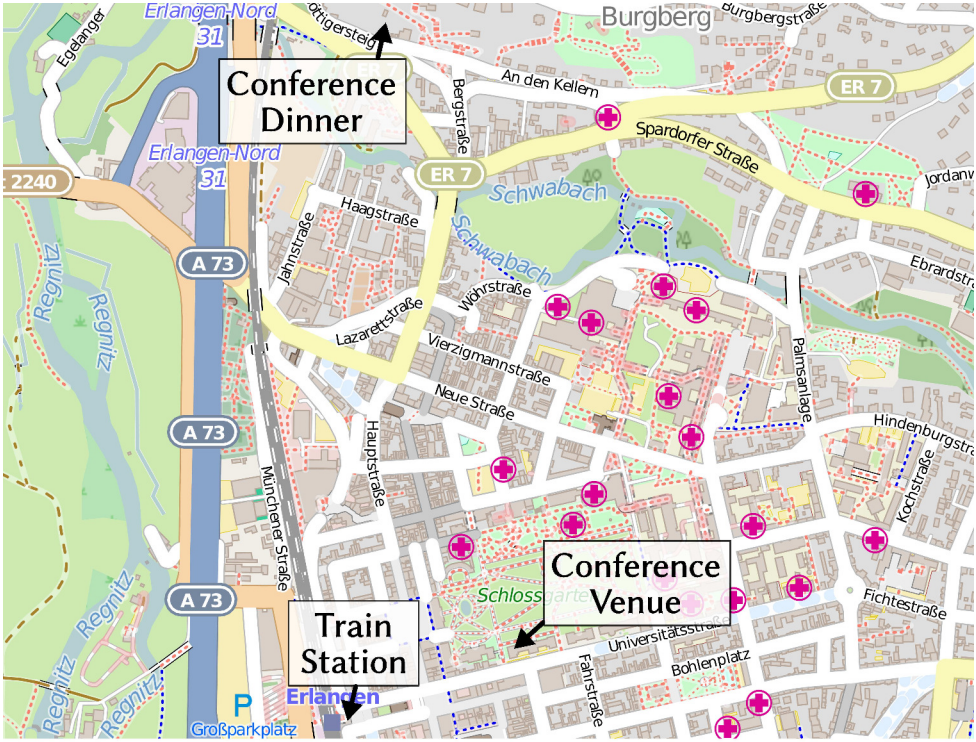
Particle Simulations

particle-simulations.de

September 21 – 24, 2015
Erlangen, Germany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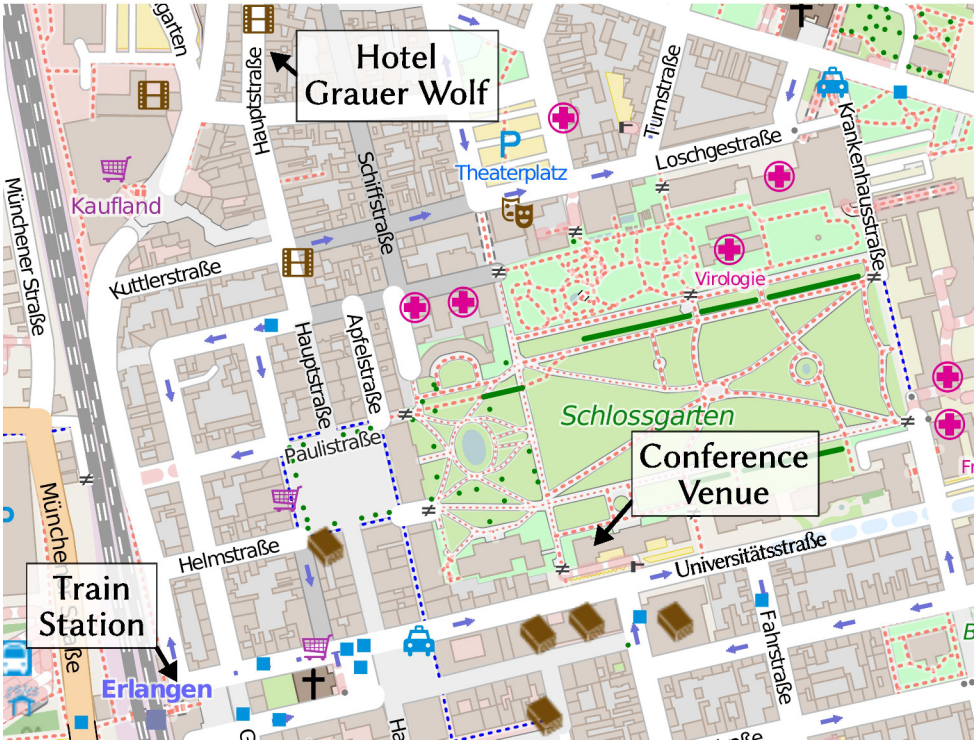
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Particle Simulations

Erlangen, 21-24 September 2015

Dear Colleagues,

A very warm welcome to Erlangen and thank you for joining 'Particle Simulations'!

Contemporary particle based simulations involve methods where physical particles are modelled as well as methods where quasi-particles are either used to discretize continuum problems or to represent abstract quantities. Reaching from atomistic systems to systems of macroscopic particles to hydrodynamics, particle simulations cover a wide range of applications on all scales. They enable promising strategies for the simulation of multiphase flows, phase transitions and the treatment of complicated shaped or free boundaries.

It is the aim of this workshop to bring together scientists working in the field of particle simulations from all fields of research. We welcome our interdisciplinary group of participants and wish to discuss the subject from different perspectives such that applications benefit from fundamental insights, and applications may stimulate fundamental research.

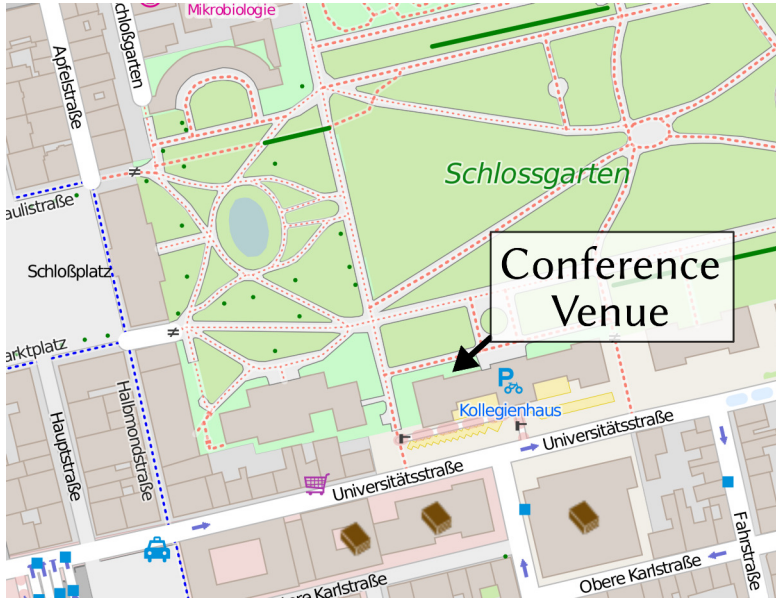
The conference is made possible by generous support of the DFG funding initiative 'Engeneering of Advanced Materials' Cluster of Excellence, the Institute for Multiscale Simulation of Particulate Systems, the Zentralinstitut für Scientific Computing and the SFB 814 - Additive Manufacturing.

We hope you'll enjoy the conference and your time in Franconia!

Thorsten Pöschel, *Patric Müller*, *Christian Scholz*

Conference venue

The conference venue is the Kollegienhaus, close to the University Villa, the central Market square and the Schlossgarten in Erlangen. It is within a few minutes walking distance of cafés and restaurants, the central train station and all conference hotels. The street address is **Universitätsstraße 15, 91054 Erlangen**.



Conference venue in the Kollegienhaus. GPS: 49.597190N, 11.006624E

For a bigger map of the conference venue location see the inside of the front cover. The conference will take place in two lecture halls, while oral session will take place in KH 01.011 and the poster session, as well as coffee breaks will be held in KH 00.014.

Session Format and Talk Style

Keynote lectures: 35+10 : 35 minutes talk time plus 10 minutes discussion

Contributed talks: 15+5 : 15 minutes talk time plus 5 minutes discussion

Poster Session : Monday 6 - 9pm

Posters are displayed for the duration of the conference in room KH 0.044. There is a dedicated **Poster Session** on **Monday from 6 to 9pm**.

Please take note of the **'People's Choice Best Poster Award'**. Your conference booklet contains a ballot slip for your choice of the three best posters. Please hand in your **completed ballot slip by Wednesday's afternoon coffee break**. The winners will be announced at close of the last session on Wednesday afternoon.

Wireless Internet Access : SSID 'FAU-Guest'

In the conference map is a detailed instruction how to use the wireless network: Connect your mobile device to the network with SSID 'FAU-Guest'. Once connected open a webpage and you should see an input field for your credentials. **Your personalized username and password is provided in your registration bag.** Or you may simply try to connect via **eduroam**.

Social events

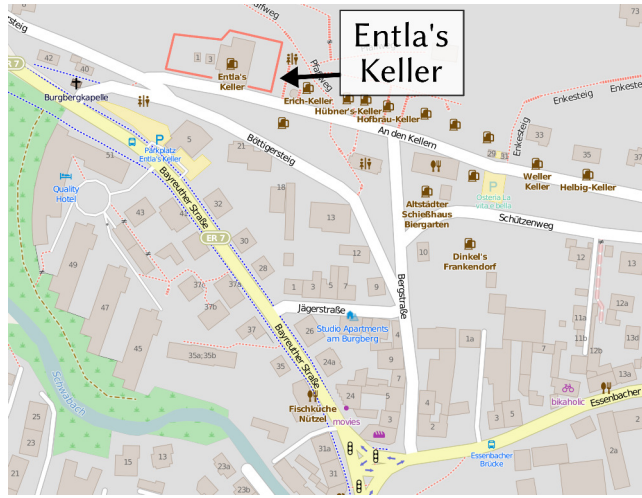
Welcome drinks – Sunday 6 - 9pm

Please join us for casual welcome drinks to kick off the conference on Sunday 20^{th} September from 6 to 9pm at the conference venue, the Kollegienhaus Room KH 0.014.

Conference dinner – Tuesday 6pm at 'Entlas Keller'

You are cordially invited to a true-blue Franconian experience for our conference dinner, to be held at the picturesque beergarden 'Entlas Keller' at the site of Erlangen's famous May-beer festival 'The Berg'. The street address is **'An den Kellern 5-7'** which is a short 20 minutes stroll from the conference venue. This beergarden (or in case of bad weather their cellar bar) is situated on the flanks of a hill with deep horizontal cellars that were excavated for the purpose of keeping beer cool during the brewing processes of the 17th and 18th century. The conference dinner will kick-off with a tour of the cellars starting at 6pm sharp, followed by the dinner starting at 6:30pm. While the Franconian cuisine is hearty and often meaty, vegetarian options will be available. Partners, wives & husbands all very welcome; please let us know in advance.

Please bring warm clothes as we are likely to enjoy **al-fresco outdoor dining**.



Conference dinner venue. GPS: 49.608083N, 11.003415

Monday

08:50 – 09:00	**Welcome**	
09:00 – 09:45	**Holger Stark**	*Colloids in microfluidic flow: From dense colloidal suspensions to inertial microfluidics*
09:45 – 10:05	**Michael Engel**	*Shape control and compartmentalization in active colloidal cells*
10:05 – 10:25	**Maarten Wouters**	*Particle-based pseudo-potential model for mesoscopic multi-component and multi-phase flow*
coffee break		
11:00 – 11:45	**Dietrich Wolf**	*Shear rate diffusion during transients in simple shear*
11:45 – 12:05	**Matthias Sabel**	*Influence of the α-shape algorithm on the structural integrity in the particle finite element method for solids*
12:05 – 12:25	**Matthias Markl**	*Powder bed generation for mesoscopic additive manufacturing simulations*
lunch break		
14:30 – 15:15	**Dan Negrut**	*On the use of computer modeling to characterize the dynamics of large particulate systems*
15:15 – 15:35	**Sebastian Borrmann**	*Computational fluid dynamics (CFD) simulations with particles by means of the smoothed particle hydrodynamics method - impact on a free liquid surface*
15:35 – 15:55	**Baofang Song**	*Instability of SPH in poiseuille flow*
coffee break		
16:30 – 17:15	**Stefan Heinrich**	*Multiscale simulation of the fluidized bed spray granulation process*
18:00-21:00	**poster session & finger food**	

Keynote **Holger Stark** **09:00 – 09:45**

Colloids in microfluidic flow: From dense colloidal suspensions to inertial microfluidics

Holger Stark*

Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany

Colloidal flow through microfluidic channels is of technological importance and finds applications in industrial processes as well as biomedical applications. However, it also challenges a theoretical understanding of the underlying physics. In this talk I review some of our work on colloidal microfluidic flow using computer simulations.

At low Reynolds number dense colloidal suspensions in Poiseuille flow exhibit shear-induced migration towards regions of low viscous shear in the channel center. Bidisperse suspensions even partially demix and large colloids preferentially accumulate in the center [1]. Our simulations of hard spheres under pressure-driven flow are based on the mesoscale method of multi-particle collision dynamics and reproduce this behavior [2]. The segregation profiles are reproduced by a phenomenological model, we developed by extending an existing theory for monodisperse suspensions [3]. At densities near to random close packing, monodisperse suspensions exhibit regular oscillations [4]. We present first results towards this observation using an elastic two-particle interactions together with Coulomb friction at contact.

In the second part we focus on inertial microfluidics at intermediate Reynolds numbers. Due to inertial forces particles accumulate at fixed locations between channel center and bounding walls. This Segré-Silberberg effect can be described in terms of an inertial lift force acting on the particles. In biomedical applications it is used for particle sorting and separation [5]. Using lattice-Boltzmann simulations we demonstrate how the lift-force profile depends on the channel geometry and how its shape can be controlled by axial forces [6] as well as particle rotation [7]. Additional control force profiles along the channel designed by optimal control theory allow to steer the particle towards almost any position in the channel cross section [8]. All these methods provide a refined approach to particle steering and more efficient particle separation.

[1] D. Semwogerere, J. F. Morris, and E. R. Weeks, J. Fluid Mech. **581**, 437 (2007).

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[2] P. Kanehl and H. Stark, J. Chem. Phys. **142**, 214901 (2015).
[3] R. J. Phillips, R. C. Armstrong, R. A. Brown, A. L. Graham, and J. R. Abbott, Phys. Fluids **4**, 30 (1992).
[4] L. Isa, R. Besseling, A. N. Morozov, and W. C. Poon, Phys. Rev. Lett. **102**, 058302 (2009).
[5] H. Amini, W. Lee, and D. Di Carlo, Lab Chip **14**, 2739 (2014).
[6] C. Prohm and H. Stark, Lab Chip **14**, 2115 (2014).
[7] C. Prohm, N. Zöller, and H. Stark, Eur. Phys. J. E **37**, 36 (2014).
[8] C. Prohm, F. Tröltzsch, and H. Stark, Eur. Phys. J. E **36**, 118 (2013).

Michael Engel **09:45 – 10:05**

Shape control and compartmentalization in active colloidal cells

Michael Engel,[1,2,*] Matthew Spellings,[1,2] Daphne Klotsa,[1,2] Syeda Sabrina,[3] Aaron M. Drews,[3,4] Nguyen H. P. Nguyen,[5] Kyle J. M. Bishop,[3] and Sharon C. Glotzer[1,2,6]

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[2] *Biointerfaces Institute, University of Michigan, Ann Arbor, MI, USA*

[3] *Department of Chemical Engineering, Pennsylvania State University, University Park, PA 16802, USA*

[4] *Department of NanoEngineering, University of California, San Diego, La Jolla, CA 92093, USA*

[5] *Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI 48109, USA*

[6] *Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI, USA*

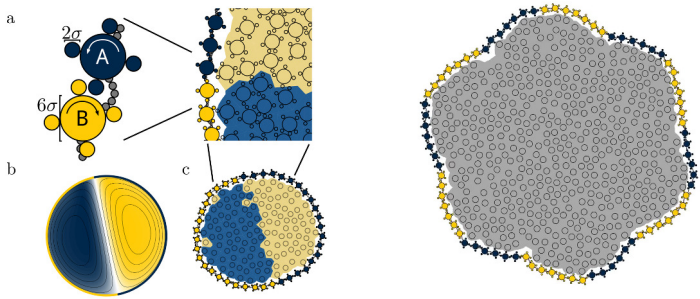

Figure 1: Left: Schematic of the confined spinner models. (a) Our active colloidal cell is made up of spinners driven counterclockwise (blue) or clockwise (yellow). Boundary spinners are connected by a flexible bead-spring chain (gray). We compare the behavior of a continuum model (b) to a microscopic model (c). The compartmentalization of interior spinners is visualized by coloring the Voronoi tessellation in the microscopic model. Right: Shape-shifting passive interior, active boundary cell. Particle flows imposed by the active boundary of a colloidal cell with a passive interior cause the shape of the cell to change in accordance with the symmetry of the boundary.

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Small autonomous machines like biological cells or soft robots can convert energy input into control of function and form. It is desired that this behavior emerges spontaneously and can be easily switched over time. For this purpose we introduce an active matter system that is loosely inspired by biology and which we term an active colloidal cell [1]. The active colloidal cell consists of a boundary and a fluid interior, both of which are built from identical rotating spinners whose activity creates convective flows [2]. Similarly to biological cell motility, which is driven by cytoskeletal components spread throughout the entire volume of the cell, active colloidal cells are characterized by highly distributed energy conversion.

We demonstrate that we can control the shape of the active colloidal cell and drive compartmentalization by varying the details of the boundary (hard vs. flexible) and the character of the spinners (passive vs. active). We report buckling of the boundary controlled by the pattern of boundary activity, as well as formation of core-shell and inverted Janus phase-separated configurations within the active cell interior. As the cell size is increased, the inverted Janus configuration spontaneously breaks its mirror symmetry. The result is a bubble-crescent configuration, which alternates between two degenerate states over time and exhibits collective migration of the fluid along the boundary. Our results are obtained using microscopic, non-momentum-conserving Langevin dynamics simulations and verified via a phase-field continuum model coupled to a Navier-Stokes equation.

[1] M. Spellings, M. Engel, D. Klotsa, S. Sabrina, A.M. Drews, N.H.P. Nguyen, K.J.M. Bishop, S.C. Glotzer, Proc. Natl. Acad. Sci., in press (2015).
[2] N.H.P. Nguyen, D. Klotsa, M. Engel, S.C. Glotzer, Phys. Rev. Lett. **112**, 075701 (2014).

Maarten Wouters 10:05 – 10:25

Particle-based pseudo-potential model for mesoscopic multi-component and multi-phase flow

M.P.J. Wouters[1,*] and J.D.R. Harting[1,2]

[1] *Department of Applied Physics, Eindhoven University of Technology, De Rondom 70, 5612 AP Eindhoven, The Netherlands*

[2] *Physics of Fluids group, Faculty of Science and Technology, University of Twente, Drienerlolaan 5, 7522 NB Enschede*

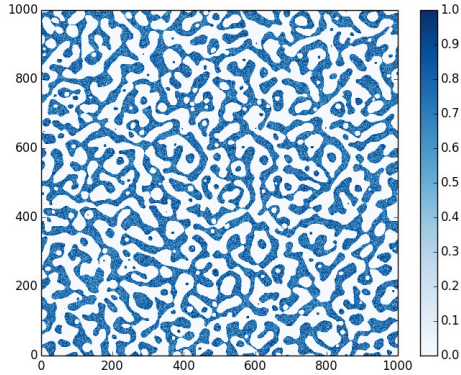

Figure 1: Snapshot of density of one component (other componenent not shown) of a binary mixture with repulsive interactions between the two components during spinodal decomposition.

There are many different models to simulate fluid flow. However, there is a gap between the macroscopic models, which lose all detail on the small scales, and the microscopic models, which are computationally too expensive to simulate large scale phenomena. To bridge this gap different mesoscopic models were developed like the lattice Boltzmann method (LBM) and multi-particle collision dynamics (MPCD) methods [2]. In the LBM the pseudo-potential model for multi-phase and multi-component flow of Shan and Chen [1] is widely used and tested. The interaction forces are modelled on a lattice, which makes the model not directly compatible with the continuous nature of particle-based methods. This work describes how the pseudo-potential method can be used in combination with the particle-based methods of the MPCD class. The method is then applied

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and tested with one member of the MPCD-class, stochastic rotation dynamics, although it can be applied to the other methods in a similar fashion.

[1] Malevanets, A., Kapral, R., *Mesoscopic model for solvent dynamics*, J. Chem. Phys. **110**, 8605, 1999
[2] Malevanets, A., Kapral, R., *Mesoscopic model for solvent dynamics*, J. Chem. Phys. **112**, 7260, 2000
[3] Shan, X., Chen, H., *Lattice Boltzmann model for simulationg flows with multiple phases and components*, Phys. Rev. E**47**, 1815-1819, 1993.

Keynote **Dietrich Wolf** **11:00 – 11:45**

Shear rate diffusion during transients in simple shear

Alexander Ries, Lothar Brendel, and Dietrich E. Wolf*

Faculty of Physics and Center for Nano-Integration Duisburg-Essen (CENIDE), University of Duisburg-Essen (UDE), D-47057 Duisburg, Germany

The transients of a sheared granular medium, before it reaches steady state flow, provide a crucial test for continuum equations of motion. We investigated these transients by Contact Dynamics Simulations for a simple shear geometry with smooth frictional walls. The particles were non-cohesive, frictional hard spheres. The initial configuration was jammed (no shear rate in the bulk). Provided the wall velocity is high enough to induce bulk flow, the shear rate spreads diffusively [1] starting from narrow shear bands at both walls, until it becomes constant throughout the bulk. Not surprisingly, the final bulk shear rate increases monotonously with the wall velocity. However, unexpectedly, the relaxation time increases linearly with the final bulk shear rate, and the local constitutive laws for solid fraction and macroscopic friction coefficient already hold during this transient. These results will be discussed in view of the theory of Kamrin and Koval [2].

[1] Z. Shojaaee, J. N. Roux, F. Chevoir, D. E. Wolf, *Shear Flow of dense granular materials near smooth walls. I. Shear localization and constitutive laws in the boundary region*, Phys. Rev. E **86**, 011301, 2012.

[2] K. Kamrin and G. Koval, *Nonlocal Constitutive Relation for Steady Granular Flow*, Phys. Rev. Lett. **108**, 178301, 2012

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Matthias Sabel **11:45 – 12:05**

Influence of the α-shape algorithm on the structural integrity in the particle finite element method for solids

Matthias Sabel,* Christian Sator, and Ralf Müller

Institute for Applied Mechanics, University of Kaiserslautern

To model the separation of material, the standard FEM can be extended by a method that periodicly detects the boundary, and remeshes the domain. A feasible realization is the particle finite element method (PFEM) that meshes particle clusters, which carry all physical quantities of the body, by finite elements. The boundary detection of the set of particles is done by the α-shape method and while the periodic redetection during simulations is the biggest asset of the PFEM, there are several possible interpretations of the boundary and the solution depends on the choice of the crucial parameter α. When applied to two dimensional problems, an intersecting circle is defined for every pairwise combination of particles with a radius scaled by α. If no further particles are located in this circle, the pair of particles forms a boundary segment. Based on this working principle we can identify two conditions wether a particle pair forms a boundary segment. The distance between two neighboring particles must not be larger than the diameter of the circle and the distance from the center of the circle to each remaining particle in the set has to be larger than the radius. If the body is subjected to a deformation, the distance between particles changes by the deformation, and with the first condition α can be identified as a maximum stretch between particles. Since α can be interpreted as a maximum stretch ratio for boundary segments, it triggers the separation of material and therefore influences the strength. Illustrative examples demonstrate to which extend this theoretical considerations apply to complex boundary value problems encountered for example in machining situations.

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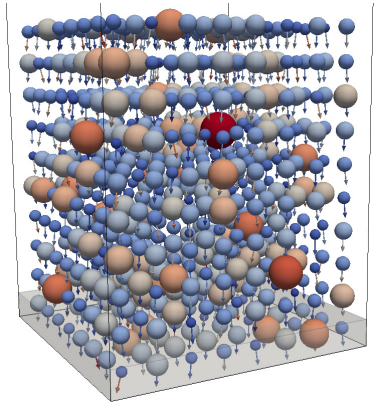
Matthias Markl 12:05 – 12:25

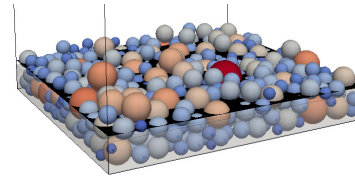
Powder bed generation for mesoscopic additive manufacturing simulations

Matthias Markl* and Carolin Körner

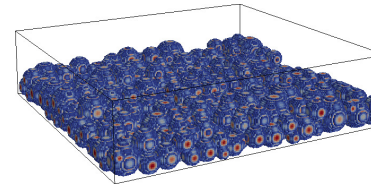
Chair of Metals Science and Technology,
Friedrich-Alexander Universität Erlangen-Nürnberg, Martensstr. 5, 91058 Erlangen



(a) Powder particles initialized.



