, we simulated the trajectories of a range of diamond shapes. The diamond shapes were simplified versions of the high-fidelity models captured with our shape sorting machine.

From each trajectory we extracted the maximum collision velocities and compared these to an in-house model for diamond breakage. This approach allowed us to make modifications to the material path through the machine and to validate that the collision velocities were below the threshold for diamond breakage.
LB-DEM simulation of particle deposition on fibers with different charge distribution models

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Keywords
LB-DEM simulation, particle filtration, charge distribution

Abstract
Electret filter material can quasi-permanently store charges and capture particles by additional electrostatic attraction, thus it has been widely used in air purification. The amount and distribution of charges in the electret filter directly affects the electrostatic field and in turn affects the particle collection performance. The paper investigates the filtration performance of electret fiber filter with three different charge distribution models by lattice Boltzmann coupled with discrete element method (LB-DEM) simulation. LBM is convenient for handling complex physical boundary, and DEM is suitable for characterizing the particle properties (eg. dielectric constant, charge density distribution).

Through the simulation of the motion and deposition of fine particles in the porous filter material under the couple of flow field and the electrostatic field, the filtration efficiency is obtained. Compared with the existing literature, it shows that the traditional assumption that the uniform charge distribution in the electret filter material will result in a low prediction of filtration efficiency, and the non-uniform distribution of bipolar charge is the most suitable.
Discrete Particle Simulation of the Spreading Process in Additive Manufacturing

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Keywords Additive manufacturing, selective laser melting, discrete particle method, spreading

Abstract Selective Laser Sintering/Melting (SLS/SLM) is an additive manufacturing (AM) process that is categorised under powder bed fusion (PBF): objects are produced by spreading successive layers of powder material and solidifying selected parts by sintering/melting them with a laser.

The process consists of different stages and for each stage different process parameters exist, figure (1) shows a schematic of the process. The powder spreading process is mainly governed by the tool geometry, material properties, and speed of the spreading tool. In addition, powder feedstock and powder characteristics play a major role in the powder layer quality, which in turn would influence the final product properties. Typically, optimising the process parameters to achieve the desired final product properties is done by performing costly experimental trials. Therefore, developing a computational tool would help reducing the amount of trials, thus reducing the manufacturing costs.

The spreading process was simulated in MercuryDPM [1], using a discrete particle model (DPM) of linear elastic, dissipative, frictional contact forces [2] and cohesive contact forces [3]. Then the layer characteristics were obtained by coarse-graining [4] which generates continuum fields e.g. density from discrete data. In this work, we investigated the DPM parameters influence on the spread powder layer characteristics, where the layer properties such as volume fraction, height, etc. were calculated and analyzed. Initial results showed that the powder layer is nonhomogeneous, possesses low volume fraction and higher particles segregation at higher interparticle friction. In addition, increasing the spreading tool speed reduced particles segregation. However, the layer porosity was increased. Further investigations will focus on experimental validation, humidity effect and spreading tool design evaluation.

Figure 1: SLS/SLM process schematic

References
Keywords
proppant, DEM, CFD, hydraulic fracture, two-phase

Abstract

This paper investigates the effects of geometrically rough surfaces on particle-fluid flow and transport, specifically for better understanding its impact on particle settling velocity. Proppant particles are injected into fractures during the hydraulic fracturing process for permeability enhancement of georeservoirs through maintaining fracture opening upon wall close-in. The propped opening of the fracture provides enhancement of the hydraulically fractured georeservoir’s productivity and project yield. Part of the successful design of a proppant injection program is the ability to predict proppant settling behavior accurately. Numerous past investigations of the injected proppant behavior in fractures have involved idealized configurations in which the proppant is injected into smooth walled fractures. The idealized conditions are however non-reflective of in field rock fracture surfaces, which exhibit complex characteristics, including geometrically roughened surfaces. Understanding of surface roughness variances’ impacts on proppant and fluid flow is essential for accurately predicting proppant behavior and improving design projects. This research uses the Discrete Element Method coupled with computational fluid dynamics (DEM-CFD) for studying effects of varying fracture surface roughness, via varied fractal dimension, on proppant settling behavior. Fracture surfaces, representative of those found in actual rock fractures, were numerically generated based on a recursive subdivision algorithm known as the ‘Diamond-square midpoint displacement’ method. This work provides an insight into the importance of fracture surface roughness analogous to actual rock surface characteristics when considering proppant behavior in fractures and of the impact of geometrically rough boundary walls on particle-fluid settling behavior in general.
A Particle Collision Selection Method Based on Monte Carlo Method

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Keywords
discrete, particle collision, collision selection, optimize, Monte Carlo method

Abstract
Calculation of rarefied gases most adopts discrete method. The number of simulated particles is an important parameter of discrete algorithm. The lighter the mass of simulated particles is, the more the number of simulated particles is, the higher the accuracy of the corresponding calculation results, and the more difficult the calculation is. Therefore, how to set the appropriate simulated particle mass has always been an important problem to be solved by discrete algorithm.

There is no solution to set the appropriate simulated particle mass in this paper, but by optimizing the conventional particle collision selection method, this paper indirectly reduces the dependence of the accuracy of calculation results on the setting of simulated particle mass, and then reduces the difficulty of calculation, so as to determine the appropriate simulated particle mass equivalently.

The particle collision selection method proposed in this paper is explained by the two-particle collision selection method in a grid in Monte Carlo method: The basic parameters of the grid and the particles in the grid are known, the original Monte Carlo method calculates the number of collision particle pairs n first, and then randomly chooses n for collision calculation; And the method in this paper is to add an influence factor m greater than 1 and select n*m pairs of particles, each pair of particles chooses whether or not to collide through probability 1/m, then the collision pairs calculated by probability are calculated. Others such as mesh generation and boundary reflection and so on, follow the original Monte Carlo method.

Assuming that the mass of the simulated particle is 1, by adding the particle collision selection method (m=2) in the Monte Carlo method, and comparing with the original Monte Carlo method to reduce the particle mass, it is found that adding the influence factor m=2 is equivalent to the original Monte Carlo method with the particle mass of 0.6 under the same convergence accuracy and the particle mass of 0.8 under the same convergence time.

It can be seen that the particle collision selection method proposed in this paper is added to the Monte Carlo method, which improves the calculation accuracy but increases the computational difficulty. However, the increase of computational difficulty is less than that of computational accuracy, which shows that this method is useful to optimize the Monte Carlo method.
277: Multiscale framework study of particle attrition in pneumatic conveying of coarse particles

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Keywords
Particle attrition, Particle breakage, Particle collision, Granular flow, Granular materials

Abstract
Research on pneumatic conveying process belongs to the field of particle science in multiphase flow. Pneumatic transportation of absorber spheres in the pebble-bed high temperature gas-cooled reactor (HTGR) is a special application of pneumatic conveying technique in nuclear engineering field. The whole conveying process is an intermittent circulation of absorber spheres between the reflector boring and the storage bin in the reactor. It consists of several sub-processes, e.g., the granular discharge from the storage bin into the boring, granular discharge from the side reflector boring into the feeder, particle entrainment in the feeder, sphere conveying in the transport pipe and gas-solid separation in the storage bin. Particle motion behaviour and particle attrition characteristics of absorber spheres are very important for the design and operation of this special conveying system. In this study, we give a brief summary of our previous experimental and simulation work for coarse particle conveying. Then, a multiscale framework for investigation of particle attrition in the pneumatic conveying of coarse particles is introduced. Further research requirements are proposed for a better understanding of the conveying process and to optimize the conveying system design.
A coupled approach of discrete element method and pore network model in the simulation of particle-fluid flows

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Keywords
Particle-fluid flow, pore scale modelling, discrete element method

Abstract
Discrete element method (DEM) has been coupled with various models (e.g., CFD, SPH and LBM etc.) for the simulation of particle-fluid flows in the past decades. DEM generally computes the dynamics of solids at a particle scale, whereas the computational scale of fluids by the other model like CFD or SPH/LBM is either larger or smaller than the particle scale. The mismatch of the scale leads to either high computational cost or uncertainties in the coupling scheme. This work presents a coupled approach of DEM and pore network model. The computation scales for solids (particle scale) and fluids (pore scale) are equivalent, thus allowing the coupling to be straightforward. Validation of the model is conducted through comparisons with experiments and LBM results for a relatively wide range of Reynolds number. The descriptions of fluid flows and calculations of particle-fluid forces are also discussed.
Investigating the jamming phenomenon of the poly-dispersed particle system via coupled CFD—DEM simulations