(b) Powder bed simulated.



(c) Suitable particles mapped.

Figure 1: (a) The powder bed generation starts with the powder particle initialization, where the color indicates the diameters according to the size distribution. The initial particle velocity is indicated by the arrows with a color distribution of the magnitude. At the bottom of the domain (black wireframe), the desired volume of the first layer is colored light gray. (b) If the average particle velocity falls under a certain velocity threshold, the simulation is stopped and particles exceeding the layer (black plane) are not mapped. (c) Final state of the powder bed after mapping into a Cartesian grid. The cell fill level is visualized by the color distribution.

Powder-bed-based additive manufacturing (AM) technologies gain more and more attention, especially in aerospace and medical engineering. However, today's low build rates cause total build times from hours to days for individual parts and issues arise in providing a constant production environment during one build process. Therefore, improved process strategies to fasten the process and achieve

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reproducible part properties need to be developed. Because the physical phenomena occurring during AM processes are not fully understood and inaccurately predictable until today, process strategies are gained by an intensive and expensive trial-and-error principle. Thus, the numerical simulation is a perfect tool to support the development of new process strategies and to circumvent the practical disadvantages.

Numerical investigations on the selective electron beam melting (SEBM) process highlight possible process strategy improvements. The simulations base on a mesoscopic numerical method operating on a Cartesian grid, which resolves each single powder particle to consider the statistical behavior of the powder bed. In this work, we present the underlying universal approach to generate the corresponding powder bed, which can be combined with any numerical method of a powder-bed-based AM process operating on the mesoscale.

The approach bases on the discrete element (DE) method and is implemented using the physics engine (*pe*) [2]. Each particle is approximated as a perfect sphere with a diameter according to a certain particle size distribution. The powder bed generation algorithm (cf. FIG. 1) covers the approximation of previous powder layers, the initialization of new particles, the free fall simulation onto the previous layer and the mapping to the mesoscopic simulation approach. In this work, the particles are converted into a Cartesian grid, which is used for a lattice Boltzmann method simulating the SEBM process.

Acknowledgments: This work was supported by the European Union Seventh Framework Program – Research for SME's with grant agreement number 286695. We also thank Regina Ammer and Tobias Preclik, Chair for System Simulation, Friedrich-Alexander Universität Erlangen-Nürnberg, for their support.

[1] M. Markl, R. Ammer, U. Rüde, and C. Körner. Int J Adv Manuf Tech **78.1-4** 239-247 (2015).
[2] T. Preclik and U. Rüde. Comput Part Mech **2.2** 173-196 (2015).

Keynote	Dan Negrut	14:30 – 15:15

On the use of computer modeling to characterize the dynamics of large particulate systems

Dan Negrut*

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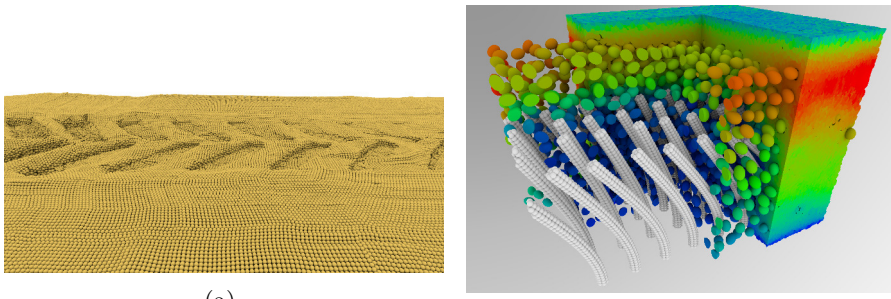

(a) (b)

Figure 1: Two examples of particulate systems simulated in Chrono. (a) Lugged tire imprint on a granular terrain made up of 10 million bodies that interact through contact, friction, and cohesion. (b) Snapshot of a fluid-solid interaction dynamics problem. The simulation relies on Navier-Stokes and SPH to capture the fluid dynamics, nonlinear finite element to capture the compliant elements, and the Newton-Euler equations of motion to represent the dynamics of the rigid ellipsoids.

This contributions concentrates on two issues: (a) a comparison of two alternatives for modeling frictional contact when simulating the dynamics of large particulate systems; and (b) a brief presentation of a software engine called Chrono that can be used to investigate the dynamics of particulate systems. For (a), a penalty approach, which is called DEM-P and relies on the local deformation at the point of contact, will be compared with a complementarity approach called DEM-C and which relies on a differential variational inclusion to model frictional contact phenomena. The two methods will be contrasted in terms of computational effort required to produce an acceptable solution, ease of implementation,

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and expressiveness; i.e., prowess in relation to capturing physics of interest. In relation to (b) the presentation will outline the structure of Chrono and showcase its use in a broad spectrum of problems — from additive manufacturing to ground vehicle mobility on deformable soils. Chrono, which is an open source software released under a permissive BSD3 license, can be used for analyzing the dynamics of particulate systems that can be dry or assume the form of suspensions. For the latter, Chrono handles the fluid-solid interaction problem by solving the Navier-Stokes equations using a smoothed particle hydrodynamics (SPH) methodology.

Sebastian Borrmann 15:15 – 15:35

Computational fluid dynamics (CFD) simulations with particles by means of the smoothed particle hydrodynamics method - impact on a free liquid surface

Sebastian Borrmann,* Anton Gladkyy, and Rüdiger Schwarze

Institute of Mechanics and Fluid Dynamics,
Technical University Bergakademie Freiberg, Germany

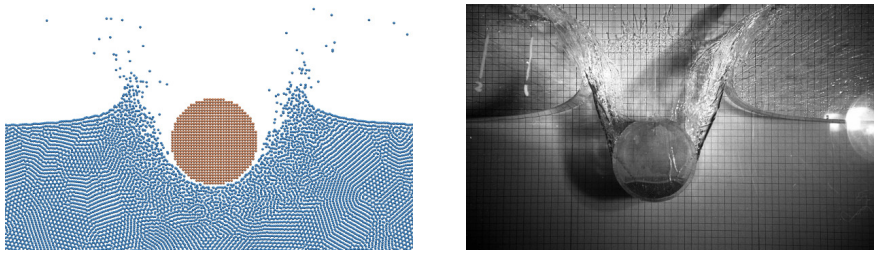

Figure 1: The left figure shows an impact simulation of a 2D rigid cylinder (orange) on a free liquid surface (blue) with SPH. The ligament formation is discernible in this stage of the simulation. The right figure shows a picture recording of circular cylinder impact experiments[2].

The interactions between rigid materials, like powder particles, granulate materials or even largar solid objects with fluids are of large interest in several fields of application. Ocean engineering or metallurcical processing are examples where such interactions appear. In the latter case the production of metal matrix composites (MMC) is on area of interest, where powder particles collide with fluid droplets for consolidation. For the numerical simulation of particle-fluid interactions it is sensible to use particle based methods for both phases. The fluid phase as well as the fluid-solid-interaction can be calculated using the Smoothed Particle Hydrodynamics (SPH) method which is completely based on particles as discrete sampling points.
In this paper, numerical simulations of a rigid body impact on a free liquid surface are perfomed with the open-source DEM framework YADE. A weekly compressible SPH (WCSPH) method has been implemented into the software using all the existing allgorithms. The interaction between particles is created

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with the Lucy kernel function[1]. The rigid bodies and walls are modelled with fixed SPH particles.
The simulations are in good agreement with experimental tests[2], both qualitatively and quantitatively. In Fig. 1 an examplary qualitative comparison is shown. The formation of liquid jets on both sides of the impact position are predicted, as well as the formation of small droplets. However, the latter effect is not physically accurate in the simulations, since surface tension is not modelled in the current WCSPH implementation.

In summary it is shown, that the WCSPH implementation in YADE provides reasonable results for the rigid body impact, quantitative results and predictions of main flow and interaction effects. For further refinement of the implementation the surface tension will be taken into account and more case-fitting kernel functions will be tested in the future.

Acknowledgments: This work was supported by the German Research Foundation (Deutsche Forschungsgemeinschaft, DFG) under Grant no. DFG SFB 799/C1 and is gratefully acknowledged.

[1] L. B. Lucy, The Astronomical Journal **82**, pp. 1013-1024 (1977)
[2] M. Greenhow and W. Lin, Nonlinear Free Surface Effects: Experiments and Theory (Report no. **83-19**.), Cambridge, MA: Department of Ocean Engineering, Massachusetts Institute of Technology (1983)

Baofang Song **15:35 – 15:55**

Instability of SPH in poiseuille flow

Baofang Song,[1,*] Arman Pazouki,[2] and Thorsten Pöschel[1]

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Smoothed particle hydrodynamics (SPH) has been widely applied to flows with free surfaces, multi-phase flow, and systems with complex boundary geometry because of its meshless and Lagrangian nature [1]. However, it is known that SPH suffers from transverse instability and fails to produce the correct solutions when applied to simple wall-bounded shear flows such as Poiseuille and Couette flows at moderate and high Reynolds number, $\mathrm{Re} \gtrsim 1$ [2–4]. The appearance of this instability casts the application of SPH to practical situations into doubt, where the Reynolds number is frequently large.

We investigated the stability of SPH for the example of plane Poiseuille flow with respect to the method parameters: smoothing length h and the ratio of smoothing length to particle spacing $h/\Delta x$. Besides, the influence of a density re-initialization technique [5, 6] on the stability of SPH is also investigated. We found that SPH can give correct results at very low Reynolds numbers ($\mathrm{Re} \ll 1$) while fails at $\mathrm{Re} \gtrsim 1$, in agreement with the finding in [2–4]. Reducing the smoothing length alone does not suffice to improve the stability of the simulation, while increasing $h/\Delta x$ for a given h significantly improves the results. Our results showed that $h/\Delta x \gtrsim 1.5$ is needed to obtain reliable results, and the density re-initialization is also necessary for simulations at high Reynolds numbers. We showed that the above arguments are relevant for other wall-shear flows too, such as pipe flow. We achieved stable and reliable results in both plane Poiseuille and pipe flows at $\mathrm{Re} = 120$, which is much higher than the usual test cases in the literature [2, 7, 8].

We identified the wall boundary approximation (see, e.g., [8]) as the main source of velocity disturbances at the wall, which eventually causes particle disorder and noisy flow fields in Poiseuille flow simulations. We further identified the sensitivity of the accuracy of SPH on particle disorder as the source of the so-called transverse instability. Our study suggested that this sensitivity can be reduced by including more neighbour particles in a particle's support, i.e., larger $h/\Delta x$. The density re-initialization also helps to reduce non-physical pressure

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and velocity fluctuations and improves the results.

Acknowledgments: We thank the German Research Foundation (DFG) for funding through the Cluster of Excellence “Engineering of Advanced Materials".

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Keynote **Stefan Heinrich** **16:30 – 17:15**

Multiscale simulation of the fluidized bed spray granulation process

Stefan Heinrich* and Maksym Dosta

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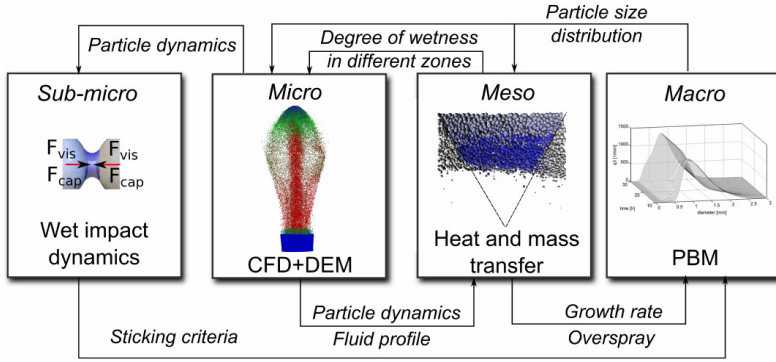

Figure 1: General representation of the multiscale architecture.

Modern production processes in chemical, pharmaceutical and biological industries are characterized by complex process structures, which consist of different apparatuses and process steps. Modeling the entire process requires simulating all units altogether, while taking into account interconnections between them. Nevertheless, in the area of solids processing, there is nowadays an unfilled gap from the side of computer support of process modeling in allowing effective optimization and prediction of the behavior of the whole plant. In this contribution the application of a multiscale simulation strategy for modeling of the fluidized bed spray granulation process will be presented. The kinetics of the granulation process is governed on the microscale. While the global process time is in the order of hours, the underlying micro-mechanisms have much smaller time constants in the order of seconds. This is a challenging situation in the field of process modelling, as a detailed simulation cannot cover the entire process time, while on the other hand a macroscopic model cannot take into account material micro-properties. On the macroscale, a Population Balance Model (PBM)

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is used for calculation of the time-dependent particle size distribution (PSD) and for description of the corresponding particle growth in the apparatus. Afterwards, according to the results obtained from the macroscale and other process parameters, such as apparatus geometry, gas flow rate, etc., the models on the micro- and mesoscales are generated. On the microscale the fluidized bed process is simulated using a Discrete Element Method (DEM) coupled with Computational Fluid Dynamics (CFD). The particle trajectories and the fluid profile obtained by this modeling are transferred to the mesoscale, where the simulations of particle wetting and transport processes, like drying, are performed. The model on the sub-micro scale is developed to calculate the collision of single particles considering the influence of the liquid layers on their surfaces by solving of the force balance, which includes the capillary and viscous forces. As a result from this model the particle sticking criterion is estimated.

Tuesday

9:00 – 9:45	**Hans Kuipers**	*Recent advances in the direct numerical simulation (DNS) of mass, momentum and heat transfer in multiphase chemical reactors*
9:45 – 10:05	**Severin Strobl**	*Event-driven particle tracking in complex geometries*
10:05 – 10:25	**Raphael Münster**	*Particulate flow simulations with complex geometries using the finite element-fictitious boundary method*
coffee break		
11:00 – 11:45	**Fathollah Varnik**	*Rheology, diffusion and correlations in sheared athermal suspensions of deformable particles*
11:45 – 12:05	**Sebastian Kapfer**	*Event-chain Monte Carlo applied to large-scale particle systems and 2D melting*
12:05 – 12:25	**Eric Opsomer**	*Segregation in a driven bi-disperse granular gas*
lunch break		
14:30 – 15:15	**Charles Radeke**	*Challenges and Applications in the Chemical and Pharmaceutical Industry*
15:15 – 15:35	**Anton Gladkyy**	*Bulk flow DEM simulation on a pelletizing table*
15:35 – 15:55	**Xiaodong Jia**	*DigiPac/DigiDEM and applications*
coffee break		
16:30 – 17:15	**Frédéric Dubois**	*Non Smooth Contact Dynamics, a relevant framework to model divided media*
18:00-22:00	**Conference dinner**	

Keynote	Hans Kuipers	09:00 – 09:45

Recent advances in the direct numerical simulation (DNS) of mass, momentum and heat transfer in multiphase chemical reactors

J.A.M. Kuipers*

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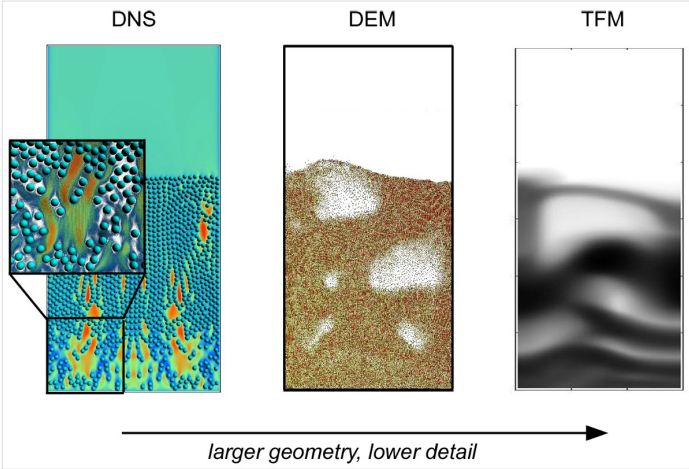

Dense gas-particle flows involving momentum, mass and heat transfer are frequently encountered in industrial processes involving granulation, coating and polymerization. In dense gas-particle flows both (effective) fluid-particle and (dissipative) particle-particle interactions need to be accounted for because (the competition between) these phenomena to a large extent govern the prevailing flow phenomena, i.e. the formation and evolution of heterogeneous structures. These structures have significant impact on the quality of the gas-solid contact and as a direct consequence thereof strongly affect the performance of the process. Additional complexities arise due to enhanced dissipation due to wet particle-particle collisions.

Due to the inherent complexity of these multiphase flows the authors have adopted a multi-scale modeling approach in which both fluid-particle and particle-

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particle interactions can be properly accounted. The idea is essentially that fundamental models, taking into account the relevant details of fluid-particle interaction (DNS) and particle-particle interaction (DEM), are used to develop closure laws to feed continuum models (TFM) which can be used to compute the flow structures on a much larger (industrial) scale. In this presentation recent advances in the DNS of dense gas-particle flows will be highlighted with emphasis on coupled mass, momentum and heat transfer. In addition, areas which need substantial further attention will be discussed.

Severin Strobl **09:45 – 10:05**

Event-driven particle tracking in complex geometries

Severin Strobl* and Thorsten Pöschel

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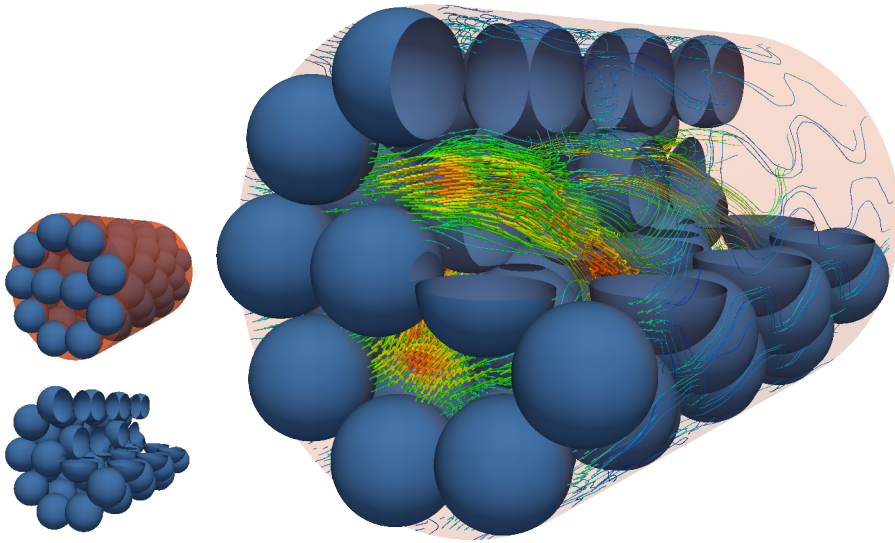

Figure 1: Simulation of a fluid flow through a fixed packing of spheres bounded by a cylinder using a particle-based method. The geometry of the cylinder is modeled using a unstructured hexahedral grid whereas the CSG approach is employed for the sphere packing.

Lately, particle-based simulation frameworks have started to support computational domains described by unstructured grids routinely used in Eulerian methods. Driven by this, the tracking or tracing of the trajectories of particles as they move through unstructured meshes has become a well-established technique (e.g. [2, 3]). We show that a wide range of the algorithms used for particle tracking already presented in the literature are a special case of Event-Driven

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Particle Dynamics (EDPD). This allows improvements regarding the numerical stability of EDPD recently developed in [3] to be applied to the problem of particle tracking. A number of problems present in many tracking algorithms are avoided or resolved in a numerically stable manner, as is shown by the investigation of some critical cases.

Building on this Constructive Solid Geometry (CSG) is introduced as an efficient scheme to define complex geometries for particle-based methods. In CSG composite objects are defined by applying the Boolean operators *union*, *intersection*, and *difference* as well as geometric transformations to simple (solid) geometric objects termed primitives. The benefit of using CSG over complex meshes resulting from the mathematical definition of the surface is highlighted using the example of porous media. We present the results of simulations of fluid flows through various complex domains, ranging from packing of spheres to foam-like structures, modeled after open-cell foams.

Acknowledgments: The authors would like to acknowledge the funding of the Deutsche Forschungsgemeinschaft (DFG) through the Cluster of Excellence Engineering of Advanced Materials.

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Raphael Münster **10:05 – 10:25**

Particulate flow simulations with complex geometries using the finite element-fictitious boundary method

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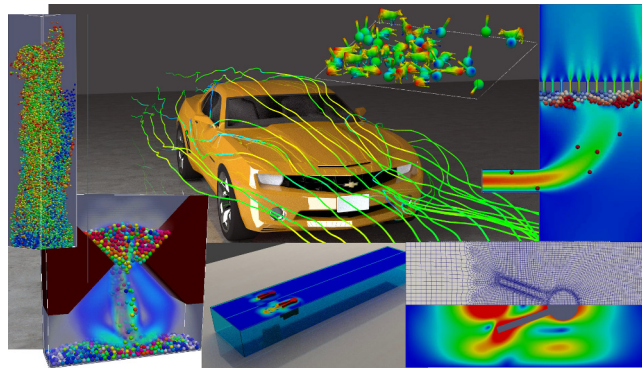

Figure 1: The FEATFLOW package: A CFD-framework that is able to handle a large variety of flow configurations including particulate flows with complex geometries.

The numerical simulation of particulate flows is an interdisciplinary scientific topic. Scientists from mathematics, physics, engineering and computer science are involved in particulate flow research, theoretical modelling, software creation and verification with standard benchmarks and real experiments. As diverse as are the participants in the topic are the approaches to develop a solver framework for particulate flow simulations. The main approaches include the Lattice-Boltzmann method, the Finite Volume Method, the Discrete Element Method and the Finite Element Method. This contribution chooses the FEM-based software FEATFLOW as its solver for the incompressible Navier-Stokes equations. Particulate flow codes require a way of including particles or general rigid bodies in their simulations, in the FEATFLOW solver this is realized by the Fictitious-Boundary method (FBM). The FBM is a technique for the direct numerical simulation of particulate flows, meaning that the particles are fully resolved by the computational mesh. Directly resolving the particles with the

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computational mesh requires a highly refined mesh in order to yield accurate results. Solving the fluid equations on these kinds of highly refined meshes is challenging task that needs efficient algorithms throughout the whole simulation pipeline to compute results in an acceptable time. The FEATFLOW solver package includes for this task a domain decomposition approach and solves the subproblems on the individual domains with a parallel Newton-Multigrid scheme. The FEATFLOW particulate flow solver includes several acceleration techniques for the computation of the hydrodynamic forces that are needed to compute the two-way interaction of the particles and the fluid. In our particulate flow solver we have included several modules of the simulation that run on GPU hardware to benefit from their massively parallel architecture. To improve the numerical efficiency and accuracy we have added mesh r-adaptation techniques to improve the mesh resolution locally around the particles and to accurately resolve their shape by the mesh. Furthermore, we implemented in our software packages methods that are able to handle complex arbitrarily shaped geometries and handle collisions between those complex objects, these kind of particulate flow simulations we call complex geometry particulate flows.

Acknowledgments: The research in this work was funded by the Deutsche Forschungsgemeinschaft (DFG) as part of the project DFG (NV): TU 102/43-1. We would like to thank the DFG for their support and interest.

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Keynote	Fathollah Varnik	11:00 – 11:45

Rheology, diffusion and correlations in sheared athermal suspensions of deformable particles

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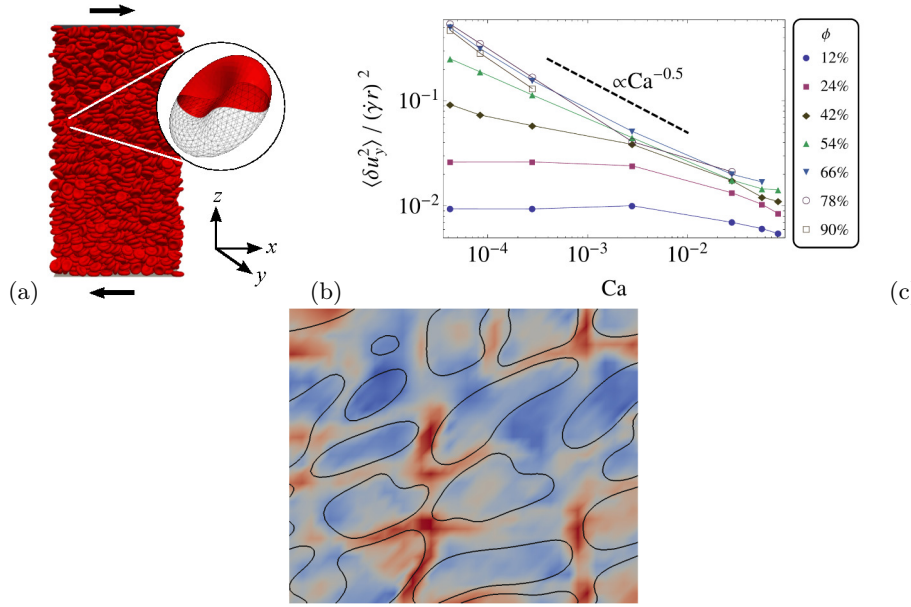

Figure 1: (a) Sketch of the simulation setup. Walls move with constant velocity in $\pm x$-direction to impose shear. (b) Particle velocity fluctuations versus capillary number for various volume fractions. (c) A snapshot of stress distribution within a plane. Particle contours are shown as solid lines. The highest solvent stress (red) occurs in the narrow regions between particles. Using this fact, one can rationalize the scaling behavior seen in panel (b) in terms of viscosity. The images (adapted) are from [10].

Athermal suspensions of deformable particles occur manifold in nature and technology. A statistical description of these far from equilibrium systems is, however,

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a challenging task. Central to the understanding of these systems is the fact that they can 'jam', i.e., they acquire a solid-like character above a certain critical particle concentration, yet often remain amorphous in structure [1, 2]. The jamming transition is typically associated with the emergence of correlated particle motion and dynamical heterogeneities [3]. While this issue has been the subject of numerous studies in the case of Brownian systems and athermal granular suspensions, concentrated soft particle suspensions consisting of vesicles or capsules have received less attention with regard to dynamic correlations and shear induced fluctuations [4, 5].

In view of the above mentioned theoretical interest and their relevance for biological and technical applications, we study here via computer simulations fluctuations of particle displacements and stresses in a sheared athermal suspension of deformable particles, covering volume fractions from the dilute up to the deeply jammed regime. Particles have the shape of red blood cells and interact only via hydrodynamics and short-range repulsive forces [6, 7]. Fluctuations are found to be generally anisotropic and the flow organizes into temporary shear bands at large particle concentrations. Fluctuation variances and relaxation times scale canonically with shear rate in the Newtonian regime and show a characteristic power-law scaling in the jammed state [8].

The statistical properties of the displacement and stress fluctuations are intimately related to the rheology and can be rationalized in terms of a dissipation balance that relates the variance of the instantaneous velocity fluctuations to the power injected by the shearing [9, 10]. Within this simple picture, the dependence of shear rate $\dot{\gamma}$ of the velocity fluctuations $\langle u^2 \rangle^{1/2}$, diffusivity D and velocity relaxation rate $1/\tau_v$ are all predicted to scale as $\propto \dot{\gamma}\eta^{0.5}$, with η being the effective viscosity. Simulation results are consistent with this theoretical expectation [10].

Acknowledgments: We thank Claus Heussinger and Timm Krüger for useful discussions. Financial support by the DFG (project VA205/5-2) is also acknowledged.

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Sebastian Kapfer **11:45 – 12:05**

Event-chain Monte Carlo applied to large-scale particle systems and 2D melting

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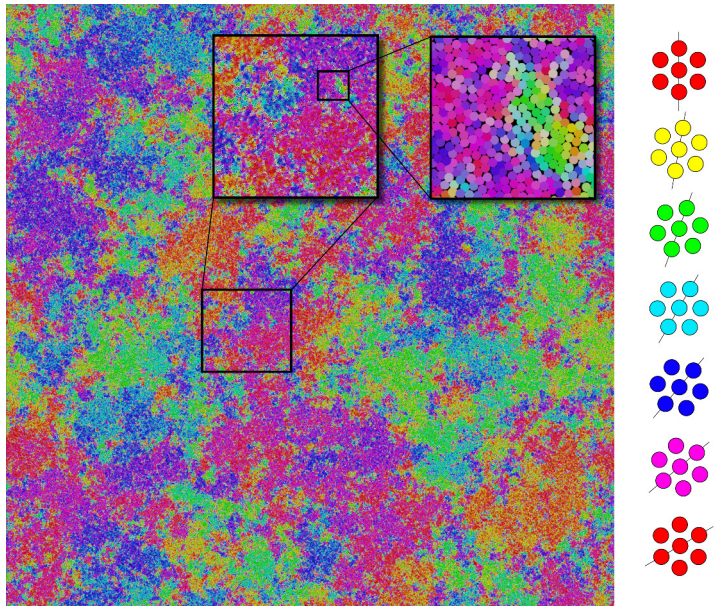

Figure 1: Two-dimensional fluid of particles interacting with an $1/r^n$ potential. The color code corresponds to the local orientational order parameter Ψ_6 (see key on the right-hand side). Note the substantial correlation length, with typical clusters of homogeneous orientation of ~ 100 particle diameters.

The melting transition of two-dimensional solids has been the subject of continued research for more than fifty years, with the prevalent scenarios being the KTHNY theory of defect unbinding and a conventional first-order liquid/solid transition. For hard disks, the KTHNY scenario has recently been essentially

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confirmed, even though the liquid-hexatic step is of first order [1]. A key problem in these simulations is the large number of particles required to faithfully reproduce physical correlation lengths (see figure).

We present a new rejection-free global-balance Monte Carlo algorithm [2] which can be applied to particle systems interacting with arbitrary pairwise potentials in the canonical ensemble. Using this new algorithm, we show that the hard disk result transfers to soft interactions with inverse power-law or Yukawa potentials [3]. The order of the liquid-hexatic step can be tuned from first-order to continuous by softening the potential. We show that there is always a hexatic phase separating the liquid and solid phases, and identify two regimes of the hexatic with vastly different correlation lengths. These results rationalize a plethora of simulation results obtained in the past, and could be verified in charged-colloid experiments.

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Eric Opsomer **12:05 – 12:25**

Segregation in a driven bi-disperse granular gas

E. Opsomer,* F. Ludewig, and N. Vandewalle

University of Liege

Driven granular gases present rich dynamical behaviors. Due to inelastic collisions, particles may form dense and slow regions in the system. These clusters emerge naturally during cooling phenomena but can also be observed while the system is continuously excited [1, 2]. Among other parameters, the formation of such aggregates is related to the size of its constitutive particles [3] which motivated us to study the dynamics of a bi-disperse granular gas. Given the need of microgravity conditions, our study was realized via MD simulations. However, an experimental counterpart is planned for the VIP-GRAN [4] instrument on the International Space Station in 2018.

In order to prepare the future series of experiments, we simulated a granular gas made of small and large bronze spheres within the geometry of the VIP-GRAN cell. The differences in size and in mass of the particles modify the collision dynamics and the energy propagation in the system. This has a dramatic impact on the cluster's formation. Moreover, under certain conditions, segregation can be observed. In that case, the system is composed by a cluster of mainly large grains surrounded by a gas of small grains. Thanks to our numerical simulations, we established a phase diagram recovering all encountered dynamical regimes and a developed a theoretical model predicting the clustering of a bi-disperse granular [5].

Acknowledgments: This work has been supported by Prodex (Belspo, Brussels) and the European Space Agency program TT VIP- GRAN/SpaceGrains. We also thank the Shape-SPS project (Wallonia) for supporting the development of our numerical model.

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Keynote	Charles Radeke	14:30 – 15:15

Challenges and Applications in the Chemical and Pharmaceutical Industry

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Research Center Pharmaceutical Engineering GmbH, Graz, Österreich

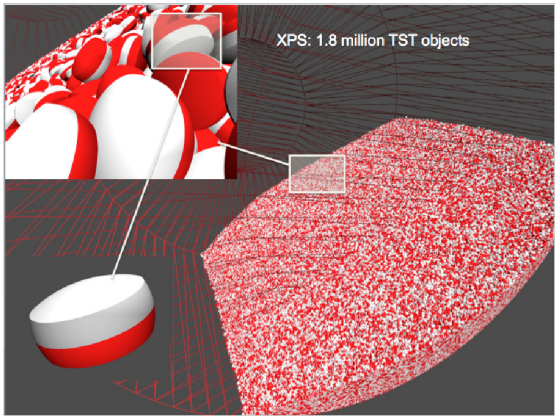

Figure 1: True Shape Tablets (TST). Modeling of bi-convex tablets using real tablet in a drum coater geometry at industrial scale. (XPS: eXtended Particle System; a simulation software)

DEM is typically used to solve physical aspects in granular flows, such as mixing, segregation effects or mechanical loading on particles. In the academic community simple geometric boundaries and particles in vacuum are sufficient, in order to model a particle system in most cases. Compared with the requirements in the industry, an extension of DEM is important. Processes in pharmaceutical and chemical engineering applications often incorporate airflow, liquid spray and heat transfer in complex shaped equipment.

Moreover, tiny slits or gaps are dominating many unit operations, where particles have to pass through, which prevents the use of larger particles. Many processes are under investigation for the so called up-scaling. Here, large-scale simulations can help to prevent simplifications in terms of particle numbers, getting realistic models for comparisons at different scales.

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Anton Gladkyy **15:15 – 15:35**

Bulk flow DEM simulation on a pelletizing table

Anton Gladkyy,[1,*] Holger Lieberwirth,[2] and Ruediger Schwarze[1]

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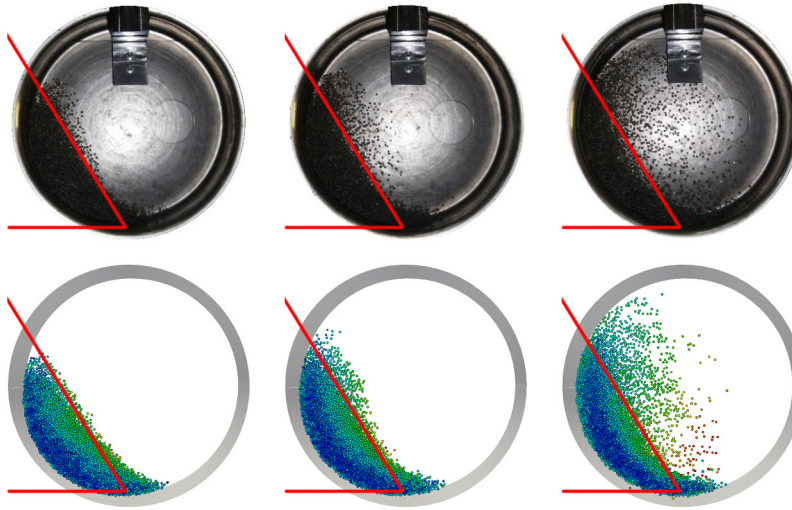

Figure 1: Qualitative comparison of experimental and simulation data: $\beta = 40°$ and $\psi = 0.5$, 0.7 and 1.0

This talk will be mostly focused on the bulk material behavior on the pelletizing disc, which is used for agglomeration of small particles into larger ball-shaped forms. A weakly wetted model bulk material (glass beads) is agitated on a small-scale pelletizing disc with different rotational speeds. Corresponding DEM simulations are performed with the open-source DEM software YADE. The linear viscoelastic model in combination with the capillary bridge models of Willett or Rabinovich/Lambert are used to simulate the wet contacts between two glass beads [1].

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Experimental observations and snapshots from the DEM simulations of the bulk material behavior are in good qualitative agreement in the entire operating regime of the pelletizing disc. On the base of particle and contact information provided by DEM, different rotational movement regimes of the particles are identified and correlated to the rotational speed of the pelletizing disc. Especially the critical rotational speed, at which the bulk material circulates along the edges of the disc, differs significantly from values which are expected from an estimation based on a well-known heuristic equation.

Further quantities, such as the total number of contacts, coordination number, length of the rotational body and others are used for a more detailed evaluation of the internal dynamics of the bulk material on the pelletizing disc. In summary, it is shown that DEM is able to predict main parameters of bulk flow on the pelletizing disc. This information can be used for the optimizing the operating modes of the technical equipment in the industry.

Acknowledgments: The authors express their thanks to the Deutsche Forschungsgemeinschaft, which supported this work within the DFG/STW project SCHW 1168/6-1

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Xiaodong Jia **15:35 – 15:55**

DigiPac/DigiDEM and applications

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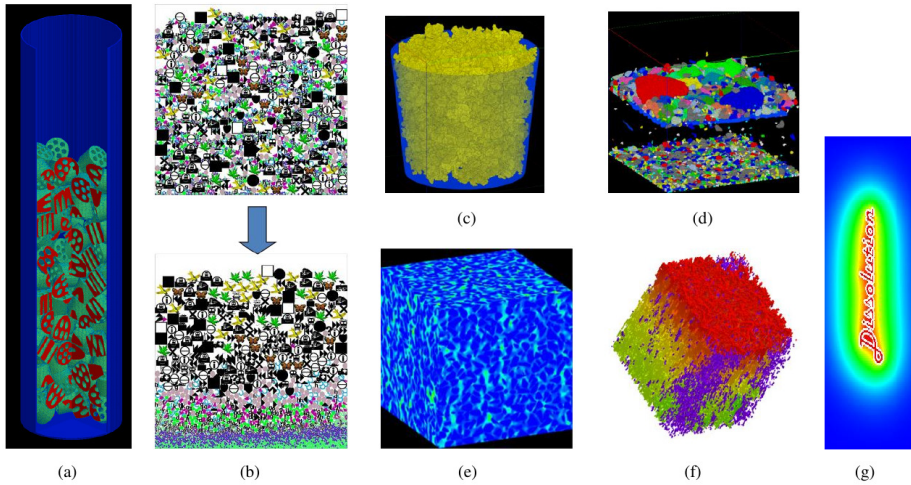

Figure 1: (a) Packed column. (b) Segregation. (c) Popcorns. (d) Vibrating screen. (e) LBM simulated flow in porous medium. (f) Temperature distribution through a porous material. (g) Concentration distribution of dissolving solids.

Here we describe a group of particle packing simulation models, all based on a digital representation of the particles, the container and the packing space. They are implemented as software programs called DigiPac and DigiDEM. DigiPac is a collection of four packing models: random-walks (DigiRWP) [1], collision-guided (DigiCGP) [2], random-placement (DigiRPP) and optimal stacking (DigiOSP) [3] packing models respectively. For complex and arbitrary shapes, the use of voxelated objects has the advantages that complex shapes can be handled by simple and efficient computer code for collision and overlap detections and for

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packing property calculations, and the computing time does not increase with shape complexity. Applications of DigiPac models will be illustrated with examples such as packed columns [2] (Fig.1a), segregation [4] (Fig.1b) and porpcorns [5] (Fig.1c). DigiPac packing models are typical Monte Carlo simulations where probabilities are used to control particle movements. It is good at providing packing predictions for trend analysis and is generally much faster than DigiDEM. DigiDEM, on the other hand, tends to provides more quantitatively accurate results and can simulate dynamic processes as well as the packing structures, but at a high computational cost. This is because DigiDEM is a lattice implementation of the Discerete Element Method where which way and how much each particle moves are determined by calculating physical interaction forces and solving Newton's equations of motion in very small time steps. Potential applications of DigiDEM are illustrated through sieving by vibrating screen (Fig.1d) and stirring of packed bed, etc. In addition to packing, the software suite also contains modules to calculate some properties of common interest, such as permeability (using Lattice Boltzmann Method) [6] (Fig.1e), effective thermal or electrical conductivity (using Finite Difference Method) (Fig.1f), dissolution [7] (Fig.1g) or chemical reaction in porous media, sintering, and light scattering etc. In all these calculations, the aim is to link particle characteristics to microstructure of packing then to their properties. Difference between the different models will be explained and illustrated. Challenges, bottlenecks and possible solutions will be described, and finally future development will be highlighted [8-9].

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Keynote **Frédéric Dubois** **16:30 – 17:15**

Non Smooth Contact Dynamics, a relevant framework to model divided media

Frédéric Dubois*

LMGC - CNRS - Université de Montpellier

Deriving a relevant numerical approach to model divided media raises many issues especially due to the fact that it mixes various time and space scales. In the present work we focus on a fully implicit approach, the Non Smooth Contact Dynamics method (NSCD), initiated by J.J. Moreau [1] and M. Jean [2], and implemented in the LMGC90 software [3]. The interaction laws, such as frictional contact, are written as multi mappings relating contact unknowns (impulse and relative velocity) without any additional regularization. In the frame of Convex Analysis proposed by J.J. Moreau a modified dynamics formulation is used, which is able to deal with non-smoothness; it is integrated with a first order scheme. Impulses account for all events supposed to occur during a time step: external loads, single or numerous impacts between pairs or agglomerates of contacting bodies. An iterative contact solver is necessary in order to exhibit the values of the unknowns. The method allows reasonably large time steps.

Progressively the models simulated by non-smooth DEM become more complex:

- Interactions between contacting bodies may be physically quite complicated. Primary phenomena depicted by an interaction law are impenetrability of materials and dry friction. Other phenomena like rolling friction due to roughness, cohesive behavior, local plastic deformation, viscous friction or wear should be also taken into account.
- Particle geometries become more complex introducing clusters of basic shapes, polyhedron or possibly non-convex shapes.
- Multiple physics couplings: chemistry, electrical or thermal effects.
- Multi-phase mixture: gas-grain or fluid-grain media.
- Complex grains behavior: elasticity, plasticity, fracture, etc.
- Phase changing: solid/solids (fracture, sintering) or solid/fluid, etc.

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As it will be detailed in this talk the Non Smooth Contact Dynamics method (NSCD) is a powerful modeling framework to derive numerical strategies. NSCD has been successfully used to study the behavior of granular materials and structures. It has been also used to study the behavior of masonry under seismic load, rock mass stability, fracture, multiple physics coupling, etc.

Acknowledgments: LMGC90 platform is a free collaborative software developed by several researchers, engineers and students: Michel Jean, Mathieu Renouf, Gilles Saussine, Alexandre Martin, Rémy Mozul, Dominique Ambard, Cyril Bordreuil, FrÃ©dÃ©ric Pérales, etc.

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Wednesday

9:00 – 9:45	**Stefan Sokołowski**	*Models and results of theoretical calculations and computer simulations for systems involving patchy particles in bulk and in confined phases*
9:45 – 10:05	**Nikola Topic**	*Packings of complex shaped particles in cylinders*
10:05 – 10:25	**Stanislav Parez**	*Unsteady granular flows down a slope*

coffee break

11:00 – 11:45	**Ken Kamrin**	*Continuum modeling and continuum simulation tools for granular materials through their various regimes of behavior*
11:45 – 12:05	**Hadi Mehrabian**	*Soft particles at a fluid interface*
12:05 – 12:25	**Davod Alizadehrad**	*Simulation of cellular blood flow using particle methods*

lunch break

14:30 – 15:15	**Jens Harting**	*Self-assembly and deposition of colloidal suspensions*
15:15 – 15:35	**Simon Bogner**	*Lattice Boltzmann method-based study of the drag correlation of dilute and moderately dense fluid-particle systems*
15:35 – 15:55	**Georg Hammerl**	*A particle based parallel four-way coupled Euler–Lagrange approach for simulating cavitation*

coffee break

16:30 – 17:15	**Holger Steeb**	*SPH modelling of pore-scale events in particulate media*

17:15 poster award presentation

Keynote	Stefan Sokołowski	09:00 – 09:45

Models and results of theoretical calculations and computer simulations for systems involving patchy particles in bulk and in confined phases

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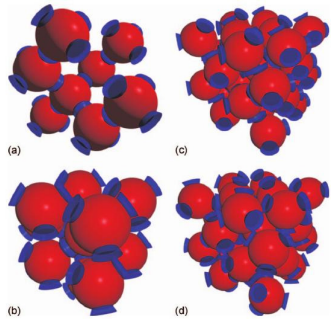

Figure 1: Possible crystal structures: (a) Diamond Crystal, one unit cell, composed of eight atoms; (b) BCC, eight atoms in the vertices of a cube around the central one; (c) FCC $2 \times 2 \times 2$ unit cells, composed of four atoms each; Orientationally disordered FCC, FCC-d, $2 \times 2 \times 2$ primitive cells, composed of four atoms each (from [2]).

The aim of this talk is to present some selected models of patchy particles. We concentrate on the cases of the so-called site-site models and focus on the description of their phase behavior[1–5]. Two basic models are considered in details, namely the four-site (four-patch) model and the two-site model with a possibility of the formation of double bonds. In the first case we discuss the existence of different solid phases, see Fig. 1. In the second case – the possibility of the existence of the re-entrant transition for bulk and for confined systems. An example of such a behavior, predicted by the Density Functional Theory and the second-order Thermodynamic Perturbation Theory of Wertheim for a fluid confined in slits is displayed in Fig. 2. However, the Monte Carlo study has excluded the re-entrant behavior. We discuss the reasons for the discrepancies

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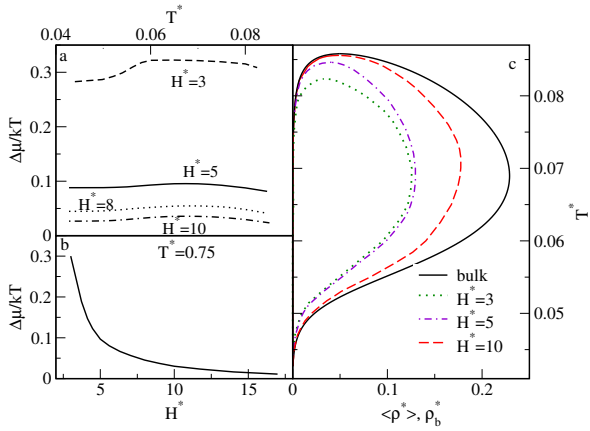

Figure 2: (a) Phase diagrams in the chemical potential-temperature plane. Pore widths are given in the figure. (b) Dependence of the chemical potential on the pore width at $T^* = 0.075$. (c) Phase diagrams in the density-temperature plane for $H^* = 3$, 5, 10 and for the bulk system. (From Ref. [4].)

between the theory and simulations. Finally we present selected results of Monte Carlo simulations of bilayers of Janus-like particles in a lattice model.

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Nikola Topic **09:45 – 10:05**

Packings of complex shaped particles in cylinders

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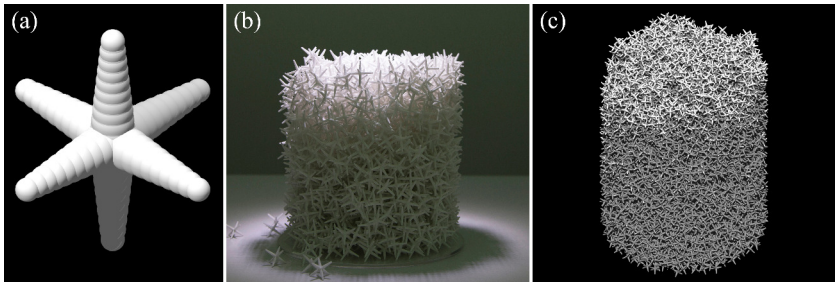

Figure 1: (a) Example of a six-armed non-convex particle. (b) Experimental packing test of complex shaped particles in a cylinder. (c) Simulation of a packing of complex shaped particles in a cylinder.

In many situations in nature and industry the macroscopic hard particles that make up the densely packed system are non-spherical, [1]. Despite their common occurrence some simple questions are still being answered e.g. the relation between the particle shape and the properties of packings. Non-convex particle shapes are especially challenging since they display effects non-existent for convex shapes, e.g. interlocking and entanglement. The influence of such effects on the properties of packings is still being characterized, [3, 4].

A model for deposition of spherical particles that produces dense packings and enables simulation of large number of particles has been developed by Visscher and Bolsterli, [5]. In this model, particles are dropped one by one onto a surface, and each particle follows the path of the steepest descent on the surface of previously deposited particles, until a particle reaches a position where it cannot descend anymore. In this position the particle is fixed and cannot be displaced by the following particles. The model can be implemented in an event-driven way. Recently, an event-driven generalization of the Visscher-Bolsterli model to

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complex shaped particles has been developed, [6, 7]. In this model the complex shape of a particle is described using the multi-sphere method. The complex shaped particle follows the path of the steepest descent of the center of mass, while rolling and falling on the surface of the sediment.

In this contribution we apply the generalized Visscher-Bolsterli model to simulate packings of non-convex 3 dimensional shapes in cylindrical containers (a simple case of a container with walls). We consider a variety of particles shapes and focus on the packing density of such sediments. Packing density is a core parameter in many industrial applications for evaluating fabrication methods versus overall fabrication costs. Reliable modelling tools thus not only accelerate but also diversify this decision making process.

Acknowledgments: We acknowledge the funding by the German Science Foundation (DFG) through the Cluster of Excellence Ëngineering of Advanced Materials".

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Stanislav Parez **10:05 – 10:25**

Unsteady granular flows down a slope

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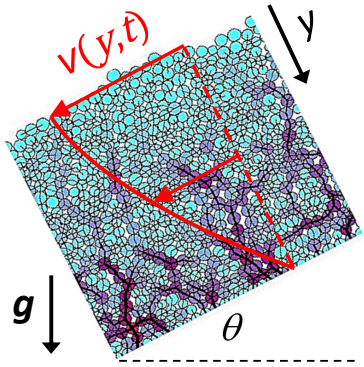

Figure 1: A snapshot from a DEM simulation of the studied system. An infinite granular layer flows down a slope inclined at an angle θ. The red line denotes an instaneous velocity profile. Colours of the grains indicate contact stress: the dark grains are most stressed.