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Keywords
Jamming, Fluid-driven particle flow, CFD-DEM, Particle size distribution, Jamming arch

Abstract
The jamming of a dense stream of particles when passing through an orifice is a general phenomenon that exists both in daily life and many industrial fields, such as the grains clog the silo during discharging, and the granular material jam the conduits which are designed to carry them smoothly. Over the years, there have been intense researches focusing on the occurrence of the jamming phenomenon and the influence of the underlying factors on it. However, most of the previous studies work on the mono-dispersed, bi- and tri-dispersed particle system, and the researches on the poly-dispersed particle system with the continuous particle size distribution is lack. Many natural particles, such as the atmospheric aerosols and the soil particles, of which the particle size is log-normal distributed, also occur many jamming phenomena in chemical and civil engineering projects. Therefore, this work aims to study the jamming of this type of poly-dispersed particle system by performing a three-dimensional simulation via the coupled Computational Fluid Dynamics—Discrete Element Method (CFD—DEM) model. The DEM model simulated the particle motion, and the coupled procedure of CFD and DEM model models the fluid-particle interaction force which drives the particle to flow. The agreement between the simulation results and the experimental results demonstrates the capacity and validity of the CFD-DEM model on simulating the fluid-driven jamming of the poly-dispersed particle system. From the simulation results, the jamming probability and the critical orifice-particle ratio size are both strongly dependent on the size of the large particles, especially the characteristic particle diameter \(d_{90}\) such that 90% of the sample by weight consists of finer grains. The critical orifice-particle ratio size also exists in the poly-dispersed particle system when the orifice-particle ratio size is defined as the ratio of orifice size to \(d_{90}\). Moreover, benefit from the DEM model, we capture the particles that form the particle jamming arch and analyze the proportion of those particles according to the particle diameter \(d_p\). It is observed that the particle jamming arch is mainly formed by large particles. Since those large particles form the particle arch and lead to the jamming happening, the size of large particles, e.g. \(d_{90}\), prominently influence the occurrence of the poly-dispersed particle jamming.
Experimental investigation of flow and segregation of non-spherical particles in rotating cylinder.

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Keywords
Segregation, Rotating Cylinder, Non-spherical particles, Granular materials

Abstract
Segregation particles (spherical as well non-spherical) is very common phenomena during flow. Granular materials segregate due to differences in size, shape & density. We have studied this phenomena in a two-dimensional rotating cylinder (axial length is much smaller than the diameter). Cylinder is driven by a computer-controlled stepper motor having radius 16 cm and length 1 cm. Mixtures of different pulses (moong-daal, rice etc.) are used to investigate the segregation phenomena. Parameters varied in the experiments are composition, rotational speed (4-8 rpm) to obtain different concentration profile. Image analysis is done to detect the position of the particles. Area fraction and number fraction profiles are plotted along the flow path. Segregation patterns are obtained for each case studied. As rotational speed increases segregation equilibrium was achieved sooner.
282: Parametric study of factors affecting the dust emission from poultry litter bed with DEM-CFD coupling technique

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Keywords
Dust Emission, Poultry Farm, Computational Fluid Dynamics, Discrete Element Method.

Abstract
Poultry farming is one of the major agricultural sources of PM10 emission into the environment. Fine dust emission from poultry litter bed has a significant effect on human health, equipment, animal welfare, and the environment. According to a report in 2015, about 17% of total fine dust in the Netherlands is caused by poultry houses which worries citizens and Dutch governments, and thus have to be reduced.

The properties of the litter bed, chicken activity, and micro-climate conditions of poultry house are a number of factors that affect the dust emission rate from poultry litter, but precise quantitative effects and their interactions are hardly known. The aim of this study is to conduct a parametric numerical analysis on the effect of poultry litter particle size distribution, litter density and its moisture content along with the airflow velocity and its direction on the dust emission rate. In this study, a CFD-DEM model as a numerical technique was set-up to simulate the dust emission process from a poultry litter bed.

The CFD-DEM simulation results indicated that less dust is emitted from a litter bed with higher moisture content which is in agreement with the scientific reports. We observed that fine dust cannot be liberated from the litter bed by the airflow in the absence of interaction between litter bed and an external moving object such as a chicken claw. This can be interpreted that the fine particles are trapped between the coarse particles and consequently they are not able to exchange sufficient energy with the airflow to be released as dust particles. In addition, the parametric study on the direction of the airflow over the litter bed indicated that more momentum is exchanged between fine particles and the airflow at bigger angles of contact and more fine particles are released from the litter bed into the environment.
A Coupled DEM-SPH Modelling and Calibration Method for Mineral Slurries

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Keywords
DEM, SPH, Slurry, Mineral, Tailing

Abstract
Mineral processing is the most important stage of copper and gold production, during which a comminution circuit is utilised to reduce the size of the ore materials for further mineral enrichment processing. The comminution circuit often accounts for 30\% ~ 50\% of the total production cost. The milling process, which may include systems such as ball mills, semi-autogenous (SAG) mills and autogenous (AG) mills, presents challenges when attempting to optimise the comminution circuit. This study presents a coupling and calibration framework for slurries in mineral processing circuits. A smooth particle hydrodynamics method was utilised to model the water phase and to couple to DEM. The coupling theoretical framework is developed. A rotary viscometer device was further developed for the DEM-SPH calibration purpose. A suite of slurry samples was selected to determine the rheological properties experimentally. DEM-SPH coupled simulations were subsequently performed to calibrate the modelling parameters in order to reflect the slurry properties in reality. The developed framework has demonstrated direct applicability to the large scale mining operations globally.
Hydraulic conveying is now widely applied in different industrial systems, such as mining, chemical, ocean and petroleum. Through literature review, we find most researches are focusing on macro information, like pressure drop, wear, solid concentration distribution, these parameters are controlled by these micro information, such as particle forces, particle flows, but, the analysis is yet rare. Generally knowledge is largely known due to many studies and investigations. Nevertheless, the fundamental study is still lacking, some complex phenomena, such as flow regimes and their transition are still not be fully understanding. Therefore, for better controlling hydraulic conveying system, flow regimes and their transition are quite important to be understood as it could get command of the pressure drop and wear. According to this direction, the combing of computational fluid dynamics (CFD) for liquid phase and discrete element method (DEM) for solid phase is chosen to be used in this paper, which could show the particle motion and flow characteristics. In addition, it not only has least assumptions, but also has detailed information of forces between solid, wall and liquid. This paper is going to develop the original 3D-model, and to reproduce various flow regimes and their transition with different variables, forces between particle-particle, particle-pipe wall, particle-fluid, are also be analyzed. This paper shows that this new developed model with CFD-DEM for horizontal hydraulic pipeline conveying is reliable.
285: Steady State Rheology of Homogeneous and Inhomogeneous Cohesive Granular Materials

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Keywords
Cohesion, Friction, Rheology, Contact Model, Shear Band, Shear Dilatancy

Abstract

This work aims at understanding the effect of different particle/contact properties like friction, Softness and cohesion on the compression/dilation of sheared granular materials. We focus on the local volume fraction in steady state of various non-cohesive, dry cohesive and moderately-to-strongly, wet cohesive, frictionless-to-frictional soft granular materials. The results from (i) an inhomogeneous, slowly sheared split-bottom ring shear cell and (ii) a homogeneous, stress-controlled simple shear box with periodic boundaries are compared.

The steady state volume fractions agree between the two geometries for a wide range of particle properties. While increasing inter-particle friction systematically leads to decreasing volume fractions, the inter-particle cohesion causes two opposing effects.

We have also considered here two cohesive contact models: (i) a linear reversible cohesive model for dry particles resembling van der Waals forces, and (ii) a non-linear irreversible cohesive model for wet particles resembles liquid bridges.

With increasing strength of cohesion for both soft and stiff particles, we report an enhancement of the effect of contact friction by cohesion. For soft granular materials, strong cohesion causes an increase in volume fraction due to significant attractive forces, not visible for stiff particles. This behaviour is condensed into a particle friction -- Bond number phase diagram, which can be used to predict non-monotonic relative sample dilation/compression due to the opposing effects.