The continuum description of flow of granular materials is still a challenge despite their importance in many geophysical and industrial applications [1]. We extend previous works [1, 2], which have explored steady flow properties, by focusing on the unsteady stage for flows accelerating/decelerating down an inclined plane. We derive an analytical solution for flow kinematics and compare it to numerical simulations using Discrete Element Method (DEM) [3], in which motion of individual grains is solved. The model shows why, when and how granular materials reach steady flow, including a prediction of transient velocity and stress profiles and transient time required to reach a steady flow.

Acknowledgments: The research leading to these results has received funding from the People Programme (Marie Curie Actions) of the European Union's

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Seventh Framework Programme FP7/2007-2013/ under REA grant agreement No. 316889.

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Keynote **Ken Kamrin** **11:00 – 11:45**

Continuum modeling and continuum simulation tools for granular materials through their various regimes of behavior

Ken Kamrin*

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The ability to model a large granular system as a continuum would offer tremendous benefits in computation time compared to discrete particle methods. However, two infamous problems arise in the pursuit of this vision: (i) the constitutive relation for granular materials is still unclear and hotly debated, and (ii) a numerical method for granular media must wear "many hats" as, in general circumstances, it must be able to capture and accurately represent the material as it crosses through its collisional, dense-flowing, and solid-like states; most simulation methods are specialized for one of these regimes (e.g. gas-dynamics solvers, fluid finite-volume solvers, finite-element solid mechanics solvers). This talk will survey in two parts the work we have been conducting to close the gap on both fronts.

First we will discuss the issue of granular constitutive modeling with an eye toward resolving the issue of cooperatively in the dense-flowing regime. For this we will discuss a *nonlocal fluidity* approach that directly accounts for the finiteness of the grain size, which is at the heart of the cooperatively phenomena that makes grains flow differently than fluids with a local rheology. This model will be shown to correctly capture shear-band widths in flowing systems like annular cells and split-bottom cells, while resolving other manifestations of cooperativity such as the secondary rheology phenomenon (i.e. "motion over there erases the yield stress over here") and the H_{stop} phenomenon of chute flows, whereby thinner layers behave as if they are stronger.

Then we will discuss our recent *trans-phase* continuum model and numerical implementation, which serves as a first step toward a simulation capability able to handle all regimes of granular flow. The numerical approach, which is based on a Material Point Method, utilizes a meshless solver, which enables the flows to gather extreme levels of deformation without loss of accuracy, while still resolving a tiny elastic part to the deformation as needed for granular statics. The technique also lets material enter a 'gas-like' phase so that granular disconnection can be simulated, which appears, for example, in the stream of a flowing

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hourglass. The utility of this method is demonstrated in its ability to capture the physics and flow fields from multiple drainage geometries, impact problems of objects colliding with beds of grains, runout in granular collapse geometries, and various problems where granular disconnection and reconsolidating happen repeatedly.

Hadi Mehrabian **11:45 – 12:05**

Soft particles at a fluid interface

Hadi Mehrabian,[1,*] Jens Harting,[2,1] and Jacco H. Snoeijer[1,2]

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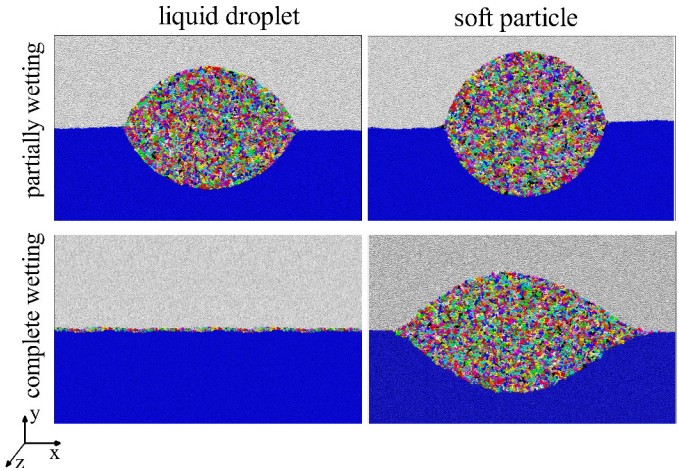

Figure 1: Snapshots from molecular dynamics simulations of soft particles at a fluid-fluid interface. They key parameters of this study are the elastic modulus and the wettability of the particles. The left panels show the outcome for a liquid drop, consisting of an non-cross-linked polymer, respectively for partially wetting (top) and complete wetting (bottom). The right panels show the corresponding particle shapes when the polymers are cross-linked and have a finite elastic modulus.

Particles added to a fluid interface can be used as a surface stabilizer in the food, oil and cosmetic industries. As an alternative to rigid particles, it is promising to consider highly deformable particles that can adapt their conformation at the interface. In this study, we compute the shapes of soft elastic particles using molecular dynamics simulations of a cross-linked polymer gel, complemented by continuum calculations based on linear elasticity [1]. Snapshots of typical

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simulations are shown in Fig. 1, where the individual polymer chains can be identified by their color. Apart from an expected dependence on the Young's modulus, governed by the dimensionless parameter $\gamma_s/(ER)$ where γ_s is the surface tension, R is the radius, and E is the Young's modulus of the particle, our key finding is that one needs to distinguish the cases where the polymer is partially or completely wetting. The left column of Fig. 1 shows simulations of the polymer *liquid*, respectively for partial wetting (upper panel) and complete wetting (lower panel). The right column shows equivalent systems, but now for *soft solid particles* that are cross-linked and thus exhibit a finite elastic modulus. We find that the partially wetting systems are very accurately described by linear elasticity, as long as the solid surface tension γ_s is large (or comparable) to that of the fluid-fluid interface. In the case of complete wetting, by contrast, the interfacial forces favor a state where the gel covers the entire interface but this is prohibited by the network elasticity. This leads to an intricate elasto-capillary balance, where the elastic response is highly nonlinear. In addition, we observe an important influence of molecular details of the cross-linking, signalling a breakdown of continuum theory.

Acknowledgments: We are grateful to Martien Cohen-Stuart, Jasper van der Gucht and Joris Sprakel for many discussions on the adsorption of microgel particles. HM acknowledges financial support from NWO through VIDI Grant No. 11304. JS acknowledges financial support from ERC (the European Research Council) Consolidator Grant No. 616918.

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Davod Alizadehrad **12:05 – 12:25**

Simulation of cellular blood flow using particle methods

Davod Alizadehrad* and Dmitry A. Fedosov

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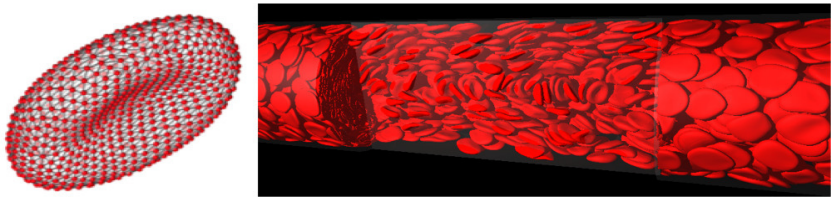

Figure 1: A red-blood-cell model (left) and an example snapshot of blood simulation, where the domain is cut in the central plane of the vessel (right).

In cellular flows through microfluidic devices and in small blood vessels, i.e. capillaries, arterioles, and venules, the motion, deformation, and hydrodynamic interactions of the cells play a dominant role in various physiological and pathological processes. These processes range from enhanced mixing and diffusion of chemical substances to adhesion of the cells in blood-related diseases such as malaria, cancer, and pathogenic infections. To understand these processes, we have developed numerical models of meso-scale cellular flow based on particle methods including moving particle semi-implicit method (MPS) and dissipative particle dynamics (DPD) [1–3].

In this presentation, we will give an overview and comparison of these simulation techniques. We will review modeling of a single cell and its suspension (blood) in microvessels (Fig. 1). The implementation of boundary conditions and the coupling of the fluid to cell membrane will be explained on the basis of these approaches. We validate these models through the analyses of apparent viscosity and formation of cell free layer, and the numerical results will be compared with experimental data [1–5]. We will then present the effect of flow parameters on red-blood-cell deformation and distribution of fluid particles at dense cellular flow. Finally, we will show our recent progress in modeling of microvascular

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bifurcations toward study of hemodynamics in complex networks of microvasculature. These results will provide a theoretical basis for further understanding of the cellular flow and mass transport in microcirculation, but also for design of microfluidic devices for blood diagnostics.

Acknowledgments: Acknowledgments: We acknowledge funding by the Alexander von Humboldt Foundation and a CPU time grant by the Jülich Supercomputing Center.

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Keynote **Jens Harting** **14:30 – 15:15**

Self-assembly and deposition of colloidal suspensions

Jens Harting,[1,2,*] Stefan Frijters,[2] Qingguang Xie,[2] Dennis Hessling,[2] Gary B. Davies,[3] and Timm Krüger[4]

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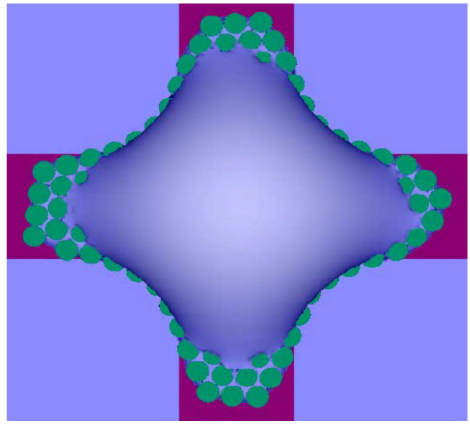

Figure 1: Snapshot showing an evaporating colloidal suspension droplet deposited on a chemically patterned substrate.

Colloidal particles suspended in fluid mixtures can interact in many ways, e.g. by electrostatic interactions, van der Waals interactions, capillary interactions, or interactions mediated by patterned substrates and external fields. In this presentation we show results from hybrid lattice Boltzmann and molecular dynamics simulations [1, 2]. We demonstrate the self-assembly of anisotropic particles at

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fluid interfaces under the influence of magnetic fields and present a new model for evaporating fluids allowing to investigate the deposition of colloidal suspensions on chemically patterned substrates (see Fig. 1) [3–6]. These examples are relevant for applications such as the self-assembly of new soft materials, conventional inkjet printing or printing of organic electronics.

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Simon Bogner **15:15 – 15:35**

Lattice Boltzmann method-based study of the drag correlation of dilute and moderately dense fluid-particle systems

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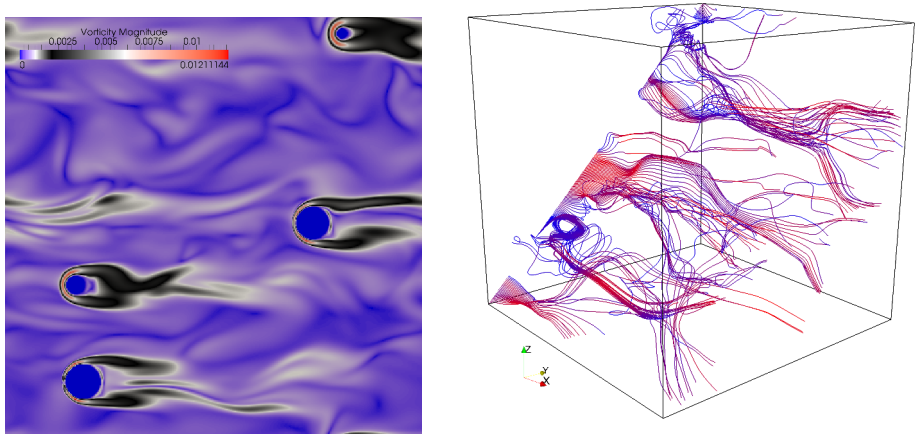

Figure 1: Left: Visualization of unsteady flow (Re=300, color indicates vorticity) through particle bed of solid volume fraction 1 %. Right: Streamline visualization of flow in particle bed of solid volume fraction 35%.

With the advent of high-speed computers, gas-solid systems have become accessible to direct numerical simulation. Particle-resolved computations help to improve understanding of the phase interaction as it appears for instance in fluidized bed reactors.

In this talk a numerical study of the drag on monodisperse, spherical particles is presented. We apply a lattice Boltzmann method based on a two relaxation time collision operator to obtain reliable predictions of the average per-particle drag force [1]. From these predictions a closure relation $F(Re_p, \varphi)$ of the drag

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force dependency on the bed density φ and the particle Reynolds number Re_p is derived. We have included bed densities φ ranging from 0.01 to 0.35 and Reynolds numbers Re_p up to 300. At low solid volume fraction, the obtained correlation is close to the widely-used Wen & Yu – correlation.

We also compare our results to previous numerical studies: Recently, there has been reported a discrepancy between results obtained using different numerical methods, namely the comprehensive lattice Boltzmann study of [2] and the predictions based on an immersed boundary - pseudo-spectral Navier-Stokes approach [3]. The present study excludes significant finite resolution effects, which have been suspected to cause the reported deviations, but does not coincide exactly with either of the previous studies. This indicates the need for yet more accurate simulation methods in the future.

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Georg Hammerl **15:35 – 15:55**

A particle based parallel four-way coupled Euler–Lagrange approach for simulating cavitation

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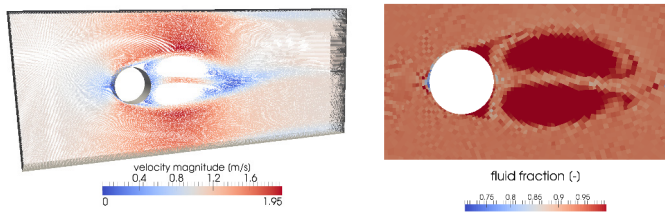

Figure 1: Bubble velocity (left) and close-up of fluid fraction in mid-plane (right).

A particle framework is developed to simulate bubbles in a fluid flow in an Euler–Lagrange framework. Each bubble corresponds to a single particle which is assumed to be of spherical shape whereas the fluid is modeled as a continuum. The small size of the bubbles and the surface tension of the liquid permits the use of a spherical geometry which enables a description based on the position, the radius and a homogeneous density inside. Bubbles are tracked throughout the simulation considering a four-way interaction including fluid-bubble, bubble-fluid and bubble-bubble interaction. Bubbles submerged in fluid are the basis for simulating cavitation. Bubbles start from small nuclei (also of spherical shape) which can be found numerously in any liquid. They emerge to vapor bubbles when the local fluid pressure goes below the vapor pressure of the liquid. Collapsing bubbles can be highly detrimental to structural surfaces as possible at ship propellers. The aim is to track the path of each bubble in order to predict the region of collapse where cavitation damage might occur.

The continuous liquid phase is considered by the volume averaged incompressible Navier-Stokes equations. The continuity equation is reformulated as in [1] leading to a non-divergence free fluid field. The final equations are solved on an unstructured grid using a stabilized finite element formulation as applied in [2].

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The trajectory of each bubble is tracked using Newton's second law including gravity, drag, lift, virtual mass, pressure and viscous force. In order to complete the four-way coupled approach, bubble-bubble interaction is modeled with a soft sphere contact model as common in plane particle simulations.

The number of nuclei/bubbles can be very large in real problems ($\mathcal{O}(10^6 \dots 10^9)$) and thus our framework allows for a parallel computation of the multi-phase problem. A binning strategy is applied for efficient neighborhood search and data transfer with the underlying fluid domain. First, the fluid domain is partitioned on the respective processors considering load balancing issues. Next, the Cartesian grid aligned bins are distributed to match the fluid element distribution. Due to the unstructured grid, a perfect match is impossible requiring for an extended ghosting of the fluid field to fit at least one full layer of bins at the processor interfaces. Bubbles are assigned to bins and tracked throughout the simulation, hence the underlying fluid element for each bubble is located on the same processor. Neighborhood search during collision detection can be limited to neighboring bins. This algorithm does not rely on fully redundant data which would limit the problem size.

The numerical test case considers flow in a channel with a cylindrical obstacle which can be seen as a simplified geometry of a hydrofoil. Nuclei are released close to the inflow boundary and a small random offset is added to the initial position to break symmetry. In Fig. 1 (left) the nuclei are depicted and colored with their velocity magnitude. The boundary surfaces of the fluid are also included in the figure but the front and rear surface are removed. Vortex shedding is about to start in the wake of the cylindrical obstacle. Due to bubble Reynolds number smaller one, the bubbles follow the fluid flow quite accurately and can be seen as markers in the fluid flow. At the stagnation point of the obstacle, bubbles are slowed down and extensive inter-particle contact as well as contact with the cylindrical surface occurs. In this region, fluid fraction goes down to about 70 % as depicted in Fig. 1 (right).

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Keynote	Holger Steeb	16:30 – 17:15

SPH modelling of pore-scale events in particulate media

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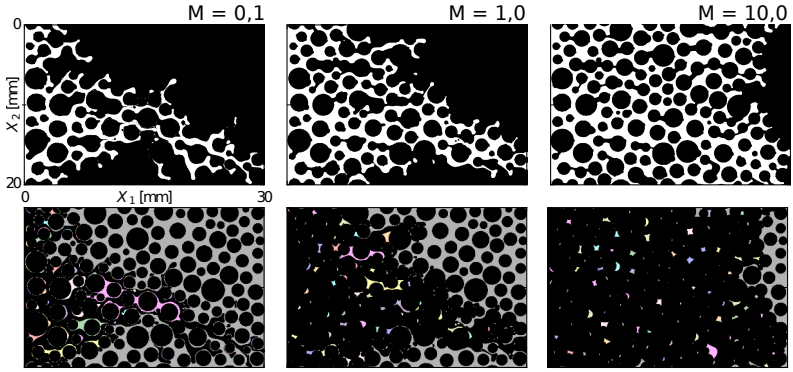

Figure 1: Pore-scale simulation results of saturation-controlled drainage at moderate capillary numbers ($\mathrm{Ca} = 10^{-2}$) and small Reynolds numbers in terms of non-wetting phase distributions (top row) and segmentations of residual wetting phase (bottom row) at percolation breakthrough. Different displacement patterns evolve depending on the viscosity ratio M, i.e. ratio of invading fluid viscosity to defending fluid viscosity, referred to as viscous fingering (left column), stable displacement (right column) and transitional pattern (middle column). Residual wetting phase, highlighted in color, is observed to form wetting films for $M = 0.1$ while compact clusters are formed for the remaining cases resulting in considerable differences with respect to interfacial areas.

Classical macroscale approaches to modeling two-phase flow of immiscible fluids through particulate media are based on a phenomenological extension of Darcy's law and an additional closing equation which relates macroscopic capillary pressure, the difference in mean phase pressures, to saturation. Hysteretic effects and non-equilibrium contributions are typically lumped into an algebraic capillary pressure-saturation relationship wherefore corresponding fitting coefficients lack general validity. Contemporary approaches explicitly acknowledge the role of interfacial area in hysteresis and saturation rate in dynamic capillary pressure. However, these macroscale approaches introduce new balance equations

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with unknown microstructure-dependent terms yet to be explored. Besides fast, e.g. x-ray tomography-based experiments, pore-scale direct numerical simulations must be considered a valuable complementary tool for these problems [1, 2].

Our approach to pore-scale resolved multiphase flow simulation is a weakly compressible Smoothed Particle Hydrodynamics (SPH) scheme which incorporates the Navier-Stokes equations together with a diffuse-interface continuum surface force model to account for the interfacial momentum balances [2]. Attractive features of SPH in this context include its Lagrangian nature due to which non-linear convective terms are not required to be modelled enhancing stability for locally large Reynolds numbers. The latter reveals to be particularly useful for non-Darcian multiphase processes since the phase indicator field is intrinsically advected through particle motion and no additional advection equation potentially prone to numerical diffusion, as used in the classical Volume of Fluid method, is considered.

The aim of our contribution is to discuss the influence of microstructure and fluid properties on phase distribution, dynamic capillary pressure and non-equilibrium processes characteristic of non-Darcian flow. We perform numerical multistep outflow experiments screening various artificial microstructures, viscosity ratios, capillary numbers and saturation rates.

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[3] P. Kurzeja and H. Steeb, Phys. Fluids **26**, 042106 & 042107 (2014).

Thursday

9:00 – 9:45	**Markus Uhlmann**	*Interface-resolved DNS of fluid-particle systems*
9:45 – 10:05	**Stefan Liebenstein**	*Simulations and experiments of confined compaction of snow*
10:05 – 10:25	**Johan Gaume**	*Modeling of crack propagation in weak snowpack layers using the discrete element method*
coffee break		
11:00 – 11:45	**Marcus Bannerman**	*Modern Event-Driven Particle Dynamics*
11:45 – 12:05	**Maksym Dosta**	*Usage of bonded-particle model for DEM simulation of particulate materials*
12:05 – 12:25	**Timo Bihr**	*Diffusion limited growth of metal patches on colloidal particles*
lunch break		
14:30 – 15:15	**Martin Sommerfeld**	*Multiscale approach for calculating drug powder delivery by dry powder inhalers*
15:15 – 15:35	**Denis Davydov**	*On the roots of continuum formulations in particle systems: Theory and numerical examples*
15:35 – 15:55	**Sebastian Pfaller**	*Hybrid continuum mechanics and particle-based simulations: The Capriccio method*
Closing remarks		

Keynote	Markus Uhlmann	09:00 – 09:45

Interface-resolved DNS of fluid-particle systems

Markus Uhlmann,* Aman G. Kidanemariam,
Todor Doychev, and Agathe Chouippe

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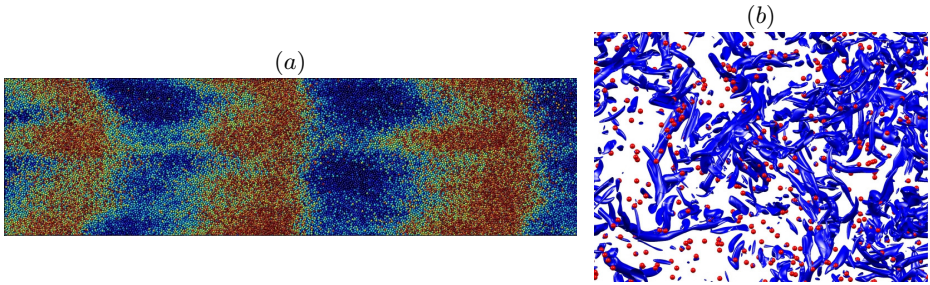

Figure 1: (*a*) Top view of a mobile sediment bed in horizontal channel flow at bulk Reynolds number of 3000 and Shields number of 0.17 at one instant in time, showing the formation of spanwise aligned dune-like patterns (color indicates vertical particle location, ranging from blue to red). (*b*) A snapshot of homogeneous-isotropic turbulence ($Re_\lambda = 120$, intense vortical structures are shown in blue) seeded with spherical particles whose diameter is equal to approximately six times the Kolmogorov length, with a solid volume fraction of 0.005.

Fluid-particle mixtures are commonly encountered in a variety of technical as well as natural systems where they often play a key role in physical, chemical or biological processes. The range of applications involving particulate flow systems is extensive; it includes chemical engineering processes, combustion devices and geophysics (e.g. in meteorology, river and marine dynamics). Although the fluid mechanical description of the motion of solid inclusions in a viscous fluid has attracted considerable attention over the past, today's understanding is still far from complete. Some examples of long-standing open questions are the following: how does a turbulent flow affect the spatial distribution of particles, and how - in turn - does the presence of particles modify the carrier fluid flow

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field? What are the mechanisms of erosion and deposition of sediment particles in a wall-bounded shear flow? Answers to the above questions provided by past studies have not been able to encompass the entire multi-parameter space. In particular, many numerical approaches target situations where the local flow field around the particles can be approximated by analytical solutions valid in the Stokes regime (or corrections thereof), essentially allowing for a simplified treatment of the disperse phase as non-resolved "point particles". This approximation has its limitations when finite-size and finite-Reynolds-number effects become significant.

On the other hand, fully resolving the fluid-solid interface in numerical simulations of configurations with linear dimensions much larger than the typical particle diameter is a formidable challenge even for today's high performance computer systems. Except for a handful of pioneering attempts, computational studies of this type have only begun to emerge during the last decade.

In this contribution results from simulations of many-particle systems in two configurations will be presented. The first is concerned with the erosion and pattern formation of an initially flat sediment bed consisting of up to 10^6 rigid, spherical, non-cohesive particles exposed to (turbulent) flow in a horizontal channel (Fig. 1*a*). In the second configuration we focus on the particle and fluid motion in unbounded domains with and without forced background turbulence in the presence and absence of gravity (Fig. 1*b*).

Acknowledgments: Funding from DFG (grants UH 242/1-1, UH 242/1-2 and UH 242/2-1) as well as generous allotment of computing time at JSC Jülich and LRZ München are gratefully acknowledged.

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Stefan Liebenstein **09:45 – 10:05**

Simulations and experiments of confined compaction of snow

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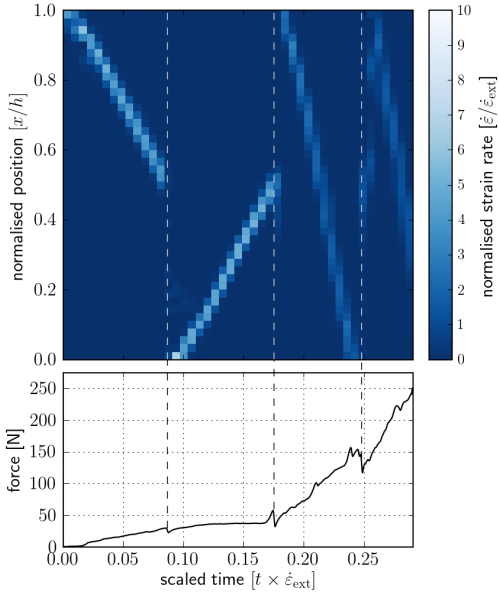

Figure 1: Top: space-time plot of evolution of deformation activity obtained from digital image correlation of artificial snow. Bottom: corresponding force-time curves, measured at the anvil which compresses the material.

The inelastic deformation of porous granular materials is governed by local interactions (as e.g. sliding) and deformation of particles. Macroscopically this

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manifests in nucleation and propagation of small concentrated zones of deformation. Often these zones appear as shear localization, e.g. in compaction of rocks. For other materials, as for example snow, porous sandstone but also non-granular materials as e.g. open-cellular foams, these zones show primarily a compaction localization [1]. These so-called compaction bands are usually observed in the first stage of compression of the material, where a single band moves through the material. However, for the compaction of snow one can observe for certain strain rates repeated band nucleation and propagation, and in particular compaction bands running opposite to the deformation direction. This behaviour is mainly governed by three mechanisms: Softening as a result of bond breaking, hardening as a result of densification and hardening as a result of rapid sintering ('healing') of bonds. Whereas the first two mechanism are common to a wide range of materials, the sintering is almost unique to snow. It is only possible because of snow's high homologous temperature which results in quick diffusion processes and enables a healing of bonds on the timescale of the deformation.

We present a continuum approach based on the proposition of [2], who developed a pressure dependent plasticity model, which includes non-locality and strain localization phenomena. This model is extended to account for breaking of ice granules upon shear deformation [3] and the interplay with the sintering process. It is developed in the framework of continuum visco-plasticity, coupled with ordinary differential equations for the sintering process. We show experimental results for artificial and natural snow, as shown for example in Fig. 1), and compare them to simulations. Special attention lies on the spatio-temporal patterns and their dependence on the strain-rate.

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Johan Gaume 10:05 – 10:25

Modeling of crack propagation in weak snowpack layers using the discrete element method

Johan Gaume,[1,2,*] Alec van Herwijnen,[1]
Guillaume Chambon,[3,4] and Jürg Schweizer[1]

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[2] *ETH Zurich, Switzerland*
[3] *IRSTEA, UR ETGR, Genoble France*
[4] *Université Grenoble Alpes, Grenoble, France*

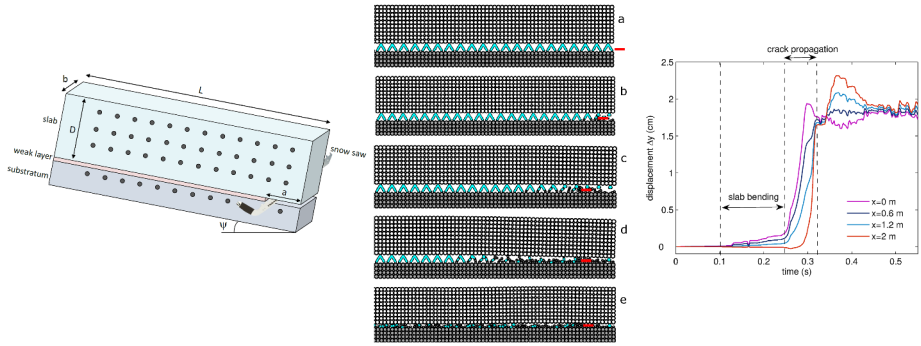

Figure 1: Left: Schematic representation of the propagation saw test (PST). Middle: Snapshots of a discrete element simulation of the propagation saw test (PST). The blue lines in the weak layer represent the bonds between the grains. (a) Initial stable state before cutting inside the weak layer. (b) The saw initiates a crack of length a inside the weak layer. This crack induces the bending of the slab but the system remains stable. (c) The saw reaches the critical cut length a_c which induces the onset of rapid crack propagation in the weak layer (d). (e) The entire weak layer has collapsed. Right: Evolution of the vertical displacement of the slab for different horizontal positions.

Dry-snow slab avalanches are generally caused by a sequence of fracture processes including (1) failure initiation in a weak snow layer underlying a cohesive slab, (2) crack propagation within the weak layer and (3) tensile fracture through the slab which leads to its detachment.

During the past decades, theoretical and experimental work has gradually led to a better understanding of the fracture process in snow involving the collapse

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of the structure in the weak layer during fracture. This now allows us to better model failure initiation and the onset of crack propagation, i.e. to estimate the critical length required for crack propagation. On the other hand, our understanding of dynamic crack propagation and fracture arrest propensity is still very limited. For instance, it is not uncommon to perform field measurements with widespread crack propagation on one day, while a few days later, with very little changes to the snowpack, crack propagation does not occur anymore. Thus far, there is no clear theoretical framework to interpret such observations, and it is not clear how and which snowpack properties affect dynamic crack propagation.

To shed more light on this issue, we performed numerical propagation saw test (PST, Fig. 1) experiments applying the discrete element (DE) method and compared the numerical results with field measurements based on particle tracking. The goal is to investigate the influence of weak layer failure and the mechanical properties of the slab on crack propagation and fracture arrest propensity. Crack propagation speeds and distances before fracture arrest were derived from the displacement field (Fig. 1, right) for different snowpack configurations and mechanical properties. Then, the relation between mechanical parameters of the snowpack was taken into account so as to compare numerical and experimental results, which were in good agreement, suggesting that the simulations can reproduce crack propagation in PSTs. Finally, an in-depth analysis of the mechanical processes at play was carried out which led to suggestions for minimum column length in field PSTs.

Acknowledgments: J. Gaume was supported by the Swiss Government Excellence Scholarship and is grateful to the State Secretariat for Education, Research and Innovation SERI of the Swiss Government

Keynote	Marcus Bannerman	11:00 – 11:45

Modern Event-Driven Particle Dynamics

Marcus N. Bannerman*

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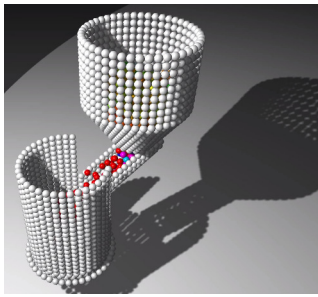
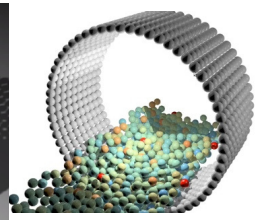
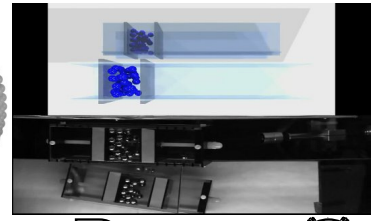

Event-Driven Particle Dynamics (EDPD) is the oldest numerical particle-simulation technique [1], appearing 10 years before Verlet's Time-Stepping (TSPD) simulations [2]. Despite its long history, EDPD has lagged behind the now-standard TSPD approach in capturing the complex geometry and material parameterisation of real granular systems. This is unfortunate as the EDPD technique is highly optimised and inherently stable as it does not rely on numerical integration, making it particularly attractive for granular systems.

One explanation for the relative lack of development is the difficulty of implementing a stable EDPD algorithm. The EDPD technique is analytically exact and does not suffer from truncation error, yet round-off errors in floating point calculations can cause the simulation to catastrophically fail [3]. This talk illustrates this problem by considering the simulation of an inelastic collapse and demonstrates the key components of a stable EDPD algorithm.

Until recently, the available force models for EDPD were limited as only certain classes of force expressions are compatible (e.g., the hard sphere or square-well potentials). Previous attempts [4, 5] to implement "soft" TSPD force models within an EDPD approach are limited to low-density systems. This talk will demonstrate how arbitrary normal forces can be simulated using EDPD using a small approximation [6]. Several extensions for dissipative forces models will also be discussed and evaluated. A new event-driven force model which is equivalent to the spring-dashpot model is introduced and used to demonstrate the

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equivalence of EDPD and TSPD. This allows particle simulations using realistic high stiffness to be simulated efficiently and without numerical instability.

Finally, an outlook on the future development of the EDPD technique and the DynamO [7] simulation package is given.

Acknowledgments: The author would like to thank his co-authors Liang Xiao, Chris Thompson, Severin Strobl, Arno Formella, Leo Lue, and Thorsten Pöschel for their contributions to the work presented here.

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Maksym Dosta 11:45 – 12:05

Usage of bonded-particle model for DEM simulation of particulate materials

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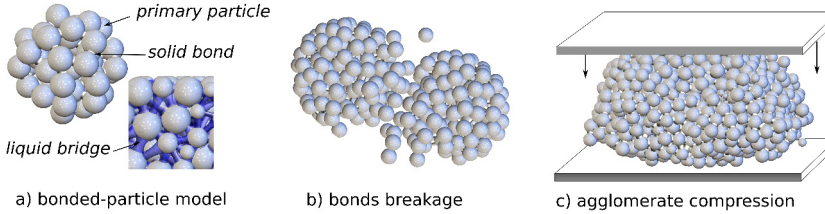

Figure 1: Usage of bonded-particle model for simulation of particulate materials.

Nowadays the Discrete Element Method (DEM) is widely used for modeling of particulate materials on the microscale. This approach allows to consider properties of individual particles and to perform simulations of particle collectives. Initially the DEM has been proposed for modeling of ideally spherical particles. Today, however, there exist several extensions and modifications of it, such as a bonded-particle model (BPM), that gives a possibility to simulate non-spherical particles, composite materials or wet granules. In this contribution the BPM, which has been implemented into the simulation framework MUSEN, will be described and its various applications for modeling of particulate materials presented.

In the BPM the primary particles are coupled with each other via solid or liquid bonds as it is shown in Fig. 1a. Similar to particles, bonds are considered as separate discrete elements and within each simulation time step the forces and moments acting in them are calculated according to the behavior of the modeled material (elastic, visco-elastic, liquid, etc.). A criterion of bonds breakage can be also implemented into the BPM. If, for example, stress acting in a solid bond is larger than its strength [1], or prolongation of a liquid bridge is larger than

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some critical values, then the breakage or rupture can occur. Consequently, the material destruction can be modeled (Fig. 1b). It should be mentioned, that due to the minimization of a computational effort the bonds are excluded from the contact detection algorithm.

On the following examples the main features of BPM will be discussed in this contribution:

- Approximation of packing density of non-spherical particles
- Simulation of composite materials
- Breakage and deformation behavior of irregular-shaped agglomerates [2], [3] (Fig. 1c)
- Modeling of wet particles

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Timo Bihr **12:05 – 12:25**

Diffusion limited growth of metal patches on colloidal particles

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Patchy particles comprise regions of different functionality on an otherwise isotropic core. An example for such particles are polystyrene particles with gold patches. In our case, the growth of these patches is limited by the diffusion of the gold precursor on the surface of the polystyrene particle.

We study this growth process on such a small system by simulation. Thereby, we investigate the influence of the density of the tracer particles, the reaction rate and the diffusion constant. After analysis of our simulations and experiments [4], we find that decreasing ascorbic acid concentration in the solution and increasing of the temperature leads to a roughening of the dendrite structure of the patches. This is caused by the increasing diffusion which lowers the sticking probability of the gold precursor and allows small shape fluctuations to grow exponentially. With these results it is possible to tune the morphology from dense cup-like structures to pure dendrites.

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Keynote	Martin Sommerfeld	14:30 – 15:15

Multi-scale approach for calculating drug powder delivery by dry powder inhalers

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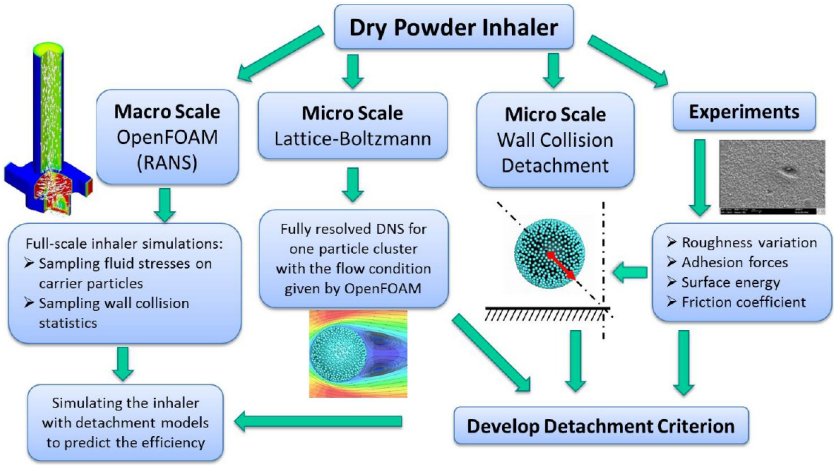

Figure 1: Summary of multi-scale approach for inhaler optimisation and design.

Pulmonary drug delivery of dry powders is increasingly being used for medical treatment because of a number of benefits associated with an inhalation therapy. Essential for an efficient use of dry powder inhalers is the pressure drop and consequently the achievable breathing flow rate as well as the fine powder delivery to the patient‘s lung. Therefore, numerous geometrical designs of inhalers are available on the market. A major requirement for the application of dry powder inhalation is that the particle diameter should be less than 5 μm in order to reach the alveoli of the lungs. Such fine powders are however very cohesive and therefore are hard to be dispersed in the highly turbulent inhaler flow. A solution to this problem is the blending of the fine drug particles with larger carrier particles (i.e. in the range between 50 and 100 μm). Consequently, the inhaler

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must insure the detachment of drug powder from the carrier. This detachment is brought about by different fluid dynamic stresses and carrier particle wall impacts. The efficiency of drug powder delivery is typically between 30 and 40 % depending on the design of the inhaler.

In order to improve the efficiency of inhalers a multi-scale numerical analysis is adopted (Fig. 1). First the fluid stresses acting on carrier particles on their way through a typical inhaler device (here the Cyclohaler® with swirl chamber is considered) are statistically analysed. For that purpose the steady flow field for a typical flow rate is numerically calculated by solving the Reynolds-averaged conservation equations in connection with the $\kappa - \omega$-SST turbulence model [3]. Then a number of carrier particles are tracked through this flow field and instantaneous relative velocities, shear rates and turbulence properties are recorded along their path. From the resulting probability density functions the most probable values are extracted [1]. Moreover, the frequency and intensity of wall collisions are registered in dependence of their location of occurrence within the inhaler.

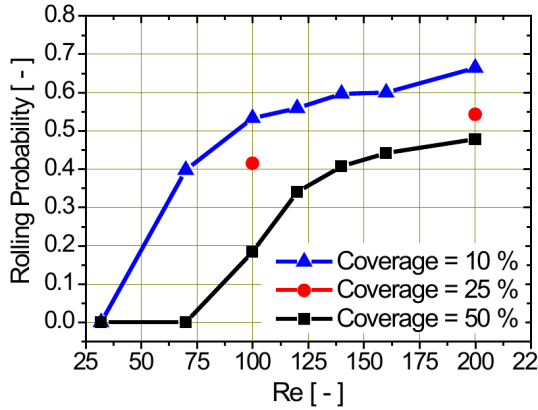

Figure 2: Fraction of fine drug particles being detached from a carrier particle by rolling as a function of Reynolds number for different coverage degree (surface treatment: TC 8 h, $D_{fine}/D_{carrier} = 5/100$).

The information on the fluid stresses is then used to simulate the flow about a fully resolved carrier particle covered with hundreds of drug particles using the Lattice-Boltzmann method (LBM). For realising this, the cluster is centrally fixed in a sufficient large cubic computational domain and exposed to laminar and turbulent plug flow as well as shear flow. From these simulations the fluid dynamic forces on the drug particles in dependence on their location on the carrier are extracted. With the help of experimentally obtained values for the adhesion force, the friction coefficient and the surface energy it is now possible to calculate detachment probabilities in dependence of relative velocity (Reynolds number), turbulence intensity and degree of drug particle coverage as well as the

surface roughness of the carrier particle.

The detachment of fine particles from surfaces is possible through three mechanisms; by normal lift off, sliding or rolling [2]. Using the appropriate conditions for these scenarios together with the measured adhesion parameters, the probabilities were calculated in dependence of the drug particle position angle on the carrier as well as for the entire carrier particle. For a laminar plug flow normal lift was found to be impossible even at the highest considered Reynolds number (i.e. Re =200). Only if a turbulent inflow is generated in the LBM simulations the normal fluid force may exceed the adhesion force. Sliding or rolling detachment may also occur for laminar conditions, where however rolling detachment generally occurs first. The overall detachment probability through rolling is shown in Fig. 2. It is obvious, that a low coverage degree yields the highest detachment probability. For only 10 % coverage, detachment trough rolling begins already at Re = 30 and reaches a probability of 65 % at Re = 200. The detachment of drug powder is of course further enhanced when turbulent flow conditions are simulated.

The analytic calculation of drug particle detachment due to carrier particle wall impact revealed that wall collisions are very efficient for drug detachment. The simulations of the entire inhaler flow and the tracking of the carrier particles showed that each particle experiences about 50 wall collisions on their way through the inhaler. Most of the wall collisions occur in the swirl chamber and the grid mounted at the entrance to the mouthpiece [3]. This detachment mainly occurs through the inertia of the drug particles at the instant of impact.

For allowing the calculation of the entire inhaler flow and the determination of the efficiency of drug powder delivery to the patient, the Euler/Lagrange approach is being used (OpenFOAM®). With the help of the LBM results and the analytical studies on carrier particle wall impact models are being developed which allow describing drug particle detachment from the carriers during their way through the inhaler. Preliminary results obtained with the wall detachment model gave a 100% detachment of the drug particles, which however does not correspond to experimental observations. It is supposed that this discrepancy is mainly associated with the assumption of the adhesion parameters. Therefore, a statistical distribution of the adhesion parameters for the drug particles on the carrier will be introduced. Moreover, the coating of the carrier particles with the drug powder in a mixer yields also clusters of drug particle being attached to the carrier. These agglomerates are most probably not dispersed again and therefore behave as larger particles and consequently do not appear in the fine particle fraction.

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Denis Davydov **15:15 – 15:35**

On the roots of continuum formulations in particle systems: Theory and numerical examples.

Denis Davydov* and Paul Steinmann

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The link between particle quantities and continuum fields has been the subject of research for at least half a century [1, 2]. Nevertheless, there are still many open questions and misleading discussions in the literature. Therefore, based on the fundamental principles of mechanics and statistical physics we construct the basic framework for the link between the particle and the continuum worlds [3–5]. In doing so considerable attention is paid to the central force decomposition and multi-body potentials. A number of general theorems related to convolution properties of statistically averaged quantities, as well as their rates are proved. The balance laws are derived. A representative numerical simulation illustrates the application of this approach to nano-structures with surface energy[6, 7].

Acknowledgments: The financial support of the ERC Advanced Grant MOCOPOLY are gratefully acknowledged.

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Sebastian Pfaller **15:35 – 15:55**

Hybrid continuum mechanics and particle-based simulations: The Capriccio method

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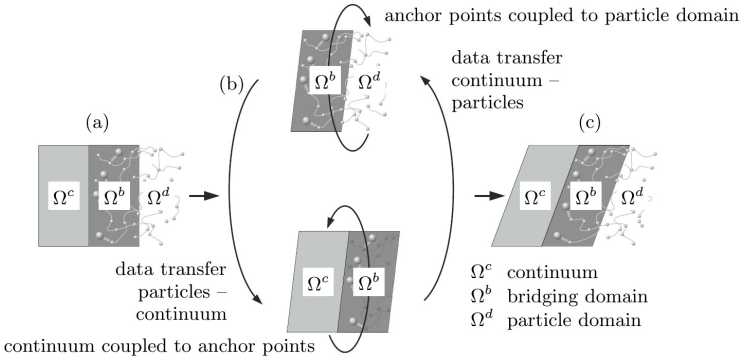

Figure 1: Capriccio method: staggered coupling scheme, small spheres: MD particles, large spheres: anchor points.

Field-based approaches are usually employed in continuum mechanics to model the mechanical behaviour of e.g. solids. However, they cannot take into account the specific atomistic or molecular structure of matter and hence are not able to consider effects originating from very small time and length scales. In contrast, particle-based approaches are well-suited to capture the associated phenomena, but are restricted to very small amounts of material due to the huge number of particles to be captured.

To combine particle-based and field-based approaches, hybrid schemes have been proposed in recent years. In our novel Capriccio method, the continuum overlaps with a particle domain in a so-called bridging domain, where an energy-based coupling together with a suitable kinematic constraint is realized. In contrast to available approaches, we concentrate on amorphous polymers and treat the particle-based region by molecular dynamics (MD) at finite temperature, whereas the continuum is solved by the finite element method (FEM). The relevant

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modifications of the MD code have been developed by our co-workers of the Theoretical Physical Chemistry Group at TU Darmstadt. Most important, the conventional periodic boundary conditions (PBC) employed in MD applications have been replaced by stochastic boundary conditions (SBC), which allow for the definition of anchor points as auxiliary particles. From the MD point of view, they are spatially fixed, confine the MD particles to the MD region, and pretend a huge amount of polymer outside the simulation box. On the other hand, the anchor points follow the motion of FE domain and thus may transfer any deformation to the MD region. Vice versa, the forces exerted on the anchor points by the MD particles constrain the anchor point displacements.

We apply a staggered algorithm to solve the coupled system. This procedure depicted in Figure 1 has been first presented in [1] and thoroughly investigated in [2]. There, we start from the initial configuration (a) and apply the staggered procedure (b) which first obtains a preliminary optimum of the continuum coupled to the anchor points (bottom). Then, due to updated anchor point positions, an MD time-stepping algorithm finds an intermediate equilibrium of the MD domain under SBCs (top) and renders new forces exerted on the anchor points. This procedure is performed until the deformed system achieves a converged state (c).

Acknowledgments: The method has been developed in close collaboration with the Theoretical Physical Chemistry Group at TU Darmstadt within the EU project "Nanomodel" and the DFG-priority programme 1369 "Polymer-Solid Contacts: Interfaces and Interphases".

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Poster Contributions

Posters are displayed for the duration of the conference. There is a dedicated **Poster Session** on Monday from 6:00pm to 9:00pm.

Please take note of the 'People's Choice Best Poster Award'. Your registration bag contains a ballot slip for your choice of the three best posters. Each poster can be identified by its number on the poster board. Note that you can only vote once for each poster. Please hand in your completed ballot slip by Wednesday's afternoon coffee break. The winners will be announced at close of the last session on Wednesday afternoon.

Jakov Lovrić

Poster 1 **Valentin Baric**

Mechanical properties of nanoparticle layers by coarse grained potential simulations

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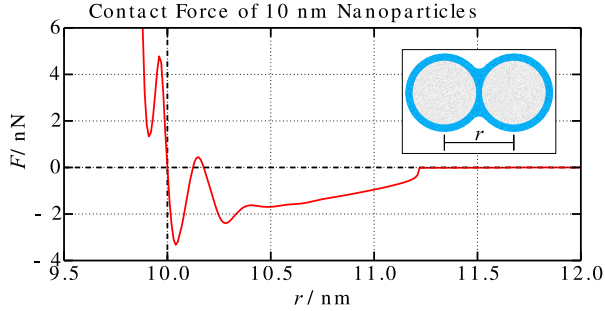

Figure 1: The resulting contact force of two 10 nm TiO_2 particles with 11 H_2O-molecules per nm^2 (70 % humidity). The distance is measured from the center of mass. The inset shows a scheme of interacting nanoparticles.

Nanoparticles are applied in many industrial and scientific applications using a broad range of processes such as fluidization and lamination. The knowledge of the underlying phenomena within the film enables us to increase energy and mass transport as well as electrical conductivity for gas sensors, batteries and catalytic processes. During the processing of nanoparticle layers the particle-particle-interactions lead to agglomeration and fragmentation that determine the properties of the layers including their pore structure, mechanical stability and electric conductivity. Restructuring occurs at a scale of a few hundred nanometers that is governed by the primary particle contacts at nanometer level. Hence,

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these effects are very difficult to measure. The utilization of particle simulations can give insight into phenomena occuring at small sizes and short timescales. However, while nanoscale contact behavior can be investigated by all-atom simulations, the simulation of nanoparticle films are expensive. Discrete Element Methods (DEM) are capable of combining high resolution contact behavior with microscale rearrangement processes and therefore allow the efficient examination of determining characteristics for application related properties.