Apart from volume fraction, the macroscopic friction increases with inter-particle cohesion following a power law trend, but not linear trend as in the previous works.
Applications of a DEM-MBD coupled model of a vibrating screen in vibration analysis

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Keywords DEM, dynamic model, vibrating screen, vibration analysis

Abstract Vibrating screen is one of the key equipment for mineral processing. Their proper operation, including accurate vibration movement and slope angle, can provide the benefits of energy savings and cost reductions in the screening process and the whole mining process [1]. The most used approach to seek the optimal screening operational parameters is by discrete element method (DEM). The input parameters of this method are the material properties, geometry parameters and vibration parameters.

To obtain the movement of the screen body dynamic models are used, in which the ore is basically regarded as a static inertia block and only improves the mass of screen body [2]. The empirical evidence shows the influence of the ore on the movement of screen body [3], for that reason, a more complex model is necessary in order to understand the operation of this machine that considers the interdependence between DEM models and dynamic models.

In this work, we present a coupled DEM-MBD model of a vibrating screen that can obtain an accurate movement of the screen body. It is useful in condition monitoring to analyze off-design conditions and provide operation ranges. Simulations are carried out with data of an industrial vibration screen used in copper industry and a laboratory scaled vibrating screen. Vibration analysis is made by means of orbital analysis and frequency spectrum. Results show good agreement with experimental data, and they are useful for condition monitoring engineers

References
State, Connectivity, and Disorder in Dense Packings of Polydisperse Spheres

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Keywords
state, connectivity, disorder

Abstract

Dense particulate assemblies arise in a remarkable number of applications, from pharmaceuticals to soils, mined materials, and metal powders. It is reasonably well-understood that the bulk behavior of granular materials is an emergent manifestation of collective interactions at the particle scale. Traditionally, structure at the particle scale is characterized by tensorial metrics that quantify the magnitude and directionality of contacts and forces between particles. These measures have been shown to be inextricably linked to the engineering-scale behavior of jammed granular matter (i.e., the so-called “stress-force-fabric” relationship). However, there is increasing interest in the quantification of granular assemblies using other microscale descriptors, e.g., betweenness centrality (connectivity), keramicity (state), and entropy (information content and disorder).

In this work, we present results of such analyses on a series of discrete element method simulations of collections of polydisperse spheres. Specifically, hydrostatic, triaxial, and shear loading conditions are applied on representative synthetic particle assemblies. The relationship between tensorial metrics and other microscale descriptors is examined. Outcomes from this study provide insights into the fundamental mechanisms that govern the statistics and evolution of microscale metrics and also promote our understanding that bridges micro- and macroscale response of granular materials.
288: A DEM investigation of the micromechanics of non-active clays
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Keywords
Clays, Compressibility, Particle-scale behaviour

Abstract
The micromechanical behaviour of clays cannot be investigated experimentally in a direct fashion due to the small size of clay particles. An insight into clay mechanical behaviour at the particle scale can be gained via virtual experiments based on the Discrete Element Method (DEM). So far, very few DEM models for clays have been designed, mainly on the basis of theoretical formulations of inter-particle interactions with limited experimental evidence.

This work presents a numerical investigation of the mechanical behaviour of non-active clays. The underlying microscale mechanisms were inferred by indirect experimental evidence [1] and used in this study to design the constitutive contact laws of a simple two-dimensional DEM framework. Clay platelets were modelled as rod-shaped particles made of spherical elementary units, designed to behave as single elements. New contact laws including attractive and repulsive long-range interaction were designed in order to simulate the positive/negative charge characterising the clay particle surface.

The contact laws were tested against the ability of the DEM framework to reproduce qualitatively some aspects of the one-dimensional compression and shear behaviour of clay observed experimentally. Specifically, these include the effect of pH and dielectric permittivity of the pore-fluid on the virgin loading and unloading-reloading lines, the dependency of the slope of the unloading-reloading lines on the pre-consolidation stress, contractive/dilative and monotonic/non-monotonic behaviour under shear. Despite the extreme simplicity of the proposed model [2], distinct microscale mechanisms could be effectively linked with clay response at the macroscale.


Quantification of particle-induced mechanical stress on filamentous microorganisms via CFD DEM simulations

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Keywords CFD-DEM, shake flask, mechanical stress, filamentous microorganism, cultivation

Abstract Cultivations of filamentous microorganisms are of prime industrial interest because of their production of various secondary metabolites like antibiotics. The productivity of the filamentous system, however, is closely linked to the cellular morphology, which varies between freely dispersed mycelia and dense bioagglomerates (pellets) depending among others on the mechanical stress. For Lentzea aerocolonigenes the addition of glass beads (x_mean = 969 µm, 100 g/L) to shake flask cultivations led to a 14-fold increase in productivity compared to an unsupplemented control. However, the intensity of the glass bead-induced mechanical stress is crucial for the productivity. On the one hand, the right amount of mechanical stress may loosen up the pellet structure, which then allows a better substrate and oxygen supply into the inner pellet. On the other hand, too high mechanical stress decreases the productivity due to the destruction of the pellet structure or even degradation of the microorganisms.

For a deeper understanding of these effects and further control of the productivity, CFD-DEM-simulations were used for quantitation of the mechanical stress during a shake flask cultivation. Characteristic parameters like the mean stress energy, stress frequency and particle induced power input were obtained for different cultivation parameters like shaker speed, particle size or particle concentration. Finally, experimental results like the pellet Feret diameter and the product concentration were correlated with the characteristic parameters. In future, information about the mechanical stress in shake flasks should be compared with CFD-DEM simulations of stirred bioreactors for the development of scale-up criteria. Furthermore, DEM simulations of the resolved bioagglomerate will be used to investigate structural changes due to the glass bead induced mechanical stress.

The authors gratefully acknowledge financial support from the German Research Foundation (DFG) in the Priority Programme 1934 DisPBiotech – Dispersity, structural and phase changes of proteins and biological agglomerates in biotechnological processes.
Decades of progress in Discrete Elements modelling enabled us to tackle problems of increasing complexity and scale from many different areas of study. One of these is particle deformation and breakage. Deformation of particles is key in fields such as powder compression and tableting or soil mechanics; while breakage plays an important role in milling and geotechnics.

We present a model of deformable and breakable granular assemblies where elementary DEM particles are brought together and form a stable cluster due to an attractive cohesive interaction. Clusters can have arbitrary convex shapes and are mechanically stable like usual multi-spheres, but unlike the latter bonds between components are not rigid and allow the elements to change their relative distance. In this way, when subject to a sufficiently strong external force, the particle arrangement can change and the body is permanently deformed. For even stronger tensile forces particles can overcome their cohesive bonds and separate, with consequent local fracture that can trigger the cluster breakage.

Using a simple cohesion interaction to hold the agglomerates together is less computationally expensive than using multi-spheres, where the rigid body dynamics has to be prescribed. In our implementation the collective dynamics is inherited by each single particle interaction, like what actually happens in nature. Moreover, since clusters are obtained by direct compression of the particle ensemble, the main properties of the former can be computed in advance. For instance, radius and porosity of spherical clusters are analytically related to the components particle properties, allowing an extensive control on both micro and macro structures of the agglomerate generated.

The ability to control not only hardness and shape, but also the internal structure makes the model ideal to replicate the behaviour of porous plastic or brittle materials, such as soil, pharmaceutical powders and catalysts. Because cohesive interactions work also between particles of different clusters, multiple granules can be directly compressed together to form a bigger ensemble. This feature makes the model very promising for the study of powder compaction.
291: Discrete element modeling as a tool for oscillatory cutting of rock

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Keywords

Rock cutting, equipment, particle bonding, oscillations

Abstract

Rock cutting is a challenging process. Heavy equipment, large cutting forces, high wear rates and large amounts of required energy are common challenges when cutting rock. Traditionally, rock cutting is based on a linear motion of the cutting tool. However, a significant improvement on the cutting performance is expected when using non-linear cutting techniques. Non-linear cutting can be achieved by using an actuator to create a vibrating or oscillating motion on top of the linear forward motion of the cutting tool. The focus in this paper is on the oscillating undercutting disc cutter. This disc attacks the rock like a chisel or pickpoint, aiming at a cutting process dominated by tensile failures.

Although the discrete element method has been successfully used for various rock cutting processes, all these processes are based on linear rock cutting tools and most of these researches are based on 2D simulations. The use of a 3D approach is necessary to enable the simulation of oscillatory rock cutting tools.

This paper utilizes discrete element method in 3D to investigate non-linear cutting processes, especially the effects of the design parameters such as frequency, velocity and eccentricity of the cutting tool. To resemble rock-like materials the particles are placed in a dense particle assembly and they are bonded together through perfect brittle elastic bonds. The bonds can fail in shear and in tension, allowing the dominant failure mechanisms, i.e. shear and tensile cracks, to occur. After failure of these bonds, particles can still interact through collisions.

The simulation results show the effect of the tested design parameters and are compared with analytical models and actual experiments of oscillating undercutting discs.
3D DEM analysis of deformation and failure in inherent anisotropic rocks

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Keywords Anisotropic rocks, Weak layers, Smooth joint contacts, Nonlinear bond model

Abstract A class of rock-like materials such as sedimentary and metamorphic rocks are inherent anisotropic rocks. Deformation and strength properties of such rock materials are strongly dependent on the loading orientation with respect to the fabric elements. Despite significant advances in analytical approaches including experimental and phenomenological ones, the key issue remains the description of the local cracking mechanism of anisotropic rocks. In this paper, a three dimensional discrete element (DEM) is proposed in the framework of the particle flow code (PFC). Compared with many existing studies on anisotropic rocks, the emphasis is devoted to capturing the failure process of cohesive interface at particle-based dimensional in inherent anisotropic rocks under a large range of confining stress. For this end, a numerical procedure for the generation of anisotropic rock samples is first presented in which the mechanical behavior of the matrix is described by bond contacts while that of weak layers by smooth joint contacts. Unlike general simple bond models using a linear failure criterion, a unified non-linear bond model is proposed and introduced in both band and smooth joint contacts. For this model, the elastic and strength parameters depend on the orientation of bond contacts. In particular, its shear strength is a non-linear function of normal stress, which has the ability to reproduce the mechanical strength of rocks in a wide range of confining stress. The proposed model is implemented into the standard particle flow code. Comparisons between experimental data and numerical predictions performed on a representative inherent anisotropic rock, Tournemire shale, have shown that the proposed model was able to well reproduce the effect of confining stress on the elastic and strength properties of anisotropic rocks. Further, a series of three-dimensional numerical simulations are performed for different orientations of weak layers and confining stresses. The effect of weak layer and confining stress on both local cracking process and macroscopic failure mode of rock samples is investigated and discussed. Correspondingly, the failure mechanism respectively in matrix and weak layer has been studied, especially capturing the failure evolution from the diffused micro-cracks to forming local fracture band.

Figure 1: Spatial distribution of diffused micro-cracks and displacement in samples (1Mpa)
Abstract

In the mining industry very large grinding mills are the work horse of grinding ore particles from 0.2 m size to a size below 150 microns. Since these mills consume anywhere from 2 MW to 20 MW power, the prediction of power in such mills was pursued by the lead author in 1990s using DEM. In the beginning, mill power was predicted with two-dimensional DEM simulation in which a thin slice of the mill was simulated, and the computed collision energy was summed. Later, three-dimensional simulations came into the fore, yet due to the very large size of mills, the prediction of mill power with these codes was done only in a select few studies. Besides, in all these simulations, the rock particles and steel grinding balls were modeled as spheres. However, some other authors attempted representing irregular shapes with jointed-spheres and the like.

We present a fresh attempt at predicting power by modeling the rock particles as polyhedral particles with angular edges. The Blaze-Dem code with GPU computing capability is used in these simulations. The polyhedral representation is as close to one can get to replicating rock particles. Of interest here is the semi-autogenous grinding mill in which very large rock particles and grinding balls undergo tumbling motion inside the cylindrical mill body. These mills draw power in the range of 10 to 20 MW. First, we present experimental results in a 90 cm diameter mill in which various ratios of rock to particle mass is filled and operated at different mill speeds. The power draw of the 90 cm mill varies between 450 to 820 watts depending on the charge filling and mill speed. We then show that the linear spring-dashpot model with history dependent tangential spring-dashpot can predict the mill power as well as charge motion. Next we present the corresponding spherical particle simulations and show the differences in charge motion due to angularity of the particles and smoothness of the particle surface. Next, we present the three dimensional DEM simulation of plant scale simulation of two semi-autogenous mills, 12.6 m diameter and 7.6 m long and 10.98 m diameter and 8.08 m long. The comparison of polyhedral DEM simulation with plant data confirms the capability of such simulations.

The polyhedral particle simulation with GPU computing is a key advancement in the discrete element algorithms. Such simulations lead to optimum design of lifters in mills as well as pointing the way for random fracture of particles in DEM simulations.
Coarse-grain DEM (CG-DEM) is a practical modeling approach to simulate a commercial scale system. In CG-DEM, the simulated grains generally have neither the size nor the shape of actual particles. Typical figures are coarse-grain one order of magnitude bigger (diameter wise) than particle and having a spherical shape. At the microscale, the coarse-grain then only has a weak physical connection to the actual particle. Hence, as generally accepted, a macroscopic perspective is preferred for calibration of CG-DEM parameters. The angle of repose (AOR) indeed sits among the most popular and accessible macroscopic measurement for that purpose.

However, due to the relatively large size of coarse-grain, it is not granted that a lab scale AOR experimental procedure is suitable for direct replication in CG-DEM simulation setup. The truth is, there is no need to simulate the experiment directly, given the property of interest is experiment independent, which should, theoretically, be the case when defining AOR as the steepest slope that the material can be heaped without collapsing. Although not as easy as it might appear, AOR experimental determination is a one-time effort for a given material. It is a different story for CG-DEM simulation when seeking to calibrate a parameter set. In that case, several simulations are to be performed.

Current study hence explores CG-DEM simulation procedure for the determination of the angle of repose (AOR) with shortest simulation time duration and as few as possible particles. Various methods are explored and varied in term of absolute geometry size. A hybrid and progressive approach are suggested, starting by quickly forming the bulk of the heap to end by slow pouring. A minimum heap size is also suggested, relative to grain size. A case study is shown, mapping AOR as a function of rolling resistance, static friction, and dynamics friction, performing several hundred simulations within a reasonable timeframe. Result forms a 3D space for which solution for a given granular material lies on a surface. Although insufficient to identify a unique parameter set, the method is useful when part of a broader series of experiment, including, as an example, hopper flow rate or the likes.
A Coupled CFD-DEM Simulation of Transport, Settlement and Plugging Behavior of Polydisperse Particles in Narrow Rectangular Channels

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Keywords
CFD-DEM, polydisperse particles, transport, settlement, plugging, narrow rectangular channel

Abstract
Transport, settlement and plugging behavior of polydisperse solid particles inside a fracture plays a vital role in many on-site operations during exploration and development of hydrocarbon resources. For instance, mud cake formation, lost circulation control, proppant placement, water injection, sand control, etc. These operations are usually unpredictable due to the lack of understanding of particle motion behavior feature. However, conventional laboratory experiments usually can only obtain macroscopic results instead of the microscopic mechanism. To solve this issue, we developed a numerical model to study the multi-scale behavior of the polydisperse particles inside narrow rectangular channels.

An unresolved CFD-DEM model for polydisperse particles flowing inside a narrow rectangular channel is developed based on an open source framework CFDEM®, which is a couple of OpenFOAM® and LIGGGHTS®. Validation of the model is completed by comparing numerical results and experimental results of particle settling and proppant displacement. Influence of size distribution, concentration, physical properties of the particles, flowing parameters and channel geometry on the polydisperse particles motion is discussed.

The transport, settlement and plugging behavior of polydisperse particles inside a narrow rectangular channel is significantly depending on the particle, fluid and flowing channel. In the low particle concentration case, large particles transport a longer distance and settle faster than small ones. Two distinguishing particle settlement zones are obtained: one large particles settlement zone near the inlet and another small particles settlement zone far from the inlet. As the particle concentration increases, the positions of the two particle settlement zones are reversed because of the interaction between particles. When a critical concentration is approached, a plugging zone is observed, which is formed through two primary mechanisms: gravity settlement and constriction capture. The far moving large particle can directly bridge and plug the nature constriction in a narrow rectangular channel. The flowing particles will be captured by the previously settled particles and bridge in the secondary constriction to form a strong plugging zone. The plugging zone usually experiences multiple forming-breaking-reforming cycles depending on channel compliance and keep moving toward the narrow rectangular channel outlet during the plugging process.