While the particle breakup forces have been thoroughly examined by Atomic Force Microscopy (AFM) and the combination of Transmission Electron Microscopy with AFM (AFM-TEM) [1], the complete layer rearrangements triggered by greater mechanical stresses are analyzed with a combination of a Nano-Indenter and a Scanning Electron Microscope (SEM). However, the effects on the primary particle level can not be resolved with these techniques. Therefore, we have developed a comprehensive simulation strategy to gain insight into restructuring events within nanoparticle films. These include a versatile model for film generation based on thermophoretic deposition of nanoparticle aggregates, which gives information about the structure of nanoparticle layers, i.e. porosity, pore size distribution, percolation and electric conductivity [2] [3]. In combination with the knowledge gained by all-atom simulations on the interaction forces between nanoparticles [1] we have been able to set up a Coarse Grained potential (FIG 1) to perform Molecular Dynamics (MD) simulations at mesoscopic level of whole particle films. We can mechanically stress the particle layers by compaction and elongation as well as indentation in order to reproduce realistic conditions. This gives us the ability to reproduce AFM experiments on particle-particle contacts and to carry out detailed investigations of the trajectories observed by means of AFM-TEM. Furthermore, we can investigate the mechanical stability and electric conductivity of the layers.

With this knowledge we expect to be able to optimize the synthesis of nanoparticle layers and subsequently the film properties according to their specific applications.

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Poster 2 **Ramon Cabiscol**

Assessment and calibration of DEM parameters for macro-scale simulation of pharmaceutical tablets

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Attrition and breakage of pharmaceutical tablets are major problems faced by industry during manufacture and transportation, as a result of non-optimal parameters for tablet compaction. To avoid this and to obtain a final product with adequate mechanical properties, the compaction conditions are carefully adjusted for new formulations of powders.

In order to fully comprehend the interplay of process parameters and formulation properties as well as their influence on the mechanical characteristics of the powder compact (pharmaceutical tablet), we apply a discrete simulation approach. In the scope of Discrete Element Method (DEM), the behaviour of a powder mixture under certain conditions can be described mathematically using single particle properties. Within this scope, after a successful calibration of simulation parameters, kinematic behaviour of tablets can be observed on a process scale.

Calibration of DEM simulation parameters for a system of non-spherical particles can become a tedious process. In this work, we demonstrate and depict the calibration of DEM parameters for cylindrical tablets, mainly rolling and sliding coefficient of friction and coefficient of restitution, which we pointed out as the most significant in sensitivity analysis. Simulation results are then collected and compared quantitatively and qualitatively to experimental data, extracted from static and dynamic angle of repose experiments. We address some key issues and setbacks when attempting to predict tablet attrition and wear in industrial transport systems.

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Poster 3 **Karola Dierichs**

Non-convex designed aggregates as architectural material systems

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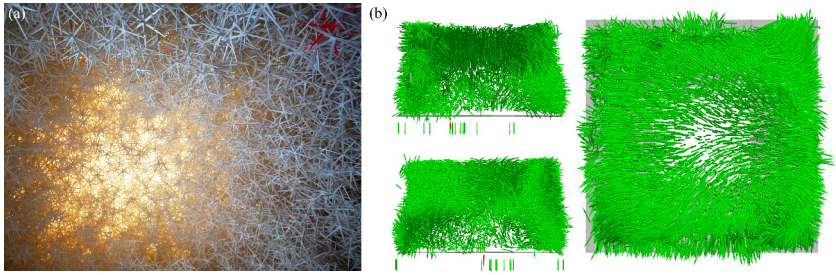

Figure 1: (a) Bottom view of aggregate vault constructed through clogging. (b) DEM simulation of aggregate vault showing particle speeds and directions in x-, y- and top z-view.

Designed aggregates are large particle systems which are made from synthetically produced granules. Over the past ten years they have been increasingly recognized as architectural material systems which allow for both rapid re-configuration and functional grading, [1, 2].

Various particle geometries have been explored, such as convex, non-convex and double non-convex hooky aggregates, [3, 4]. The research presented here is focused on non-convex particles as architectural construction systems, which work mainly under compression forces, such as columns, walls, arches or domes. Research is mainly conducted with small-scale experiments, full-scale prototypes as well as simulations using a state-of-the-art Distinct-Element Modeling (DEM) software package, [5].

Small-scale experiments investigate packing densities as a function of arm length and arm amount in order to identify particle geometries which are both cheap to produce and effective with regards to architectural performance criteria such as stability. Full-scale prototyping for columns, walls, arches and walls were

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conducted — with domes being the most challenging formation. The most stable construction method for vaults has so far been a large-scale tank with an outflow hole at the bottom. Vaults are formed through clogging of the granular system, redundant particles can in a next step be removed to be recycled. The process has been simulated using a DEM software package. Particles are modelled using the multi-sphere method and randomly generated in a box, the bottom lid is removed after cycling and particles are deleted using a sphere filter. So far a maximum of 25000 particles has been used in the model. Simulations mainly serve to gain an increased understanding of the micro-mechanical behaviour of a given particle geometry in a larger aggregate structure. Current research is conducted into larger spatial formations that combine different structural compression-types. These larger structures use different non-convex geometries such as cumulated tetrahedra as well as short-armed and long-armed cumulated cubes.

Further research will be conducted into aggregate systems that mix geometric particle types from different groups - such as non-convex and double non-convex particles - in order to achieve further structural functional grading and consequently an expanded catalogue of architectural prototypes.

Acknowledgments: We acknowledge the funding by the Itasca Educational Partnership Program (IEP).

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Poster 4 **Manuela Göbelt**

Silver needle webs for electrode applications — experimental basis for optimization of electro-optical properties based on picture algorithm developments using electron microscopy data

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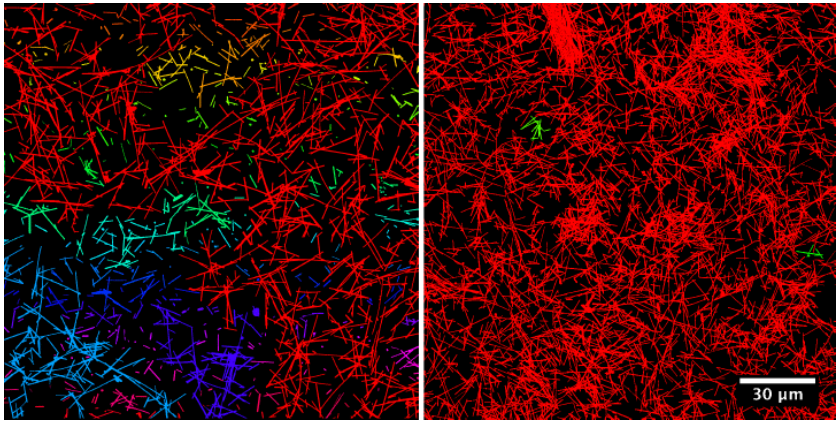

Figure 1: Connected region in a non-percolated (left) and an percolated sample (right)

Transparent conducting electrodes are a critical component in optoelectronic devices like solar cells. The replacement of Indium containing electrodes by more abundant elements is of major economical interest. One approach is the utilisation of metal nano-wires for this purpose. Silver nano wires with high aspect ratio are produced by chemical synthesis based on the reduction of AgNO3 in Etylengycol with an additional capping agent [1]. The raffinated solution is dropcasted and spray coated on silicon or glass as a substrate. This procedure results in a homogeneous random web, that exhibits different degrees of interconnectivity

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depending on the geometry and the cover ratio of the nanowires [2]. Micrographs of the random web were recorded using a scanning electron microscope SEM and were analysed by picture analysis / pattern recognizion algorithms developed for this task presented in this congress by the co-authors. The electrical conductivity and transmission in the UV-VIS of the nanowire webs were measured. In contrast to the microscopic investigations those methods average over a large number of wires. The picture analysis permits to connect the results of the microscopic and integral methods and has been proven to be a powerful tool for the optimisation of transparent conducting electrodes for solar cells. Fig. 1 shows the micrographs for different coverage with nanowires. The percolation of the nanowires is essential for a good overall conductivity of the network as being dependent on the overall connectivity between wire ensembles.

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Poster 5 **Johan Gaume**

Granulation of snow: from tumbler experiments to discrete element simulations

Johan Gaume,[1,2,*] Walter Steinkogler,[1,3] Henning Löwe,[1] Betty Sovilla,[1] and Michael Lehning[1,3]

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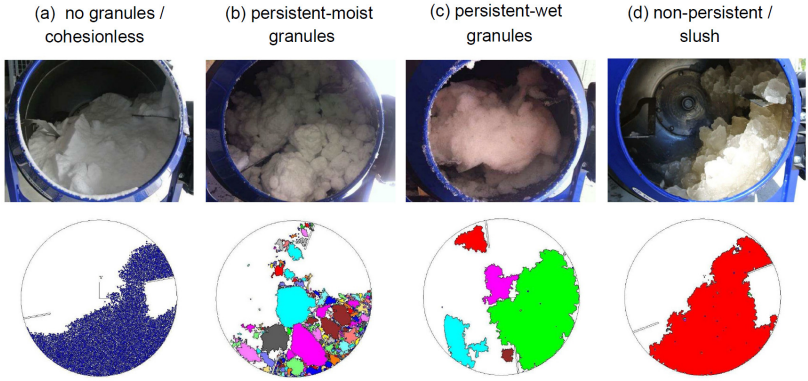

Figure 1: Illustration of the granulation regimes observed in the experiments (top) and reproduced using cohesive discrete element simulations.

It is well known that snow avalanches exhibit granulation phenomena, i.e., the formation of large and apparently stable snow granules during the flow. The size distribution of the granules has an influence on flow behavior which, in turn, affects runout distances and avalanche velocities. The underlying mechanisms of granule formation are notoriously difficult to investigate within large-scale field experiments, due to limitations in the scope for measuring temperatures, velocities, and size distributions.

To address this issue we present experiments with a concrete tumbler (Fig. 1, top), which provide an appropriate means to investigate granule formation of snow. In a set of experiments at constant rotation velocity with varying temperatures and water content, we demonstrate that temperature has a major impact

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on the formation of granules. The experiments showed that granules only formed when the snow temperature exceeded -1°C. No evolution in the granule size was observed at colder temperatures. Depending on the conditions, different granulation regimes are obtained, which are qualitatively classified according to their persistence and size distribution.

The potential of granulation of snow in a tumbler is further demonstrated by showing that generic features of the experiments can be reproduced by cohesive discrete element simulations (Fig. 1, bottom). The interparticle contact laws used in the simulations are classical [1,2]. The normal force is the sum of a linear elastic and of a viscous contribution (spring-dashpot model), and the shear force is linear elastic with a Coulombian friction threshold. Cohesion was added to the particles by adding a bond to each contact with specified shear and tensile strengths. In addition, a new bond can be created at a new contact between two particles if the total contact force exceeds a specific aggregation value.

The proposed discrete element model mimics the competition between cohesive forces, which promote aggregation, and impact forces, which induce fragmentation, and supports the interpretation of the granule regime classification obtained from the tumbler experiments.

Acknowledgments: Funding for this research has been provided through the Interreg project STRADA by the following partners: Amt für Wald Graubünden, Etat du Valais, ARPA Lombardia, ARPA Piemonte, Valle d'Aosta, and Regione Lombardia. J. Gaume was supported by the Swiss Government Excellence Scholarship and is grateful to the State Secretariat for Education, Research and Innovation SERI of the Swiss Government

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Poster 6 **Alexander Haarmann**

Simulation of a particle-wall contact and validation through experiments

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If one concerns the behavior of fine particles in questions of conveying and handling, the contact mechanics between the particles themselves and the particles and the surroundings are crucial. If one wants to predict the behavior of a particle-collective one first step is the examination of a single particle-particle or particle-wall contact. As the adhesion of a particle to a wall has been examined numerous times, the restraining force against particle-rolling caused by an external force - the adhesion moment - has not been examined in such an intense way. The authors developed a simulation based on C++ to predict both the adhesion force and moment. With the technical equipment consisting of an Environmental Scanning Electron Microscope (ESEM) with micromanipulators and a spring table it is now possible to measure the adhesion moment and compare the simulated values to experimental data [1, 2]. Aim of the project is to simulate the contact of a particle with a wall in gaseous environment. Two different contact cases are examined, a smooth particle on a wall and a rough particle with two contact points on a wall. For these cases distribution functions, especially for the adhesion-moments, were developed to predict the strength of the contact against external stress. As a further step in the project experiments will be made. The adhesion moment will be measured using a spring table with the corresponding measuring software inside of an ESEM. There are test particles matching the simulated particles, especially the rough one, very well. The experimental data will be used to verify the simulation, while the simulation will be used to predict the results of further experiments [3]. The ESEM was equipped with micromanipulators. The manipulators can be used to move particles in a very defined way while one can observe the whole process using the microscope. To measure the adhesion moment of the particles a spring table was installed. The measurement is performed as follows. Several particles are isolated on a stub by using the manipulators. This stub is then placed in the spring table. Then the manipulators are used to stress the particle sideways. The spring is bend to a certain degree and then the contact breaks and the table returns to its starting position. According to the spring constant of the table and the deflection the necessary force to break the contact can be measured. According to the point

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where the particle was stressed by the manipulator a lever arm can be observed and the adhesion moment can be calculated. The simulation calculates reasonable values for the adhesion force and moment for both the smooth and the rough particle. As there is not much comparable experimental data, the decision was made to measure the adhesion moment at the own institute. The results of this measurements will be shown, compared to the simulated values and the results of this comparison will be discussed.

Acknowledgments: The authors would like to thank the German Research Foundation (DFG) for the financial support of the project in the priority program "PiKo".

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Poster 7 **Michael Haderlein**

A framework for numerically efficient simulation of multiphase precipitation processes

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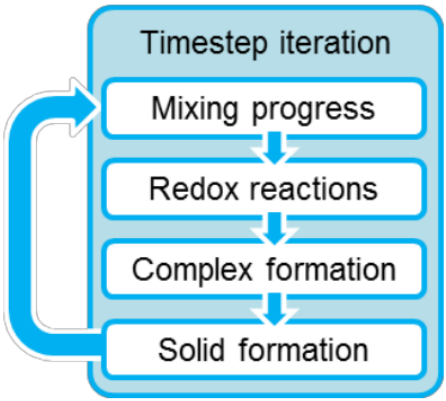

Figure 1: Sketch of processes modeled every timestep iteration

This submission is part of the DYNSIM project.
The simulation of precipitation processes is an important tool for process engineering. If multiple solid phases are involved, the complexity of the system rises and the experimental effort increases. Especially for such cases, efficient and accurate numerics can reduce costly experimental work. In particular, process engineering involves the optimization of process parameters like temperature profiles or flow patterns which requires a large number of simulations. Particular attention is therefore paid to the numerical efficiency to keep the computational cost at a reasonable level even in the latter case. The objective of this contribution is the development of a simulation tool for precipitation which is directly applicable to different materials.
In general, precipitation in liquid phase involves multiple process steps: Two or more liquids need to be mixed, redox reactions might take place, complexes

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might form and finally solids will precipitate. The solid formation itself occurs by nucleation and growth. As sketched in Figure 1, all these processes need to be considered simultaneously for a proper description of precipitation. Mixing controlled precipitation in a T-mixer could already be modelled very well in excellent agreement with experimental data [1]. In the next step, we extend this approach to complex reaction networks and reaction controlled systems. When reaction kinetics are quite fast a quasi-equilibrium can be assumed. The complex reaction equilibria are described by a nonlinear system of equations whose convergence is accelerated by the analytically derived Jacobian. Finally, the solid formation is modeled by means of population balances. Multiple phases are described by independent population balances which are coupled via mass balances. To ensure numerical efficiency, the direct quadrature method of moments is applied here [2].
The implementation of this general tool is validated by different examples. First, the implementations of the mixing model and the redox reaction kinetics are validated by comparing the product of the Villermaux-Dushman reaction with literature data [3]. Second, the mixing controlled single phase synthesis of barium sulfate is modeled for multiple concentrations and power inputs [3]. Finally, the multiphase precipitation of copper salts is investigated [4]. All results match well with literature data and are produced within short computational time. The combination of flexibility, accuracy and numerical efficiency is considered to provide the way towards a powerful simulation tool which is applicable to many material systems.

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Poster 8 **Young-Hoon Jung**

Origin of stress-dependent elastic properties of granular soils: Contact stiffness and contact density

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Stress-level-dependent elasticity is a major feature of soil behavior that needs to be investigated independently within the framework of micromechanics theory. The nonlinear anisotropic elastic response can be represented by a well-know empirical equation of three-dimensional elastic moduli given by [1]

$$G_{ij} = C_{ij} p_a f(e) (\sigma'_i / p_a)^m (\sigma'_j / p_a)^n. \quad (1)$$

where G_{ij} is the elastic shear modulus in the i-j plane, C_{ij} is a dimensionless constant relating to the directional properties of the elastic shear moduli, p_a is the atmospheric pressure, used as a normalizing constant, $f(e)$ is the void ratio function, σ'_i and σ'_j are the principal stresses in the i and j directions respectively. The sum of exponents m and n, hereinafter designated by s, determines the magnitude of the stress-level dependency of soil elasticity has long been known, the physical origin of this relationship has not yet been clarified. Recent experimental study shows that for both sands and clays s varies between approximately 0.4 and 0.6, with a value of 0.5 having been observed by many researchers.
To investigate the origin of the stress-level dependency of soil elasticity, we focused on the significance of microscopic parameters such as contact geometry, the evolution of the contact distribution, and changes in contact densities. Two synthetic specimens, one loose and the other dense, were used for the simulations. The stress path experiment was simulated under various contact conditions which can be analytically realized via a contact stiffness model proposed by Jager [2]. The geometry of the contact body was assumed as an elastic sphere with local, axi-symmetric irregularity. Using this model, discrete element modeling (DEM) code was modified to accomodate the three contact models with s=0.5 for conical contact surface, 0.33 for the spherical surface, and 0.0 for the flat surface. Axi-symmetric stress loadings on an assembly of 10,000 spherical particles with the diameter of 0.5 mm were simulated using a non-commericial DEM code developed by Kuhn [3] . Both loose and dense specimens were prepared by adjusting the frictional coefficient between the particles.

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For the dense specimens, the contact geometry had a decisive influence on the sum of the exponents, expressed as s. The simulation results show that $s = 0.5$ for the conical contact surface, 0.33 for the spherical surface, and 0.0 for the flat surface. These values are exactly identical to the value of the exponents for the expressions of the contact stiffness equation. For the loose specimens, however, the value of s is much higher than it is for the dense specimens such that there is no correlation between the value of s and the exponent in the contact stiffness model. Microscopic data explains the reason why the loose and dense specimens exhibit different degrees of stress-level dependency with regard to the elastic shear moduli. For the dense specimens with high coordination number, the internal structure represented by the degree of fabric anisotropy and the coordination number value remain unchanged during shearing, thus leading to the coincidence of the s value and the exponent in the contact stiffness model. For the loose specimens with a low coordination number, however, the fabric structure evolves continuously during shearing, which results in an increase in the exponents in the power function of the elastic modulus. The rearrangement of particles and the transition of contact force chains with the evolution of the fabric manifest themselves as increasing dependency with regard to the elastic moduli on the stresses in the loose specimens.

Acknowledgments: This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government(MSIP) (No. 2015R1A2A2A01005969).

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Poster 9 **Jonathan Kollmer**

Absence of subharmonic response in vibrated granular systems under microgravity conditions

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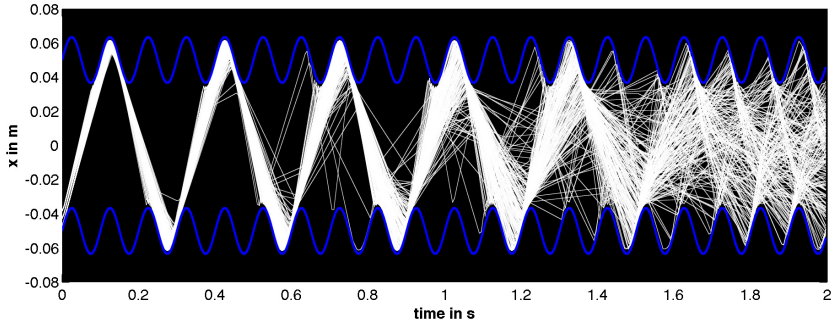

Figure 1: Space-time plot obtained from a MD simulation of a 5x5x10 cm box containing 473 particles with a diameter of 4mm. For a coefficient of restitution ε of 0.2 subharmonic motion is unstable.

Experiments in microgravity conditions have shown that granular systems subjected to sinusoidal vibrations respond either by harmonic or gaslike dynamics, depending on the parameters of the vibration, amplitude and frequency, and the container size, while subharmonic response is unstable, except for extreme material properties and particular initial conditions. The absence of subharmonic response in vibrated granular systems implies that granular dampeners cannot reveal higher-order resonances, which makes them even more attractive for technical applications. By making extensive use of molecular dynamics simulations we explain this behaviour [1].

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Poster 10 **Jakov Lovrić**

Morphological measures of randomly packed ellipses in 2D

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We simulate random packing of non-overlapping ellipses over a broad range of the particle aspect ratios and area fractions. We construct Voronoi tessellations from the centers of mass of the randomly packed particles, as well as the particle boundaries. We systematically analyze a number of morphological measures and their mutual correlations. We find the best fitting function for the distributions of the given measures, which seem to resemble generalized Gamma distributions in limited range of parameters. While these type of distributions have been suggested previously in the literature in the context of area distribution of randomly packed particles, we find that this is not always the case. Furthermore, we analyze the correlations between pairs of morphological measures and find that they depend strongly on the shape of the ellipses only at high area fractions. For circles at the area fraction of 80% the most correlated measures are area and perimeter of a given Voronoi cell, whereas for elongated particles, highest correlations appear between the mean contact length between cells and the number of neighbors.

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Poster 11 **Christopher McHardy**

Lattice Boltzmann method for the simulation of radiation transport in microalgae-biosuspensions

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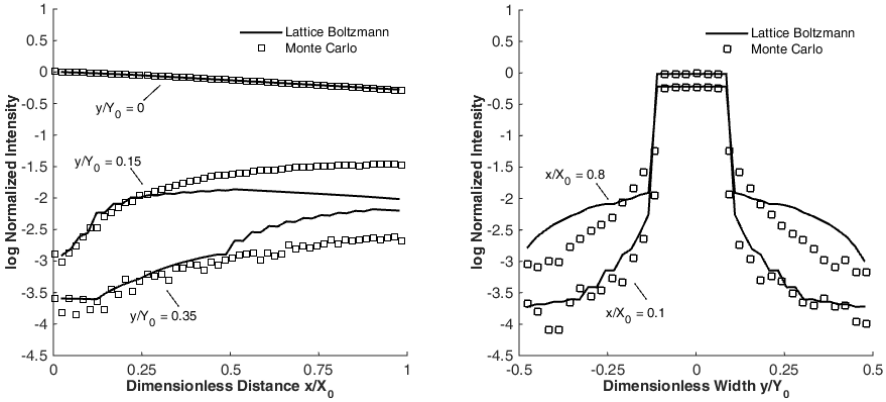

Figure 1: Profiles of specific intensity predicted by lattice Boltzmann method and Monte Carlo method on the xy-plane at $z/Z_0 = 0$. The center of the collimated beam located at $y/Y0 = 0$. Left: intensity with respect to traveled distance; Right: intensity with respect to domain width[5].

The technical cultivation of phototroph microorganisms, such as microalgae, depends on an efficient supply of light in photobioreactors. While insufficient supply of light limits cell growth, high light intensities lead to inefficient metabolic utilization of the supplied radiative energy or even may cause inhibition of growth. In photobioreactors, the solution of the radiative field is connected to the flow field inside the reactor because optical properties of the biosuspension depend on local concentrations of cells and gas bubbles, which are usually non-homogenously distributed.

The transport of electromagnetic radiation can be modeled by the Radiation Transfer Equation (RTE). To solve the RTE, different numerical methods, such

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as Discrete Ordinate Methods or Monte Carlo Methods, can be applied [1]. However, these methods cause either high computational costs or require different numerical grids from those used in Computational Fluid Dynamics. Thus, the interpolation of information between the different numerical grids becomes a necessity for the determination of local optical properties of biosuspensions. A new approach is to use lattice Boltzmann methods to calculate radiative transfer. Those methods potentially enable the usage of the same grids for the calculation of flow and radiative fields. Since the RTE can be directly derived from the Boltzmann equation by treating radiation as a "photon gas", particle-based lattice Boltzmann methods seem to be a natural choice for the calculation of radiative transfer.

The subject of the present contribution is the discretization of the RTE by means of a lattice Boltzmann method to compute the stationary intensity of monochromatic light in three dimensions inside an absorbing and scattering biosuspension. Based on recent literature [2–4] the directions of light propagation are discretized in the cubic grid. To estimate light scattering by cells, representative averages of the scattering phase function are calculated for scattering angles between each discrete direction of propagation. Absorption and scattering are included in the model as source and sink terms. The method was implemented in MATLAB and compared to Monte Carlo simulations of radiation transport. Furthermore, the method was used to predict the attenuation of light by a homogeneous suspension of microalgae and validated by experimental measurements.