Increasing the particle size and concentration will improve the plugging probability and decrease plugging penetration depth. A low particle density leads to a long transport distance and a far settlement and plugging zone. Nonuniform size distribution and high-friction particles facilitate narrow rectangular channel plugging more effectively than the uniform ones. An optimal flow rate range exists for a solid, tight and stable plugging zone. The vertical channel is found to be more feasible to plug than the horizontal one and rough channel is more likely to be plugged than a smooth one.
Contribution of Frictional Interactions to Discontinuous Shear Thickening

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Keywords
Discontinuous Shear Thickening, friction, roughness, rolling resistance

Abstract
Discontinuous shear thickening (DST) of concentrated suspensions (either Brownian or non-Brownian particles in a Newtonian liquid) is a remarkable phenomenon which arises as a drastic increase (several orders of magnitude) in viscosity at a critical shear rate/stress. Recent studies attributed the driving mechanism of DST to the transition from lubricated to frictional contacts [1-3]. While recent experimental [1] and numerical studies[2-4] aim to shed light on the underlying details of this transition, there is also a need for numerical studies to characterize the effect of frictional interactions among the dispersed particles. For this study we have focused on the minimum set of required components to capture (D)ST behavior in dry particulate media. To demonstrate the sole contribution of frictional interactions; we neglect hydrodynamics, electrostatics, and inertia effects. We demonstrate that frictional contact forces can be responsible for shear thickening as the particle volume fraction increases. After a certain volume fraction, DST can be observed. We studied this behavior over a range volume concentrations and different combinations of sliding friction and rolling resistance. The main novelty lies in the use of the rolling-resistance, which represents a torque without force, and makes a direct link to particles with varying surface properties ie., surface roughness. Starting from smooth spheres, sliding friction and rolling resistances has been systematically varied and their influence on the rheology was obtained in the form of relevant dimensionless variables.
A discrete approach for modeling of anchoring bolting in rock masses

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Keywords Bolting, excavation, reinforcement effect, anisotropy, shear band

Abstract In the framework of the extended rigid block spring method (RBSM), a numerical algorithm is proposed for simulation of anchoring bolts in rock masses. This algorithm is based on two assumption: (1) Only axial tensile stress is considered in bolts, shear stress along or across bolts not considered; (2) anchor bolts are fixed at both ends. The perfect elastic plastic model is used to describe the stress-strain relationship and failure behavior of bolts. The model is firstly used to investigate the effects of bolts on uniaxial compressive strength (UCS) of isotropic rocks. Four numerical UCS tests are conducted, respectively with 0, 4, 9, 19 hair-like anchor bolts. The stress-strain curves for UCS tests with different number of bolts are shown in figure 1. It can be observed that peak strength, residual strength and Young’s modulus are all increased compared to the test with no bolts. Peak strength are increased by 8.08%, 15.19% and 27.6%, respectively for rocks with 4 bolts, 9 bolts and 19 bolts. The micro-failure mechanism is investigated, it is found that as bolts number increases, the ratio of shear crack number to tensile crack number increases. The effects of bolts on strength anisotropic degree of anisotropic rocks are also investigated. Results for UCS of rocks with different bedding plane orientation reinforced by different number of bolts are shown in figure 2. The relationship between UCS anisotropy and bolts number is shown in figure 3. It is very clear that the UCS anisotropy degree decreases as bolts number increases. Finally, the model is further applied to model anchoring effects in an excavated tunnel. It is found that bolts can significantly reduce the size of excavation damaged zone and convergence displacements.

Figure 1 Stress-strain curves for uniaxial compressive tests with different number of bolts

Figure 2 UCS of rocks with different bedding plane orientation reinforced by different number of bolts

Figure 3 Relationship between strength anisotropy and number of bolts
Working principles of the viscosity of nanoparticulate suspensions derived from CFD-DEM simulations

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Keywords
viscosity, suspension, CFD-DEM, genetic algorithm, nanoparticle

Abstract

The viscosity of nanoparticulate suspensions is known to be dominated by particle-particle interactions due to surface forces. Yet, quantitative characterization of these interactions is demanding, which is why a quantitative modelling of the viscosity has proven to be difficult. DEM allows a detailed characterization of the interaction forces and, coupled with CFD, was used to elucidate the working principle that links interaction forces with the rheological behavior of the suspensions. From the elucidated relationship, a mechanistic model for the viscosity of nanoparticulate suspensions could be derived and used to predict the viscosity based on physical material and system parameters. Required proportionality parameters were obtained by subjecting the derived model to an approximation with a genetic algorithm.
Direct simulation of wave propagation in fully saturated granular packings using coupled LBM-DEM

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Keywords
Wave propagation, Lattice Boltzmann method, Discrete element method, Biot's theory

Abstract

Biot's theory predicts wave velocities in a saturated granular medium using the properties of the solid skeleton and pore fluid, but neglects the interaction between constituent particles and local squirt flow, which becomes essential as the wavelength decreases. In this work, we explore the missing ingredients in Biot's macroscopic description of wave propagation, by mean of particle-based numerical simulations. The lattice Boltzmann method (LBM) and the discrete element method (DEM), which resolve the pore-scale hydrodynamics and intergranular behavior, respectively, are two-way coupled to simulate wave propagation in saturated granular packings.

After comparing existing the two existing coupling schemes, we apply isotropic compression on a fully-saturated packing of polydisperse, frictional spheres to study the influence of the pore fluid on the acoustic behavior. An oscillating pressure boundary is used to emit acoustic waves from the fluid boundary.

The dispersion relations of the saturated granular packings are obtained from coupled LBM-DEM simulations, while DEM simulations provide the dispersion relations of the corresponding dry solid skeleton, as well as its long-wavelength elastic moduli. Using these as input, the wave velocities in the saturated system are computed with Biot's theory and compared with the numerical results from the LBM-DEM simulations.
Particle contact parameter calibration with response surface method: an example of particle charging in the ironmaking blast furnace

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Keywords
Contact parameter calibration, Repose angle, Repose surface method, Blast furnace

Abstract

Contact parameter calibration is critical to predict interparticle interactions in the discrete element method (DEM) simulation. This work employed a general and efficient method for contact parameter (coefficient of static friction, rolling friction and rolling viscous damping) calibration with the use of the response surface method (RSM) and the repose angle experiment. The DEM simulations based on Hertz-Mindlin model and elastic-plastic spring-dashpot rolling friction (EPSD) model were carried out, and three significant prediction models for coke, sinter and pellets were established. According to the prediction model, three contact parameters can be calibrated. Then, the investigation of parameter sensitivity suggests that coefficients of static friction and rolling friction have remarkable influence on the repose angle. Further investigations of the model robustness prove the suitability of the three models in predicting the reliable contact parameters between particles with different particle density, particle size distribution and particle shape.
Keywords
Cohesion, Bond number, Formulation, Prediction, Flowability, Distinct Element Method

Abstract Particulate solids are one of the key ingredients for products manufactured by many industries such as pharmaceuticals and food. Several types of particulate solids are typically mixed to manufacture the final product with a certain specifications. As a consequence, these powders undergo various manufacturing processes such as, mixing, storage, conveying, etc. In all these manufacturing processes the physical behaviour of the powder is at least as important as their chemistry. Stability, content uniformity, manufacturing difficulties, and performance of the products are mainly determined by decisions made during the formulation process. Therefore, a need for more fundamental understanding of performance and behaviour of formulated products is needed.

Virtual Formulation Laboratory (VFL) collaborative project between University of Leeds, University of Leicester, University of Greenwich, and Imperial College of London is formed to address this gap. The aim here is to develop a software tool for prediction and optimisation manufacturability and stability of advanced solids-based formulations, specifically for evaluation of their flow, extent of segregation, degree of mixing, and compatibility. The overall aim of the project are (a) to develop the science base for understanding of surfaces, particulate structures and bulk behaviour to address physical, chemical and mechanical stability during processing and storage and (b) to incorporate these into a software tool (VFL) which accounts for a wide range of material types, particle structures and blend systems to enable the formulator to test the effects of formulation changes in virtual space and check potential problems covering the majority of manufacturing difficulties experienced in production plants.

In this study, we present our work on prediction of flowability of binary and ternary mixtures under dynamic conditions using Discrete Element Method analysis of Freeman FT4 rheometer. It is found that granular bond number, which is the ratio inter-particle adhesion force to gravitational force correlates well with the flow energy measured by Freeman FT4 rheometer for binary mixtures. Three averaging methods are used to calculate the mixture bond number by introducing a weighing factor based on fractional surface area of each component in the mixture. The granular mixture bond number is varied by modifying interfacial surface energy, density and size of each mixture components. The outcome of this study can be used to expand its applicability for prediction of flowability of multi-component powder mixtures.
Analysis of the Dynamics of Acicular Crystals in an Agitated Bed

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Keywords
DEM, Particle Shape, Agitated Beds

Abstract

Agitated filter bed dryer is the unit operation of choice in the pharmaceutical industry for separation of the solids from mother liquor after crystallisation process. The impeller is rotated intermittently to promote homogenous heat transfer within the wet cake. However, the shear deformation induced by the impeller could lead to unwanted breakage of the crystals, adversely affecting the product quality and processing of the solids.

A large fraction of active pharmaceutical ingredients are acicular in shape and are very prone to breakage during the agitated drying process. Apart from shear deformation, highly acicular particles are also subjected to bending when the particles in front of the blades are ploughed over the blades, snapping them into smaller fragments. Discrete element method (DEM) is used in this work to simulate the dynamics of faceted particles with high aspect ratio in an agitated bed. Particle shape is modelled using faceted polyhedron. The simulation is validated experimentally by comparing the torque recorded in a custom-built miniaturised agitated filter bed dryer. The effect of particle shape on the stress and strain distributions within the particle bed are analysed, in addition to the influence of impeller rotation speed. The outcome of the work is reported, providing an insight into the role of particle shape, especially faceted and acicular, as well as platy-like, in the particle bed dynamics and the prevalent particle breakage behaviour in agitated beds.
303: Particle shape effects for industrially relevant simulations using polyhedra particles

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Keywords
Polyhedra, DEM, Large Scale, Packing

Abstract
In blast furnaces, burden topography and packing density affect the stability of the burden, permeability of gas flow as well as the heat transfer efficiency. A fundamental understanding of the influence and interaction of coke and ore particles on the burden topography and packing density is therefore essential, in particular the influence of particle shape polydispersity and particle size polydispersity. In this talk we look at the effect of particle shape and size polydispersity on the coke and ore charge distribution inside a bell-less blast furnace using the discrete element method (DEM). A comparative study between spheres, with rolling friction to account for shape, and polyhedra is conducted for shape and size polydisperse particle systems. In
Advances in DEM simulations using GPUs

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Keywords
GPU, Polyhedra, Large Scale

Abstract
The Discrete Element Method (DEM) is the most commonly used numerical method for the simulation of granular material. However the computational cost of the DEM has limited the number and shape estimation of particles. In this talk we look at the Graphical Processor Unit (GPU) as an alternative computing platform to the CPU that has enabled detailed particle shapes such as polyhedra as well as an increase in particle number to tens of millions within a realistic time frame. In particular we will consider the effect of particle shape in various industrial devices such as slios, mixers, mills as well as the charging process of blast furnaces in the steel making industry. We show that the effect of particle shape cannot be ignored and needs to be taken into account in the optimization/design of these process. It is also made apparent that the use of GPU computing enables a new performance level in DEM simulations making it more tractable to industrial applications and design optimizations.
305: SudoDEM: a new open-source discrete element code for modeling of non-spherical granular particles

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Keywords
discrete element, granular, non-spherical, particle shape, super-ellipsoid, polyhedron, open source

Abstract

This paper introduces a new open-source discrete element code, SudoDEM, for modelling non-spherical particles in both 3D and 2D. Developed from another popular open-source code YADE, the code inherits a classic DEM framework empowred by OpenMP acceleration, and provides a rich library of particle shapes, including super-ellipsoid, cylinder, cone, polyhedron for 3D, and disk, super-ellipse for 2D. More complex particle shapes can be readily obtained by clumping these basic shapes. Two general and efficient contact-detection algorithms, the parametric common normal algorithm and the Gilbert-Johnson-Keerthi algorithm, have been developed to handle contacts among complex shaped particles. Example simulations (including granular packing and triaxial compression) are demonstrated as validation and showcase of the robustness and flexibility of SudoDEM.
Deformable and breakable DEM particle clusters for modelling plastic and brittle porous materials

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Keywords
Clusters, deformation, breakage, elasto-plastic interaction, granules, agglomerates, porosity

Abstract

Decades of progress in Discrete Elements modelling enabled us to tackle problems of increasing complexity and scale from many different areas of study. One of these is particle deformation and breakage. Deformation of particles is key in fields such as powder compression and tableting or soil mechanics; while breakage plays an important role in milling and geotechnics. We present a model of deformable and breakable granular assemblies where elementary DEM particles are brought together and form a stable cluster due to an attractive cohesive interaction. Clusters can have arbitrary convex shapes and are mechanically stable like usual multi-spheres, but unlike the latter bonds between components are not rigid and allow the elements to change their relative distance. In this way, when subject to a sufficiently strong external force, the particle arrangement can change and the body is permanently deformed. For even stronger tensile forces particles can overcome their cohesive bonds and separate, with consequent local fracture that can trigger the cluster breakage.

Using a simple cohesion interaction to hold the agglomerates together is less computationally expensive than using multi-spheres, where the rigid body dynamics has to be prescribed. In our implementation the collective dynamics is inherited by each single particle interaction, like what actually happens in nature. Moreover, since clusters are obtained by direct compression of the particle ensemble, the main properties of the former can be computed in advance. For instance, radius and porosity of spherical clusters are analytically related to the components particle properties, allowing an extensive control on both micro and macro structures of the agglomerate generated.

The ability to control not only hardness and shape, but also the internal structure makes the model ideal to replicate the behaviour of porous plastic or brittle materials, such as soil, pharmaceutical powders and catalysts. Because cohesive interactions work also between particles of different clusters, multiple granules can be directly compressed together to form a bigger ensemble. This feature makes the model very promising for the study of powder compaction.
309: CFD-DEM modelling of non-spherical particles in an industrial context

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Keywords

CFD-DEM, DEM, drag, multisphere, non-spherical particle

Abstract

The continuous development of existing and new functional material systems, where particulate morphology differs from spherical systems (e.g. fibres, flakes, ...), demands technical know-how on the processing of non-spherical particles. Therefore, tools are needed to aid in process design and further understand non-spherical systems.

On this work, an overview of different approaches for the modeling of non-spherical particles on the context of industrial particle simulations is presented. Additionally, a novel approach for the computation of orientation dependent drag and hydrodynamic torque for multi-sphere DEM particles is presented.

First, the multi-sphere, super-quadric and convex-hull geometric DEM representations are described with industrial-relevant examples depicting its advantages and disadvantages.

Furthermore, A novel drag model for multi-sphere particles, which considers orientation dependency and hydrodynamic induced torques, is presented. The approach is inspired by Stokesian Dynamics as done by Joung (2006) with multiple bonded spheres. Its validity is shown by comparing results to analytical solutions of single non-spherical particles. A study on the number of spheres needed to correctly represent the drag behavior of the non-spherical particle is shown.