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Poster 12 **Sebastian Mühlbauer**

Gas flow over catalytic surfaces

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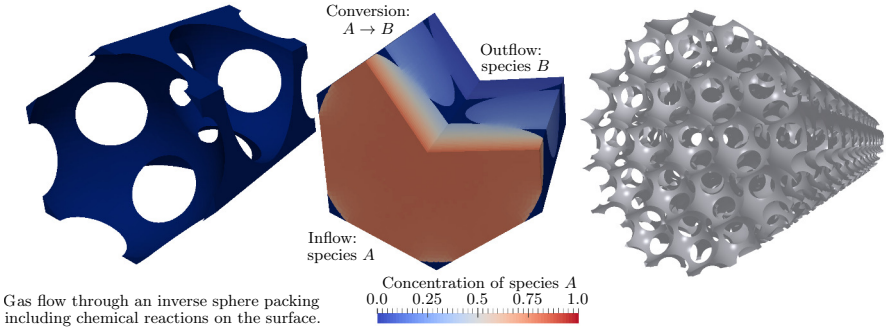

Gas flow through an inverse sphere packing including chemical reactions on the surface.

Gas flow through porous structures including chemical surface reactions is an important issue in many technical applications, first of all heterogeneous catalysis. Simulating such gas flows requires to merge reaction kinetics into gas dynamics within complex geometries. Particle based simulation methods are eminently suitable for this, while continuum methods run into two substantial problems. First, generating a mesh of sufficient quality in order to allow for employing a continuum approach appears to be very challenging, especially for complex structures, like the one depicted below. Another invaluable advantage of particle based methods compared to continuum methods is that chemical reaction models can be implemented on microscopic scale yielding results on macroscopic scale.

Employing a particle based approach, we simulate chemical reactions on catalytic surfaces in complex gas flows. The starting point is non-dissociative adsorption with subsequent desorption as can for example be observed for carbon-monoxide on a platinum surface [1]. The underlying gas dynamics is simulated using Direct Simulation Monte Carlo [2], which allows for following the trajectory of each quasi-particle. If a reactive quasi-particle impinges on a reactive surface, it is adsorbed with a certain probability. Apart from constitutive parameters defined by the particle-wall-pairing, the adsorption probability depends on the local

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temperature. Naturally, low local surface coverage, which implies an abundance of free adsorption sites, encourages adsorption. Depending on the wall temperature the particles are desorbed after a certain time. According to the prescribed reaction parameters the particles might behave differently, after having desorbed from the surface. A qualitative surface reaction model can be implemented by changing the particle behaviour after desorption such that a second adsorption is prevented. This we use in order to simulate heterogeneous catalysis in inverse sphere packings. The figure above shows an example, for which the inflowing substance is denoted as species A and converted to species B at the surface following the reaction mechanism described previously. For the given parameters substance A is consumed completely within the domain so that the gas passing the outlet consists purely of species B. Employing a multiscale approach we can investigate complicated porous structures on macroscopic scale such as an entire catalytic converter.

Acknowledgments: We acknowledge the funding by the German Science Foundation (DFG) through the Cluster of Excellence Ëngineering of Advanced Materials".

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Poster 13 **Patric Müller**

Epitaxial growth of patchy coatings on nanospheres

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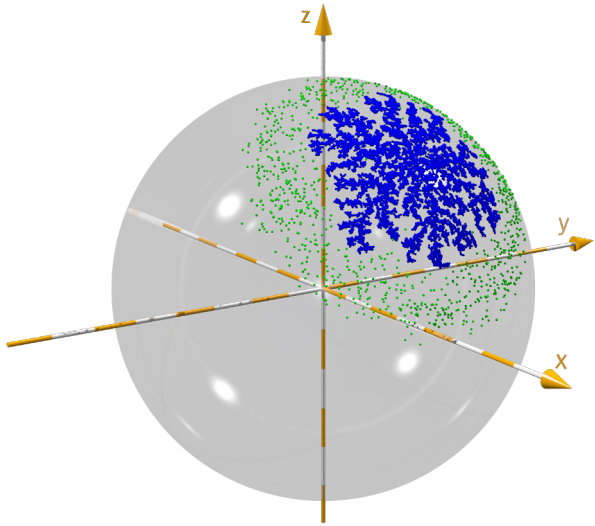

Figure 1: Diffusion limited epitaxial aggregation on a spherical surface as a model for the growth of patchy coatings on nanospheres. Preliminary simulation results of a dendritic patch morphology.

Patchy nanoparticles are characterized by heterogeneous surface properties. The resulting anisotropic chemical and physical behavior makes them interesting for novel applications. Recently a one-pot colloidal method for the facile synthesis of gold and silver patches on silica and polystyrene nanospheres has been described [1–3]. We show that the corresponding patch growth process may be described by diffusion limited epitaxial aggregation on the curved surface of the core particle. The experiments display fast diffusion limited and slow integration limited aggregation leading to either dendritic or continuous cup-like structures. Depen-

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ding on the parameters our model is able to describe both regimes of aggregation and the associated patch morphology.

Acknowledgments: We acknowledge the funding by the German Science Foundation (DFG) through the Cluster of Excellence Ëngineering of Advanced Materials".

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Poster 14 **Peter Mueller**

Impact of spheres on large thin plates

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Using a free-fall apparatus, the low-velocity impact behavior of model elastic to elastic-plastic spherical particle products (glass, steel spheres and elastic-plastic granules) impacting on large thin glass plates had been experimentally measured. The impact and rebound velocities had been determined from the time interval between consecutive impacts and thereby, the coefficient of restitution had been evaluated. The contact time had been measured from the current transmission during contact of the steel spheres (soldered with a very thin flexible conductive wire) and the plate (coated with a thin conductive layer) when a closed circuit is created. The influences of the impact velocity, the sphere size and the plate thickness on the impact behavior have been investigated.

A novel analytical approach to find a comfortable solution for the coefficient of restitution of elastic spheres impacting on large thin plates, by solving the mathematically strenuous Zener model [1] will be presented. By comparing with the coefficients of restitution evaluated by numerically solving the mathematically strenuous Zener model [1], it will be shown that the proposed simple analytical approach provides an excellent approximation of the Zener model [1] as well as predicts results accurately for the range of coefficients of restitution larger than 0.2. It will be shown that a significant dependence of the coefficient of restitution of elastic spheres on the ratio of sphere diameter to plate thickness as well as on the impact velocity (and thereby, on the inelasticity parameter) exists, which can be well described by the Zener model [1] as well as the proposed analytical approach.

The measured contact time values have been compared with the theoretical predictions of the Hertz [2] and the Zener models [1]. Thereby, a detailed discussion will be presented about the inadequacy of the Hertz model [2] to accurately predict the contact time for a sphere impacting on an infinitely extended elastic plate of finite thickness, where longitudinal and transversal waves can travel several times (below the contact area) through the plate within the contact time, whereby flexural waves arise. Similarly, the limitations of the Zener model [1] such as the overestimations of the CoR (due of negligence of energy dissipation

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by friction and viscous damping) will also be illustrated with help of experimental results and thereby, the effective limits of reliability of the Zener model [1] will be discussed considering the underestimations of the contact time for thin plates.

Acknowledgments: The authors thank the German Research Foundation (DFG) for the financial support of this study within the framework of the Research Grant: TO 156/40-1 „Statische und dynamische Beanspruchung elastischer, plastischer und viskoser Granulate“.

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Poster 15 **Eric Partelli**

Helical inner-wall texture prevents jamming in granular pipe flows

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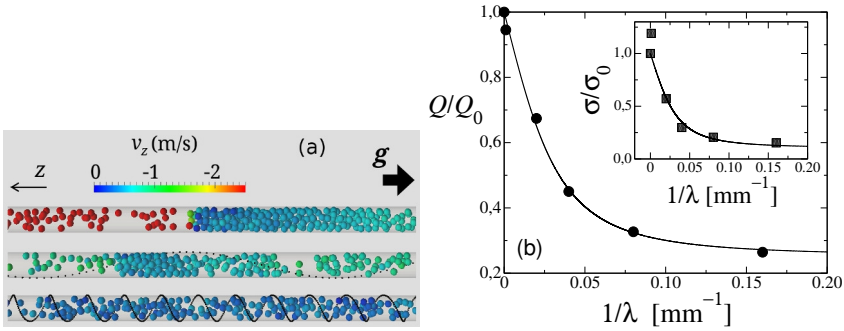

Figure 1: (a) Snapshots of simulations without helix and with helix of wavelength values $\lambda = 25\,\text{mm}$ and $6.25\,\text{mm}$ (from top to bottom). $D_\phi = 3.5$ and in the figures a 70 mm long excerpt of the pipe is shown. The small particles composing the helix are coloured black and there are 44 of such particles per helix wavelength; (b) main plot: expectation value of the mass flux Q as a function of $1/\lambda$, where λ is the helix wavelength and particle-particle interactions are computed considering viscoelastic particles and material parameters associated with aluminum particles as described in Ref. [4]. The flux is rescaled with $Q_0 \approx 7.4 \times 10^{-3}\,\text{kg/s}$ which corresponds to the calculation with no helix [4], or equivalently $\lambda \to \infty$. The continuous line corresponds to the best fit to the simulation data using Eq. (1), which gives $B \approx 0.75$. Inset: non-dimensional standard deviation of the flux, σ/σ_0, as a function of $1/\lambda$, where $\sigma_0 \approx 2.5 \times 10^{-4}\,\text{kg/s}$ is the value of σ with no helix. The continuous line denotes the best fit to the equation $\sigma = \sigma_0 \cdot \{1 - C \sin[\arctan(2\pi D/\lambda)]\}$, which gives $C \approx 0.9$ with correlation coefficient $R^2 \approx 0.983$.

Granular pipe flows are characterized by intermittent behavior and large, potentially destructive solid fraction variations in the transport direction [1–3]. By means of particle-based numerical simulations of gravity-driven flows in vertical

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pipes, we show that it is possible to obtain steady material transport by adding a helical texture to the pipe's inner-wall (Fig. 1a) [4]. The helical texture leads to more homogeneous mass flux along the pipe, prevents the emergence of large density waves and substantially reduces the probability of plug formation thus avoiding jamming of the particulate flow. We show that the granular mass flux Q through a pipe diameter D with an helical texture of wavelength λ follows the equation

$$Q = Q_0 \cdot \{1 - B \sin[\arctan(2\pi D/\lambda)]\}, \tag{1}$$

where Q_0 is the flow without helix, predicted from the well-known Beverloo equation. Our new expression yields, thus, a modification of the Beverloo equation with only one additional fit parameter, B, and describes the particle mass flux with the helical texture with excellent quantitative agreement with simulation results (Fig. 1b). The future application of the method proposed here has the potential to improve granular pipe flows in a broad range of processes without the need of energy input from any external source.

Acknowledgments: We thank the German Research Foundation (DFG) for funding through the Cluster of Excellence "Engineering of Advanced Materials" and the Collaborative Research Center SFB814 (Additive Manufacturing). We gratefully acknowledge the computing time granted by the John von Neumann Institute for Computing (NIC) and provided on the supercomputer JUROPA at Jülich Supercomputing Centre (JSC).

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Poster 16 **Eric Partelli**

Particle-based simulation of powder application in additive manufacturing

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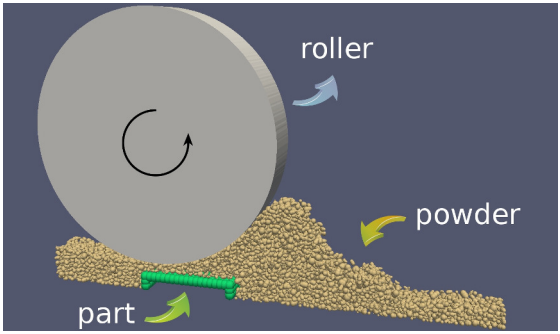

Figure 1: Snapshot of the simulation indicating the main elements of the powder application process. The roller moves from left to right thereby rotating in the counter-clockwise direction. Periodic boundary conditions are applied in the horizontal direction perpendicular to the transport, while particle motion is constrained by the presence of rough vertical walls (not shown) on the left and right ends of the simulation area.

The development of reliable strategies to optimize part production in additive manufacturing technologies hinges, to a large extent, on the quantitative understanding of the mechanical behavior of the powder particles during the application process. Since it is difficult to acquire this understanding based on experiments alone, a particle-based numerical tool for the simulation of powder application is required. In the present work, we develop such a numerical tool and apply it to investigate the characteristics of the powder layer deposited onto the part using a roller as the coating system (Fig. 1) [1–4]. In our simulations, the complex geometric shapes of the powder particles are taken explicitly into account [3, 4]. Our results show that increasing the coating speed leads to an increase in the surface roughness of the powder bed, which is known to affect

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part quality. We also find that, surprisingly, powders with broader size distributions may lead to larger values of surface roughness as the smallest particles are most prone to form large agglomerates thus increasing the packing's porosity [2]. Moreover, we find that the load on the part may vary over an order of magnitude during the coating process owing to the strong inhomogeneity of inter-particle forces in the granular packing. Our numerical tool can be used to assist — and partially replace — experimental investigations of the flowability and packing behavior of different powder systems as a function of material and process parameters.

Acknowledgments: We thank the German Research Foundation (DFG) for funding through the Cluster of Excellence "Engineering of Advanced Materials" and the Collaborative Research Center SFB814 (Additive Manufacturing). We gratefully acknowledge the computing time granted by the John von Neumann Institute for Computing (NIC) and provided on the supercomputer JUROPA at Jülich Supercomputing Centre (JSC).

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Poster 17 **Carlos Plana**

Numerical solution of population balance equations for liquid antisolvent precipitation of fenofibrate

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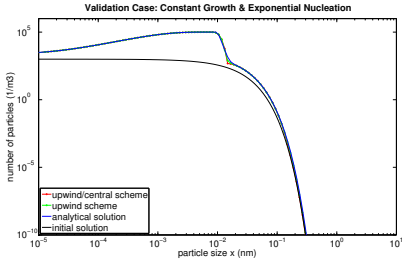
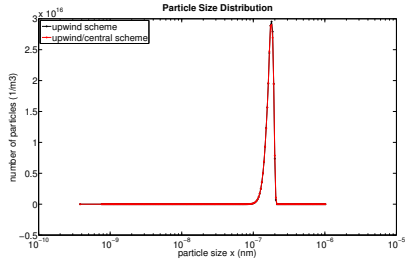


(a)



(b)

Figure 1: (a) Validation of the finite volume schemes, (b) Particle size distribution for negligible mixing time

The particle-size distribution of crystals is an important factor in the chemical and pharmaceutical industries. It is crucial in the manufacturing of pharmaceutical drugs because it affects key characteristics of the product such as specific surface area and bioavailability. A promising process capable of obtaining small

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monodisperse distributions in the nanometer range is liquid antisolvent crystallization (LAS). Here precipitation is induced by the addition of a second substance, the antisolvent, which is miscible with the solvent but has low solubility for the product. LAS is a fast process heavily influenced by the product concentration and the solvent composition, and so the mixing dynamics determine its efficiency and quality.

Our goal is to develop an accurate model of LAS of fenofibrate in a mixture of ethanol-water. For this purpose we combine theoretical derivation guided by experimental observations with efficient and accurate numerical solution of a 1-D Population-Balance Equation (PBE). The PBE is solved along particle trajectories obtained from a fully-resolved multiphase Direct Numerical Simulation of the mixing process. The PBE includes homogeneous nucleation as well as a growth term and reads:

$$\frac{\partial n(x)}{\partial t} = B_{\mathrm{hom}}(x, S, K_{sp}) - \frac{\partial [G(x, S, K_{sp}) n(x)]}{\partial x}, \tag{1}$$

where n is the number-concentration of particles of size x, B_{hom} stands for the homogeneous nucleation rate, S is the supersaturation, K_{sp} is the solubility constant and G accounts for the growth term. Both terms are influenced by the macroscopic state of the system through the solvent composition and the fenofibrate concentration [1]. This results in a strong coupling between the macroscopic variables and the crystallization terms through the mass balance equation.

The PBE was solved here by using a high-resolution finite-volume scheme in space (particle size) coupled with a semi-implicit method based on numerical differentiation formulas in time [2]. The scheme was tested against the literature [3] and validated against an analytical solution (see Fig. 1a). Finally, the results from the solution of the PBE were compared with those obtained with the simplified method of moments for the solution of the PBE and a simplified mixing model for the macroscopic fluid dynamics. Fig. 1b shows the particle-size distribution obtained from one such simulation.

Acknowledgments: We acknowledge funding from the Deutsche Forschungsgemeinschaft (DFG) through the Cluster of Excellence Engineering of Advanced Materials (EAM).

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Poster 18 **Hamzeh Pourtavakoli**

Granular dampers: Does the particle shape matter?

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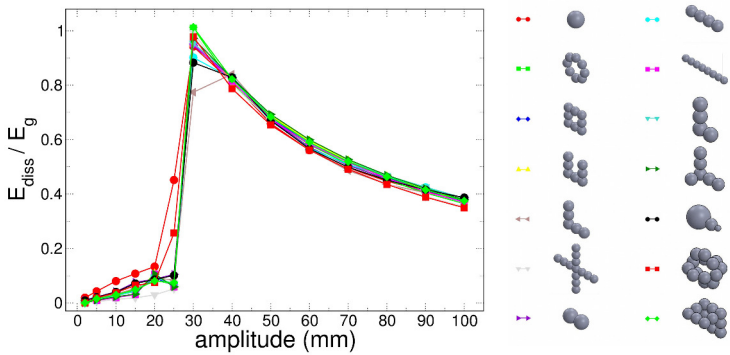

Figure 1: Non-dimensional dissipated energy per cycle of the damper oscillation. $E_{\rm diss}$ represents the average dissipated energy per period, while $E_{\rm g}$ denotes the value of $E_{\rm diss}$ corresponding to all particles colliding with the wall at maximum relative velocity (see Ref. [7]). The total mass of the granular material is the same in all simulations, for all particle shapes investigated. The parameters of the simulations, which are related to material properties, system size and oscillation dynamics are the same as in the experiments of Ref. [7].

Granular dampers — containers partially filled with granular material — are widely used as a means for attenuating mechanical vibrations in a broad range of systems. While the influence of material properties and particle size on the granular dampers' performance has been investigated in previous works (see, for instance, Ref. [1]), the role of particle *shape* on this performance has deserved much less attention. Indeed, it is well-known that dissipative properties of granular materials made of complex particle shapes may be very different from the ones of spherical particle ensembles [2, 3]. This different behavior raises the question of whether the particle shape could be used as an adjustable parameter for the optimal operation mode of a granular damper, depending on the practical

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application. Moreover, it is relevant to understand to which extent the particle shape may affect the performance of the damper.

By means of particle-based numerical simulations using the Discrete Element Method, here we address the question of how the performance of granular dampers is affected by the shape of the granular particles. Our simulations are performed under conditions of zero gravity, which corresponds to applications where granular dampers perform particulary well since gravity tends to demobilize the granulate ([4, 5]). Moreover, particles of complex geometric shapes are modeled using the multisphere method [6] as shown in Fig. 1. We find that the average energy dissipated per each cycle of the damper oscillation is independent of the particle shape, for given conditions of particle mass, material properties and number of particles (Fig. 1). In consistence with previous experiments [7], we find that the granular system is characterized by a gas-like regime for low amplitudes of the container's oscillation and by a collect-and-collide regime for intense forcing. Both regimes are separated by an optimal operation mode — the critical amplitude of the damping oscillation for which the energy dissipation is maximal — which is independent of the particle shape. The behavior of the system in the collect-and-collide regime can be described by a recently proposed effective one-particle model, which can be used to predict the dissipated energy as a function of the oscillation amplitude.

Acknowledgments: We thank the German Research Foundation (DFG) for funding through the Cluster of Excellence "Engineering of Advanced Materials" and the Collaborative Research Center SFB814 (Additive Manufacturing). We gratefully acknowledge the computing time granted by the John von Neumann Institute for Computing (NIC) and provided on the supercomputer JUROPA at Jülich Supercomputing Centre (JSC).

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Poster 19 **Stefanie Reuter**

Behavior of particle suspension flows subject to stochastic forces

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We describe a multiscale modeling and simulation approach to non-Newtonian fluid flow.

Our model is based on the asymptotic analysis of weakly inertial ellipsoidal particles in combination with a volume averaged description of particle suspensions. This leads to Navier-Stokes like equations with an additional particle stress tensor, which is characterized by stochastic Jeffery's equations.

We use our own finite element framework *Navier* to simulate the complete model. The involved particle stress tensor is computed on the microscale with a Brownian Configuration Field method, based on a Monte Carlo approach to solve stochastic differential equations, which describe the particle dynamics.

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Poster 20 **Stefan Romeis**

Deformation behavior of micron-sized polycrystalline gold particles studied by in situ compression experiments and frictional finite element simulation

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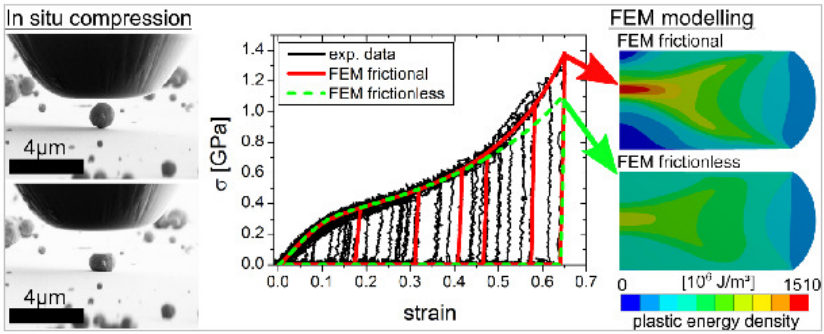

Within this contribution we present a combined experimental and finite element study on the deformation behavior of micron-sized polycrystalline gold particles which enables detailed insights into and a priori modelling of their deformation. In situ uniaxial compression experiments of the single spherical polycrystalline gold particles in the size range of 1μm were performed with a custom built manipulation device inside a scanning electron microscope. Stress-strain data and information on the particle morphology were obtained. Independent of particle size a well reproducible stress-strain behavior was observed. Furthermore, the particles showed a strain rate independent deformation behavior without plastic creep. Statistical significance was ensured by testing a large number of particles. The stress-strain behavior and geometric shape of the stressed particles was in good agreement with the elastic-perfectly plastic finite element model accounting for frictional effects at the contact interfaces. A significantly increased yield strength Y compared to bulk gold of 630 MPa was found. Grain size strengthening according to the Hall-Petch relation is assumed as the main hardening mechanism. The hardness H drops after reaching a maximum value close to

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$H = 2.8Y$ as prediction by Tabor. The strain dependence of hardness is related to the altered geometric shape of the deformed particles. Comparison to a frictionless finite element model revealed the necessity of considering the effect of friction: at small strains the particles appear softer due to a reduced dissipation of plastic energy, whilst at large strains the resistance to deformation is larger mainly due to the dissipation of frictional energy at the contact interfaces. These findings are not restricted to gold particles, but should be generally valid in case of elastic-perfectly plastic materials.

Poster 21 **Swati Sahu**

Lattice Boltzmann Simulation of a Reactive Flow in T-type micromixer

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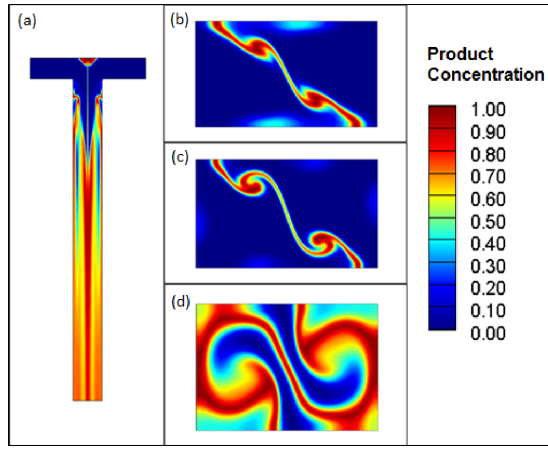

Figure 1: Product concentration profiles for the horizontal (X-Y) cross-section at (a) mid-height of the mixer (left panel), and for the X-Z cross sections of the mixing channel (right panel) at a distance of (b) 0.05mm (c) 0.1mm (d) 0.4mm from the back-wall of the inlet channel.

A three-dimensional simulation of the reactive fluid flow and its associated concentration fields in a T-mixer was performed using the models based on Lattice Boltzmann methods. The different flow regimes, namely, stratified laminar, vortex and engulfment regimes were studied by determining the concentration distributions of reactants and product. The creation of secondary flow patterns (vortex pair) at high Reynolds numbers significantly enhanced the reaction rates. The residence time distributions (RTDs) were used to characterize mixing

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at different Reynolds numbers in the T-mixer.

An experimental prototype of a T-mixer was fabricated and used for the measurement of pressure drops at different flow rates, and the validation of the model results. The results from the LBM simulations were also validated with the literature and found to be in reasonably good agreement. The study shows that RTD of the reactant and product species could be used to qualitatively characterize the mixing characteristic patterns at high and low Reynolds numbers in T-mixers.

Acknowledgments: The authors acknowledge the financial support of the Humboldt foundation.

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Poster 22 **Clara Sangros**

Implications of Hertzian-bond and elasto-plastic contact model on the granular fabrics of lithium-ion electrodes

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Lithium-ion batteries are the most popular rechargeable energy systems for portable electronics due to their high energy and power capability. Lithium-ion electrodes consist of porous composite materials (active material, conductive additives and binder) coated on a substrate. Recent work has demonstrated that the microstructural characteristics such as porosity, average particle size as well as particle size distribution and morphology have a great influence on battery performance.

Taking into account the intrinsic particulate nature of Lithium-ion battery electrodes, Discrete Element Method (DEM) simulations of micro-compression experiments are carried out in order to get a deeper look into the interactions between active material (graphite) particles. A very important aspect of DEM simulations is the suitable selection of a contact model since it has a great influence on the microstructure. In this study, two different DEM contact models are compared based on their prediction of the mechanical bulk behavior of an electrode. In particular, an anode composed of graphite particles (particle size distribution: 4-8 μm) and a total thickness of 50 μm.

The aim of this research is to compare an elastic-bond model with an elasto-plastic adhesive model in order to get a better understanding of the microscale behavior of an electrode. This examination leads to the establishment of a relation between the resulting granular fabric (microscopic level) and the macroscopic stress. The overall stresses are expressed in terms of contact forces in two different ways. The first one by statistical spatial averaging over sample volume (radially from the center of the indenter) and the second one by defining overall traction transmitted across in virtual axial layers. The results from this study will help to select a contact model that will describe the micromechanical behavior of the electrodes which will be useful to improve electrode design.

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Poster 23 **Fabian Schaller**

Locally densest packings of ellipsoids

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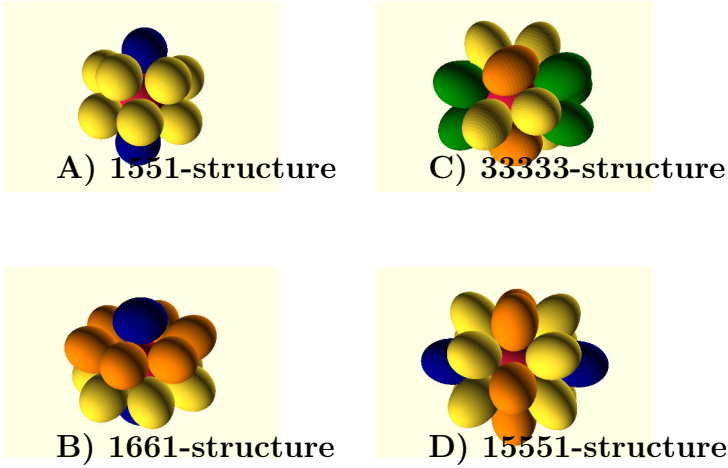

Figure 1: **A)** 1551-structure (Icosahedron) for spherical and almost spherical particles, **B) - D)** Densest structures for more aspherical particles.

Systems of jammed particles play an important role in granular matter, and the influence of the local structure to the global macroscopic properties is ongoing research. In the past universal scalings of local properties have been found for spheres [1–3] and some of them, like the scaling of the local packing fraction distributions, can be transferred to jammed ellipsoids [4, 5].

The local packing fraction can be higher than the globally densest packing, which is usually a crystal. For spherical particles, the locally densest configuration is an icosahedral cluster, about one percent denser than the crystalline fcc structure. The locally densest configuration is of relevance as a cutoff for scalings of the

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free volume distribution such as proposed by Aste et. al. [3] for jammed sphere packings. To extend this theory towards aspherical particles, the structure of the locally densest packing is crucial.

Here, we present a simulated annealing optimization method to find the locally densest configurations of prolate and oblate ellipsoidal particles. We consider a fixed central particle and its first shell of neighbors which are allowed to translate and rotate. The simulation minimizes the Set Voronoi cell volume [6] of the central particle in order to find locally densest packings.

We observe different structures for the densest packings depending on the aspect ratio of the particles, examples are shown in figure 1. A phase diagram of the different structures and their local packing fraction for the different aspect ratios is presented. Our densest configurations exceed the known-densest crystalline packings [7].

This work will help to extend existing theories for spherical particles to the non-spherical case.

Acknowledgments: We acknowledge funding by the German Science Foundation (DFG) through the research group "Geometry and Physics of Spatial Random Structures" under grant no SCHR-1148/3-2.

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Poster 24 **Tobias Schikarski**

Hydrodynamic mixing of miscible flows in a T-micromixer

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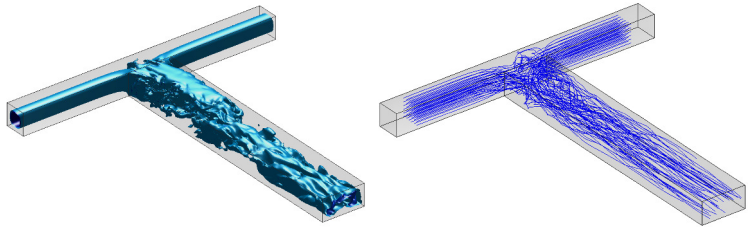

(a) Isosurfaces for $mag(u)$ and $Re = 1100$ (b) Particle trajectories for $Re = 1100$

Figure 1: Isosurfaces of the magnitude of the velocity (a) and particle trajectories (b) for Reynolds number $Re = 1100$ (water-water flow). The fluid motion is laminar at the inlet, becomes turbulent at the junction and then slowly relaminarizes toward the outlet.

Anti–solvent precipitation is a promising bottom-up process for manufacturing pharmaceutical drugs from nano–particles that precipitate in a microreactor. The quality of this chemical reaction is mainly determined by the efficiency of hydrodynamic mixing of two fluid streams, typically water and ethanol. We here investigate transition to turbulence of water–water and water–ethanol streams in a simple T–micromixer via Direct Numerical Simulation of the Navier–Stokes equations coupled with a convection–diffusion equation for the concentration. The coupling is two–way because the concentration determines the mixture's viscosity and density. In addition, we compute the concentration changes along particle trajectories and store these as input parameters for calculating the chemical reaction and resulting nano–particle size distributions.

Our goal is to investigate the hydrodynamic mixing of miscible flows in the range of operating conditions (Re up to 5000). Hence, using accurate numerical schemes and efficient algorithms for the mixture is particularly important and

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challenging. First, because of the strong dependence of viscosity and density on concentration, the Navier–Stokes equations and the convection–diffusion equation are strongly nonlinearly coupled. Second, water and ethanol have similar viscosities, but at 50% concentration the viscosity of the mixture is nearly three times higher than that of the pure components. This effect leads to qualitative changes in the fluid motion in regions of fully mixed fluids [1]. Finally, viscous momentum diffusion is much faster than molecular mass diffusion, which leads to very high Péclet numbers.

In this work we will describe the fluid motion and hydrodynamic mixing up to $Re = 2000$ and present relevant process parameters such as pressure losses, degree of mixing and turbulent statistics for the full domain and along particle trajectories (see Fig. 1).

Acknowledgments: We acknowledge funding from the Deutsche Forschungsgemeinschaft (DFG) through the Cluster of Excellence Engineering of Advanced Materials (EAM).

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Poster 25 **Philipp Schönhöfer**

Pear-shaped particles forming the gyroid in a solvent of hard spheres

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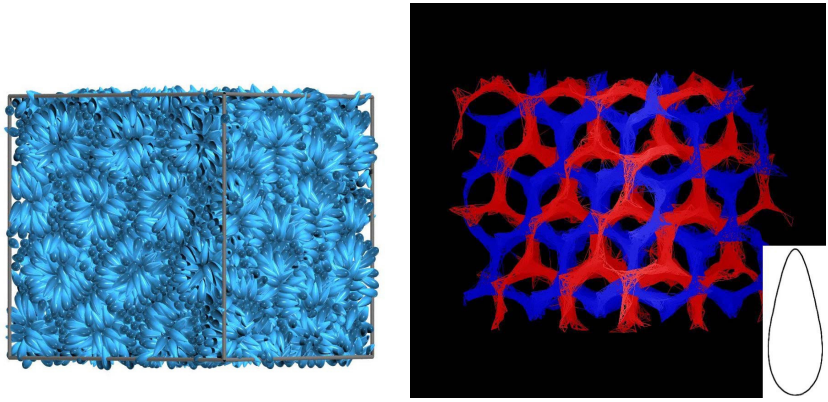

(a) (b)

Figure 1: (a) Snapshot of a system of tapered particles forming the *Ia3d* gyroid phase during the MD simulation [2]. The blunt ends are highlighted dark. (b) The gyroid network ocurrs after performing a cluster analysis on the configuration in (a) using the blunt ends of the particles. On the bottom right is the profile of a tapered particle used in the MD (k=3, k_θ=3.8) [2].

It is established that elongated liquid crystals like spherocylinders and oblate discs form phases in addition to the isotropic fluid and crystalline solid states [1]. These phases – like the nematic or smectic phase – are characterized by long-range orientational order.

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An auspicious system which forms highly complex structures is the packing of tapered or pear-shaped particles [2]. Some pears with suitable aspect ratio k and degree of tapering k_θ form the *Ia3d* cubic phase as shown in previous work (see FIG. 1a and FIG. 1b).

This structure can be reproduced by Molecular Dynamics simulations [2]. For this purpose a generalized Gay-Berne potential with a modified contact function σ is used [3]. It has to be considered that for tapered particles the length l and width d vary and are expressed as polynomials of $(\hat{r}_{ij} \cdot \hat{u}_i)$:

$$l(\hat{r}_{ij} \cdot \hat{u}_i) = a_{l,0} + \cdots + a_{l,n}(\hat{r}_{ij} \cdot \hat{u}_i)^n$$
$$d(\hat{r}_{ij} \cdot \hat{u}_i) = a_{d,0} + \cdots + a_{d,n}(\hat{r}_{ij} \cdot \hat{u}_i)^n$$

where $\hat{u}_i$ is the orientation and $\hat{r}_{ij}$ is the normalized distance vector between particle i and j. The amplitudes $a_{d,k}$ and $a_{l,k}$ are chosen such that they fit the Bézier-curve representing the pear best [3].

Figure. 1a shows a configuration of these simulations forming the complex phase between the isotropic and crystalline phase. Using cluster analysis on the blunt ends of the particles two seperate cluster systems become observable. Both cluster cross the whole system without connecting each other. The structure can be identified as the *Ia3d* cubic phase [2].

The next step is to introduce hard spheres within the simulation. These spheres will take up the role of solvent to model mixtures such as the lipid-water system. To that end, the potential between pears and spheres has to be modified again. With an explicit solvent the system should be complex enough to model most common phenomena in cubic phases yet simple enough to allow us to simulate large systems.

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Poster 26 **Christian Scholz**

FEM simulations of actively rotating granular particles

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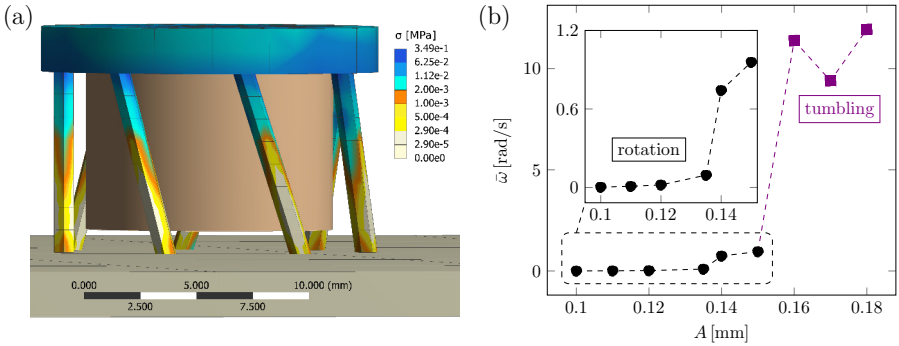

Figure 1: (a) Local stresses acting on the particle during vibrational excitaton, obtained from FEM simulations. (b) Rotational velocity ω of the particles in dependence of the excitation amplitude A for a fixed frequency of $f_D = 50\,\mathrm{Hz}$.

Particles that perform active motion store and convert energy in internal degrees of freedom to perform a locally directed motion. Here we study actively rotating granular particles using finite element simulations. Such particles, as introduced in [1], convert vibrational motion into rotational motion via tilted elastic legs in a circular arrangement at the bottom of the particle, when excited by vertical vibrations. We reproduce the motion of the particles quantitatively for realistic material properties. For small excitation amplitudes a regime of slow rotation is found and for large amplitudes a tumbling regime, where the particle start to perform a precission and overall a much faster rotation. The threshold for this transition depends significantly on the material parameters, in particular the elastic modulus of the legs.

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Poster 27 **Cristian Soitu**

Evaluating a novel particle-based method for mesoscopic computational fluid dynamics

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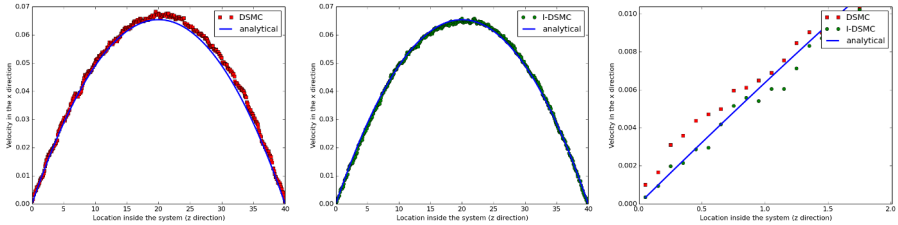

(a) Velocity profile for DSMC (b) Velocity profile for I-DSMC (c) Velocity near the boundary

Figure 1: Plot 1a illustrates the pronounced grid artifacts in DSMC due to the strong correlations between the velocities of particles in the same cell, whereas 1b shows that in I-DSMC this effect is not present. In the last plot, 1c, it can also be observed that the velocity near the boundary follows more accurately the analytical profile in the case of the I-DSMC simulation.

Direct simulation Monte Carlo (DSMC) is one of the oldest and still most powerful particle-based methods and is generally viewed as a numerical solver for the Boltzmann equation for a low-density gas. We describe the implementation details of a variant of DSMC as proposed by Donev et al. [1] which is suitable for denser fluids and eliminates the grid artifacts in the original method.

The resulting method termed isotropic direct simulation Monte Carlo (I-DSMC) is Galilean invariant as a fictional interaction range is used, leading to a spherical neighborhood instead of cuboidal collision cell typically employed in DSMC. As the dependence of the I-DSMC collision kernel on the relative velocity of potential collision partners ($K_c = 3\bar{v}_{rel}/4$) necessitates the search for the maximum velocity in the local neighborhood, the original paper estimates a decrease in

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efficiency of a factor of 2-4 compared to DSMC. However, our results show a satisfactory decrease in efficiency of only a factor of 1.5, attributed to the building of the neighborhood list required by the isotropic interaction kernel.

As a first practical example a Poiseuille flow is simulated and the results obtained are compared with those of a DSMC simulation. We find that, although less efficient, I-DSMC behaves more accurately: First, as expected, the grid artifacts are completely eliminated. Second a significantly better agreement with the analytical solution next to the wall is observed. Furthermore, we compare our results with the ones obtained by Bolintineanu et al. [2], where several variations of no-slip boundary conditions for multi-particle collision dynamics (MPCD) are evaluated. We show that I-DSMC generates similar results with no need for the complex treatment of domain boundaries required for MPCD.

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Poster 28 **Robert Stepic**

Binding of amino acids to bioactive surfaces of calcite

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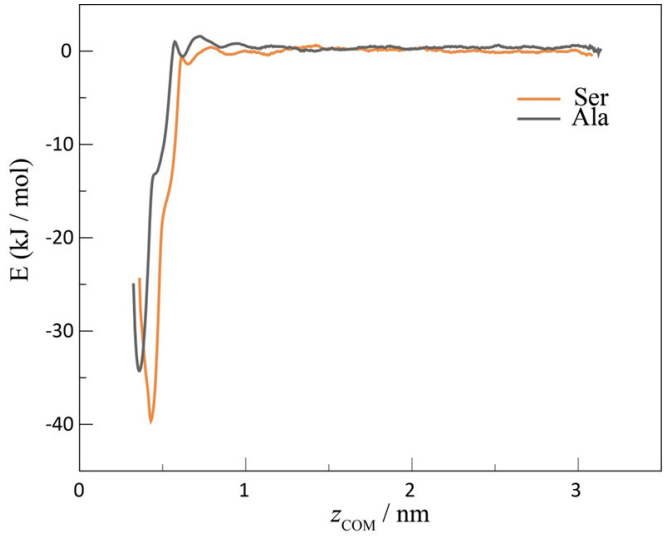

Figure 1: An example of the resulting free energy profiles for binding of amino acids serine and alanine.

Biomineralization is a process of inorganic crystal growth in the presence of biomolecules, most commonly proteins and polysaccharides, which produces crystals with vastly different properties compared to their inorganic counterparts. These environmentally friendly biominerals have a wide range of potential applications, so understanding the process of their growth on atomic level has become an imperative of many researchers in recent years [1]. In this work we focus on studying interactions of elementary protein building blocks, amino acids, with

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two important surfaces of calcite [2,3], the stable (104) surface and the growth (001) surface. We use fully atomistic molecular dynamics simulations coupled with enhanced sampling techniques in order to obtain free energy profiles for binding of various amino acids to the surfaces (Figure 1). This gives us not only the free energies of binding, but also different geometries and effective rates of binding. It is shown that amino acids with polar and charged side chains interact more favourably with the surfaces. Insights from this work might prove useful in identifying amino acids in peptides and proteins which play an important role in the mechanism of biomineral formation.

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Poster 29 **Martin Tupy**

Simulation of drying processes in nanoparticulate layers

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Particle laden processes are used in many areas of today's industry, however, only recently became of interest in the production of electronic devices. Printed electronics and coatings offer fast and cost-efficient alternatives to the long established processes. Different techniques are available to deposit colloidal suspensions on substrates, such as dip coating or convective particle assembly [1, 2]. There, it can be observed that different processing setups can introduce defects such as pores or cracks. Therefore, an understanding of the dynamics of particle suspensions during the transition from a fluid-like to a solid-like behavior is of great importance. It has been found that the initial configuration of the colloidal film regarding the particle positions as well as the distribution of the fluid in the film has great influence on the final dry structure.

A multiphase model has been developed capable of representing the dynamics of drying colloidal films. The particle dynamics are described by a force-based molecular dynamics algorithm. The liquid phase is modelled as capillary bridges between the colloids [3], thus, acting as forces in addition to the particle-particle interaction. This system is embedded in a finite difference framework handling the vapor phase by solving the diffusion equation on a coarse lattice with respect to different boundary conditions and distributed system variables needed for the evaporation process. The initial configurations are obtained with the help of the steepest descent ballistic deposition algorithm [4].

In this contribution the model is described and structure formation in colloidal films is studied with varying initial conditions depending on the distribution of particles and liquid in the film.

Acknowledgments: The authors thank Tobias Kraus for his suggestions and inspiring discussions. Moreover, the financial support through the Research Training Group 1161/2 'Disperse Systems for Electronic Applications' and the Clus-

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ter of Excellence 'Engineering of Advanced Materials' is acknowledged.

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Poster 30 **Tobias Wollborn**

Agglomerate breakage behavior in ultrasound agitated gaseous environments

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Agglomeration and dispersion of solid particles play an important role in many industrial processes. On the one hand agglomeration is desired for better transportation properties, on the other hand the existence of agglomerates is obstructive for further processing, like in mixing processes. An ultrasound agitated gaseous fluid is used to control the agglomeration by dispersion. The dispersion is performed in an indirect way by accelerating the agglomerates in the agitated fluid. Agglomerate breakage occurs by agglomerate-agglomerate and agglomerate-wall impacts. For a better understanding of the dispersion behavior, breakage of single agglomerates is investigated using the Discrete Element Method (DEM). Agglomerate compression and impact simulations are carried out using a Stiff-Bond-Modell and a simplified JKR model in a DEM software. The bondings between agglomerates are represented by the presence of solid binder (PVP, CMC). Bond breaking occurs by reaching the limit of the normal and tangential strength, which is based on the tensile strength of the binder material. The properties of the agglomerate are changed by varying primary particle size ($d_P = 30 - 250\mu m$), mixing ratios and structure by using different agglomerate designs. The simulation results are compared to agglomerates bonded by the classical JKR model. Validation of the simulation results is performed by the experimental investigation of the breakage behavior of solid particle agglomerates by compression and agglomerate-wall impact within the velocity field reached by indirect dispersion in an agitated gaseous environment.

Acknowledgments: The project is embedded into the SPP 1486 PiKo "Partikeln im Kontakt"which is funded by the German Research Foundation (DFG).

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Poster 31 **Philipp Kanehl**

Dense colloidal suspensions in microfluidic flow: size segregation and velocity oscillations

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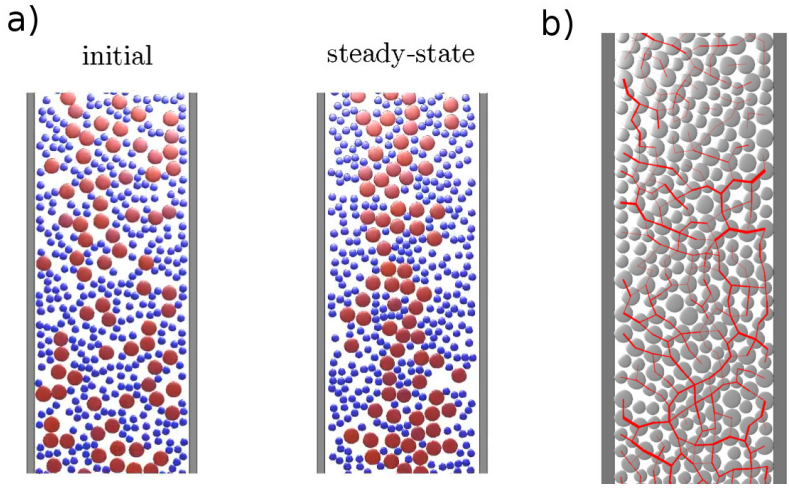

Figure 1: a) Steady state size segregation of particles with size ratio 2 in comparison to the initial mixed state at area fraction $\phi = 0.5$. b) Force chains inside a jammed colloidal network ($\phi = 0.8$) imminent to an unjamming rarefaction wave.

Colloids in suspension exhibit shear-induced migration towards regions of low viscous shear. In dense bidisperse colloidal suspensions under pressure driven flow large particles can segregate in the center of a microchannel and the suspension partially demixes [1]. In mono disperse suspensions, if the density is increased further, regular oscillations in flow velocity emerge [2].

To develop a theoretical understanding of these effects, we simulate hard spheres under pressure-driven flow in two and three dimensions using the mesoscale simulation technique of multi-particle collision dynamics. Generalizing an existing phenomenological model [3] to binary suspension, our theory accurately reproduces the segregated density profiles across the channel from our simulations.

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We present a detailed parameter study on how a monodisperse suspension enriches the channel center and quantitatively confirm the experimental observation that a binary colloidal mixture partially segregates into its two species [4]. In particular, we always find a strong accumulation of large particles in the center. Moreover, first results on velocity oscillations in suspensions near random close packing are presented. By analyzing our numerical data, we address the role of fluid permeation, colloidal friction, and channel confinement.

Our work was supported by the Deutsche Forschungsgemeinschaft (DFG) through the research training group GRK 1558.

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	Monday, Sept. 21st	Tuesday, Sept. 22nd	Wednesday, Sept. 23rd	Thursday, Sept. 24th
08:50 - 09:00	welcome note			
09:00 - 09:45	Holger Stark	Hans Kuipers	Stefan Sokołowski	Uhlmann Markus
09:45 - 10:05	Michael Engel	Severin Strobl	Nikola Topic	Stefan Liebenstein
10:05 - 10:25	Maarten Wouters	Raphael Münster	Stanislav Parez	Johan Gaume
coffee break				
11:00 - 11:45	Dietrich Wolf	Fathollah Varnik	Ken Kamrin	Marcus Bannerman
11:45 - 12:05	Matthias Sabel	Sebastian C. Kapfer	Hadi Mehrabian	Maksym Dosta
12:05 - 12:25	Matthias Markl	Eric Opsomer	Davod Alizadehrad	Timo Bihr
lunch break				
14:30 - 15:15	Dan Negrut	Charles Radeke	Jens Harting	Martin Sommerfeld
15:15 - 15:35	Sebastian Borrmann	Anton Gladky	Simon Bogner	Denis Davydov
15:35 - 15:55	Baofang Song	Jia Xiaodong	Georg Hammerl	Sebastian Pfaller
coffee break				closing remarks
16:30 - 17:15	Stefan Heinrich	Frederic Dubois	Holger Steeb	
			poster award presentation	

Sunday, Sept. 20th
18:00-21:00

welcome reception

18:00-21:00

poster session
&finger food

18:00-22:00

conference
dinner


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