Lastly, different drag correlations used in CFD-DEM coupling for multi-sphere particles are presented by evaluating a fluidized bed containing spherocylindrical particles. Calibration strategies are discussed and a comparison to experimental data is presented.
Abstract

The physical and morphological properties of particles and interphases can seriously impact the whole physico-mechanical behavior of particle-reinforced composites (PRCs). In this work, we devise a robust coupling model of the discrete element method (DEM) and finite element method (FEM) to numerically investigate the effective elastic modulus and thermal conductivity of three-phase particle-reinforced composites consisting of elliptical particles of high packing density, soft interphase and matrix, as shown in Fig. 1. In the numerical model, a novel parametric equation of the interphase is proposed to realize a soft (penetrable) layer with a constant finite thickness coated surrounding each hard elliptical particle. Additionally, a convenient strategy is implemented to cope with periodic boundary conditions containing numerous particles. On the other hand, we also apply a micromechanical theory to calculate the effective elastic modulus and thermal conductivity of such three-phase composites by incorporating the fraction of soft interfaces. We show that our numerical and theoretical models lead to predictions of the elastic modulus and thermal conductivity of particle-reinforced composites with nonspherical particles of a high volume fraction to a reasonable accuracy by comparing with available experimental data. Moreover, utilizing our models, we systematically investigate the influence of the characteristics of particles and interphase such as geometric size and aspect ratio on the elastic modulus and thermal conductivity of particle-reinforced composites. We find that these physical characteristics play significant roles in determining the physical and mechanical properties of composites, suggesting that the properties of such materials can be tailored via proper composites engineering and design.
311: Unifying size-topology relationship in random packings of polydisperse adhesive spheres

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Keywords
polydisperse, packing, adhesive, Discrete Element Method

Abstract
We study the size-topology relationship in random packings of polydisperse adhesive microspheres with a wide range of global packing fractions through a geometric tessellation. We find that the dependence of the neighbour number on the center particle size is always quasilinear, independent of the size span and interparticle adhesion. The averaged local packing fraction as a function of normalized particle size for different polydispersities is well regressed on the same profile, which increases to larger values as the mean particle size increases. The local coordination number-particle size profile coalesces into a master curve for all the adhesive particles, but will transfer to another branch for non-adhesive particles. Such size-topology relations are described theoretically by an extended geometrical “granocentric” model, which was applied previously to analyse jammed packing of granular matters and compressed emulsions. Our findings, together with the modified theory, provide a more unified perspective on the internal geometry of amorphous polydisperse systems, especially those with relatively loose structures.
Continuous-based cement hydration model of non-spherical particles and diffusivity of cement paste

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Keywords
granular materials, cement hydration; non-spherical; degree of hydration; porosity; diffusivity

Abstract
Cementitious composites as a typical granular material, their macroscopic properties are closely related to the microstructure generated by cement hydration. Currently, most of the cement hydration models are dominated by spherical particles. However, the actual shape of cement powder is non-spherical during the process of grinding of cement clinker, and the hydration of non-spherical cement particles is still an open issue. In this study, a continuous-based cement hydration model for non-spherical cement particles is proposed, which is inspired by the famous HYMOSTRUC model. In the theoretical model, the kinetics of an individual cement particle are derived via its morphological features, and two types of rate-controlling mechanisms are adopted in hydration. For a simulated cement paste with multi-sized particles, the effects of particle interaction on the penetration rate are considered in the spatial model for the presence of incompletely hydrated particles in the outer shell of the central particle. Subsequently, five kinds of polyhedron-shaped cement particle are taken as an example to illustrate the construction approaches of hydration products and unhydrated cores, and they are employed to generate the microstructure of the simulated cement paste. Furthermore, the proposed theoretical model is validated by experimental results. The evolutions of the thickness of hydration products layers and the degree of hydration of simulated cement paste over time are investigated for different diameters. Results reveal the fact that the penetration rate and the degree of hydration reduce with increasing particle diameter. Besides, results also display that the cement particle shape has a significant impact on the microstructure and diffusivity of cement paste, mainly reflect on the degree of hydration increase with decreasing of sphericity of cement particle under the same w/c ratio and hydration time conditions. It also indicates that the porosity of the cement paste increase with increasing sphericity of the particle and w/c ratio, and relative diffusivity of hardened cement paste reduces with increasing degree of hydration, with decreasing sphericity of the particle and w/c ratio. The purpose of this study is an attempt to explore a theoretical framework for non-spherical cement particles in hydration model. We expect that it will contribute to understand the influence of cement particle shapes on cement hydration and the development of the microstructure of cement paste, and further on the macroscopic properties of cementitious composites.
Influence of stress path on the contribution of fine particles in a gap-graded soil matrix

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Keywords Discrete Element Method, suffusion, stress path, semi-active fine particles

Abstract Internal erosion is one of the main causes of embankment dam failures. Internal erosion happens in different forms including suffusion, which particularly impacts the non-cohesive fine particles in a soil with a load-carrying structure made of coarse particles. Suffusion can impact a soil’s mechanical behaviour due to alteration in the soil’s stress-transmitting matrix caused by removal or relocation of fine particles. Susceptible cohesionless soils to loss of their fine particles due to seepage flow are known as “internally unstable” such as some gap-graded soils.

It is believed that the contribution of fine particles to the soil stress matrix in gap-graded soils depends on both the fines content and the gap ratio (the particle diameter ratio between coarse and fine fractions of particle size distribution curve). The fine particles’ contribution to the soil stress matrix can be quantified through their stress reduction factor ($\alpha$, the ratio of effective stress carried by fine particles to the effective stress of soil stress matrix) and their coordination number. Fine particles can sit loosely (i.e. inactive in stress transfer), provide lateral support to the soil stress matrix (semi-active) or actively carry a load at the same level as coarse particles (active). Whether fine particles will play an inactive, semi-active or active role will be crucial to their susceptibility to suffusion and will depend on a number of factors including the stress path that the soil is subjected to. The stress path can alter the semi-active fine particles’ role severely. Therefore, the most complicated scenario would happen when fine particles are semi-active.

As the direction of seepage flow can alter the stress state of soil, it is important to investigate the effect of stress path on the semi-active fine particles’ role and the impact of their removal by hydraulic forces on the mechanical behaviour of soil. Hence, this paper investigates the impact of the stress path on the semi-active fine particles in internally unstable soils with varying fine contents and gap ratios.

Discrete Element Method (DEM) modelling is employed to generate gap-graded assemblies of spherical particles with different fine contents and gap ratios using the PFC3D software package. Samples are initially isotropically compressed before being subjected to triaxial compression or extension stress paths. Semi-active fine particles are captured by considering the coordination number and more importantly $\alpha$ of each fine particle after confinement stage. Finally, the variation of coordination number and $\alpha$ values are analysed during shearing to evaluate the effect of axial compression or extension on these particles’ role in the soil matrix.

The result of DEM simulations indicates that the stress paths along with the different gap ratios and fine contents change the contribution of the fine particles in the soil stress-transmitting matrix. There is clear impact on role of semi-fine particles when the principal stress planes are rotated.
Simulation of the energy distribution of wet operated stirred media mills using a coupled CFD-DEM approach

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Keywords
stirred media mill, optimization, Rocky DEM, Fluent, coupled CFD-DEM

Abstract

Stirred media mills are very common in a wide range of industries, such as the chemical, pharmaceutical, ore, or paint industry and for fine grinding and dispersing of product particles down to fine particle sizes of a few microns or less. In addition to the fragmentation of particles, agglomerates and aggregates followed by an emulsification process, stabilization process, disruption of single-celled microorganisms, chemical reactions or particle synthesis are potential applications for stirred media mills as well. Due to the wide range of construction and processing parameters, experimental optimization and Scale-Up of wet operated stirred media mills are labor intensive and expensive. Therefore, coupled CFD-DEM simulations offer the potential to reduce the spent amount of time, money and labor.

The main aim of this study is to set up simulations to predict and optimize grinding and dispersing processes in wet operated stirred media mills. In particular, the influence of the stirrer geometry and of process parameters on the grinding performance is investigated. Therefore, coupled non-resolved CFD-DEM simulations on the macro scale were conducted with the focus on the stressing energy distribution within stirred media mills. The energy spectra are used as a measure for comminution, since a direct simulation of the product particles would require an unrealizable computing effort. The grinding media was considered as spheres. Two stirrer geometries, with and without holes, were compared.

The main information obtained from the macro scale CFD-DEM simulation is the contact frequency of grinding media, the contact energy distribution and the applied power to the different levels of energy during grinding media collisions. The distribution of contact frequency in dependency of the respective collision energies gives an indication at what rate product particles are stressed.
Micromechanical study of the elastic stiffness in isotropic frictional granular solids

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Keywords elastic moduli, fluctuation theory, inter-particle friction, isotropic assemblies

Abstract Granular materials are available in nature with large quantities and are mostly as part of raw or final products in industries. A ubiquitous type of the granular assemblies is soils, which are studied in various engineering disciplines such as Geology, Mining, and Geotechnics. Numerous field studies and lab-scale experiments have been conducted to characterize soils under various loading conditions. These studies lead to a better understanding of complexities in macro-scale response of soils. However, it is now well understood that grain scale properties are controlling the bulk-scale behavior of the granular material. Therefore, it is essential to study and determine the micromechanical mechanisms that govern various phenomena that are challenging in geotechnical engineering. Discrete Element Modelling, treats material as group of discrete particles, thus enhances the achievement of this goal.

DEM simulations are very slow when large-scale phenomena and industrial applications of granular materials are taken into account. Even with the most advanced computational techniques of today, it is not possible to simulate realistic numbers of particles with complex geometries. Thus, continuum models are more desirable where a granular medium is assumed as a continuum and principles of continuum mechanics are applied to obtain macroscopic field variables. However, besides an advantage of continuum approach, many features of granular materials at microscopic scale has to be neglected, such as restructuring, geometric non-linearity due to discreteness, explicit control over particle properties. The mechanical behaviour of the materials is presented as a constitutive relation, then the constitutive model has to be defined based on the relation between stress and strain extracted from continuum models.

In this study, assemblies of polydisperse, linearly elastic frictional spheres are isotropically prepared using DEM. In a second stage, several static, relaxed configurations at various volume fractions above jamming are generated and tested. We investigate the effects of inter-particle contact properties on the elastic bulk and shear modulus by applying isotropic and deviatoric perturbations. The amplitude of the applied perturbations has to be small enough to avoid particle rearrangement and to get the elastic response, whereas large amplitudes develop plasticity in the sample due to contact and structure rearrangements between particles. We compare the data from DEM simulations with predictions from well-established micromechanical models, namely the Effective Medium Theory (EMT) and the Fluctuation Theory (FT). Both theories do not account for the effect of different preparation history (different inter-particle friction coefficients) on the elastic moduli. The fluctuation theory is in agreement with numerical data, almost perfect for the bulk modulus and close for the shear modulus, at least in the intermediate compression regime, but does not capture the anomalous behavior where the theory overpredicts.
318: Soft-sphere models for normal collisions of spherical particles in viscous fluids

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Keywords
soft-sphere model, normal collision, contact force, lubrication force

Abstract

Even with decades of study, it is still challenging to accurately predict the motions of discrete phases (particles, bubbles, and liquid drops) in multiphase flows due to several numerical issues. One of the challenging issues is accurate and efficient modelling for the collision of particles in viscous fluids, in the framework of CFD-DEM methodology. To deal with this problem, relevant models have to consider two important forces: particle contact force and lubrication force. The former model accounts for dry collisions, i.e., collisions in vacuum or in a fluid of negligible resistance. However, the latter takes into account the influence of fluid inertia and fluid viscosity on the collision process. Even though many studies have been already done, better understanding of collision phenomena and model improvement are still needed.

In this study, the characteristics of representative soft-sphere contact models and lubrication force models are investigated to develop a better model with virtually no parameters requiring adjustment and tuning. For this purpose, previous models and our new model are validated against the experimental data of particle-to-wall collision in air and wall-bouncing particle in liquids, respectively for contact model and lubrication model. The performance of the models is evaluated and compared in terms of restitution coefficient and collision duration. The contact models considered here for viscoelastic collisions include linear spring model and Hertz-based nonlinear models. The considered lubrication models are based on the Stokes number that includes the added mass effect. Detailed results and discussion will be given in the final presentation.

This research was supported by the National Research Foundation of Korea (NRF) under grant number 2017M2A8A4018482 and 2015R1D1A1A0105 9675.
Introduction to open-source development minisymposium

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Keywords open-source, DEM, DPM

Abstract 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 different developers of open-source codes and also be a one-stop-shop for potential new users.

The session is split into three parts (two normal sessions) and a drop-in session (Wednesday afternoon in rooms 2G-2N) where developers of different codes can get together and potential users can try any of the codes represented.

There is a maximum of two presentations per code. The first talk should give a general overview of the code including main features, upcoming features, license, contribution rules, etc. The second talk can be more technical and explain the details of certain key features.

This presentation will open the session and give an overview of both open-source development and the codes represented in the session. It will cover topics including how to manage releases, what license to use etc; comparing and contrasting the ways the codes represented do this.

The following codes are represented in the session:

- MercuryDPM and oomph-lib
- Yade
- Liggghts and CFDEM
- ESyS-Particle and GenGeo
- GranOO
- MESA-PD and waLBerla
- GrainLearning
- dp3D
The granular Blasius problem: boundary layers in granular flow

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Keywords
granular flow, rheology, granular rheology, DPM, boundary layers, free surface

Abstract
The rheology of dense granular flows is important to understand for many industrial and geophysical applications, but it remains poorly understood. While depth-averaged models (based on the shallow water approach of hydraulics) are commonly used to study granular flows, such models provide no information about the internal velocity profile of a flow, but instead assume that this profile is self-similar along the current. This assumption is invalid when the basal roughness conditions vary along the flow, distorting the flow profile near the base. We demonstrate, through DPM simulations, that a step increase in basal roughness imposing a no-slip condition produces velocity profiles that are qualitatively similar to the classical Blasius boundary layer problem studied by Prandtl. We show that a variant on the commonly-used rheological model of Jop et al. (2006) quantitatively predicts the correct velocity profile.
Macroscopic single contact properties of cohesive silanised glass beads

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Keywords
compression test, contact model, particle contact, cohesion, surface modification, 11-cyanoundecyltrichlorosilane

Abstract
The flowing behaviour of granular materials is determined by the contacts between individual solid grains. This contact behaviour is highly dependent on the particle properties; in particular we are interested in the effect of cohesion. This research experimentally investigates the contact of a single pair of macroscopic cohesive glass beads. The surface of the glass beads were functionalised via chemical silanization, attaching a silane group to the particle surface by a covalent bond. Ideally, a monolayer around the bead should be observed that increases the dry adhesivity of the surface. However, findings indicate the silanization procedure to be moisture sensitive, especial when a trichlorosilane is used. Agglomerates of polymerized silanes are unequally divided over the surfaces, as shown on AFM measurements and SEM images. To measure the adhesion, a CMS NanoTribometer was used. With this device the contact force and displacement of the particle can be measured, from which the adhesivity can be extracted. The force-displacement curves of unmodified glass were compared with the Hertzian contact model and showed a good agreement. For polymerised particles, a broad variance is noticed in the results, which we attribute to agglomeration of polymerised silanes on the surface. Some of the force-displacement curves show highly irregular behaviour. A possible explanation is that the contact occurred on a high polymerized spot, resulting in a force-displacement graph which is comparable to the model “stiff particle with soft contacts” of Tomas [1] for highly adhesive surfaces. In most cases, however, a contact behaviour of the functionalised particles was observed in which the loading stiffness is slightly smaller than the Hertzian behaviour of untreated glass. When unloading, the displacement increases while the normal force decreases to a point where there is still a positive normal force, thereafter, to return almost back to the previous loading curve, in such a way that the adhesion is not depended on the applied load, see figure. The point where this phenomenon occurs is dependent on the load and the location of contact but does not seem to depend on velocity. The gradual change observed during cyclic loading and unloading is attributed to wear of the silane layer. An explanation why the displacement increases when the normal forces decreases, is still a matter to be researched.

329: Simulating particle agglomerates in MercuryDPM to study the dual-porosity in clay

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Keywords
cluster generator, plasticity depth, dual-porosity, clay, oedometer test, hydraulic conductivity

Abstract

Particle agglomerates are found in many industrial and scientific applications; for instance, particle breakage, milling, granulation, tableting, or reproducing the microstructure and study the dual-porosity of clay. The challenge addressed here is how to accurately model such agglomerates in discrete particle simulations.

For this purpose, we have implemented a new feature in MercuryDPM, an open-source software for discrete particle simulations. It is called the Cluster Generator: with a few line commands it is possible for a user to create particle agglomerates, i.e. a particle-composed entity, and insert them into a larger process simulation. The particles are formed by compressing spherical elementary particles. Due to the compression, the particle contacts deform plastically, causing increased cohesion between the elementary particles, thus forming a cluster. Varying the elasto-plastic interaction parameters, the properties of the cluster can be shaped: increasing the values of loading stiffness and plasticity depth, for example, causes an increment in solid fraction and hardness of the agglomerate.

Taking advantage of the different possibilities given by the code, an oedometric test for clay is simulated, distinguishing in particular two cases: the first one considers distilled water as interstitial fluid, the second one considers salt water as interstitial fluid. Salt water makes clay grains shrink, increasing pore diameters and also hydraulic conductivity: this particular behaviour is simulated by varying the elasto-plastic parameters, and in particular increasing the plasticity depth in order to have a decrease in micro porosity, whilst an increase in macro porosity. The ability of the code to reproduce these changes in dual-porosity and the differences with experimental data will then be investigated.
Notes