Minutes

EFCE Working Party Mechanics of Particulate Solids Workshop on Discrete Element Modeling
5th International Conference for Conveying and Handling of Particulate Solids

30 August 2006, Sorrento, Italy

Chairmen

Prof. S. Luding,	TU Delft, NL
Prof. J. Ooi,	U Edinburgh, UK
Prof. U. Tüzün	U Surrey, UK

Participants

The workshop was attended by a total of 32 people. See enclosure 5.1 for a list of participants.

1 Introduction

The WPMPS workshop is intended to increase the acceptance of DEM-codes for simulation of bulk solids behavior. This requires the codes to be validated, which in turn needs carefully selected problems with a good experimental database for test runs. The workshop shall help to identify a suitable set of problems for the quantitative validation and verification of DEM type models in the area of bulk solids handling.

Participants were invited to the workshop through the conference organizers, publications in the official EFCE journal "Chemical Engineering Research and Design" and in various other scientific journals, through email distribution lists and by direct invitation. The official announcement can be found in Enclosure 5.2.

The workshop was structured by the chairmen to have an initial session of short presentations by various participants, followed by a discussion in the plenum and a subsequent split into three working groups. A wrap up session served for the working groups to rapport their findings.

2 Short Presentations

Prof. Luding started the short presentations with an introduction into the 3 general areas of the themes:

1. Generic simulation of lab scale experiments
2. Large scale storage, conveying and handling applications
3. Multiphase processing of powders and particles

and an overview of presentations given at the conference related to DEM work. He showed that the main theme of these talks had been contact models but also large scale (hybrid) simulations and parameter identification, see Enclosure 5.4, page 9.

Dr. Feise introduced the DEM activities at BASF. He listed the identification of DEM model parameters from independent bench scale tests and the coupling of fluid – particle flow as the areas most urgently needing to be developed for industrial use of DEM tools, see Enclosure 5.5.1, page 11.

Dr. Theuerkauf showed selected samples of DEM work at Dow. So far simulations were run on shear testers, storage in silos, screw conveyers, mixers, packing structure, material testing, pneumatic conveying/fluidized beds. He posed two main questions. The first dealt with the level of complexity needed to capture the physics of the real system in the DEM simulation. For a shear tester they were able to show that various codes give similar results. He also called for a *User norm/guide "DEM101" the unique calibration parameters and procedure* to allow users to get reliable parameters estimates to use in their simulations, See Enclosure 5.5.2, page 14.

Prof. Ooi presented slides from Dr. Ramaioli, Nestlé, who was not able to attend. Dr. Ramaioli explains that Nestlé sponsors a PhD-project at EPFL with the purpose to generate a tool useable to simulate the behaviour of beverage powders in dispensers. He stresses that validation needs to be done not only for shear tests but also concerning the effects of vibration and segregation. The limitations of DEM seen by Dr. Ramaioli center around the very few real validations, the lack of a procedure to gather grain properties for the simulation and over-simplified models, see Enclosure 5.5.3, page 18.

Dr. te Kamp introduced the background of the ITASCA company to the workshop. ITASCA is traditionally a geotechnical company which focuses their work in chemical engineering on Storage, Conveying, Dosing, Agglomeration, Tableting, Sorting and Blending. Dr. te Kamp sees the keys to wider acceptance in industry as a) Validation of the DEM: run selected problems with good experimental backup, numerical prove of concepts and b) Definition of standards, e.g. influence of model setup. He pleads that researchers and software vendors strongly depend on the input from industry and the community needs to identify a few selected problems and validate DEM in order to spread the use of this engineering tool, see Enclosure 5.5.4, page 20.

Dr. Favier presented the EDEM software to the workshop. He announced that the EDEM code is available as a coupled plug-in to Fluent since June 2006. He stressed that integration with other CAE tools is advancing and will widen the use of DEM and this will be the main driver in the near future. To his understanding the challenges for industrial application of DEM are in the establishment of benchmarking for DEM codes, meaning validation against standard tests, relate DEM model to continuum model benchmarks, relate DEM simulation to alternative techniques, and the set-up of reference points for the "layman, see Enclosure 5.5.5, page 27."In any case more than one test will be required to generate the data needed to determine the DEM model parameters.

Dr. Gröger showed how various micro and macro parameters are connected. To get a well defined set of parameters, simple experiments that can easily be simulated need to be developed. This is paramount since the determination of parameters though an optimization of the simulation of a complex experiment leads to an inverse problem, where no unique solution is available; i.e. the results are never known to be right; see Enclosure 5.5.6, page 35. Nevertheless, T. Gröger showed that the concept of validation experiment vs. simulation is feasible. He could even show some first successful attempt of using this concept.

Dr. Tijskens showed examples of a successful joined project with DEM and experimental work in agricultural engineering. He sees a major difference between DEM and the much more mature FEM in the realism build into the tool. He stresses that computational cleverness allowing e.g. large problems to be solved, is no substitute for physics. Therefore efforts need to be made to tackle modeling questions such as shape, contact laws and calibration or optimization algorithms, see Enclosure 5.5.7, page 38.

In the discussion following the short presentations several points from the presentations were reinforced. Prof. Rotter emphasized the need of good reference experiments. He called for element tests which provide reliable and reproducible calibration results. Comparisons were drawn to the Caltech workshops for fluid mechanics in the 1970's which provided a range of good case studies for similar work in CFD. The need to bring fluid and particle fluid interaction effects into DEM as specifically stressed by Prof. Levi, see Enclosure 5.5.8.

3 Work Group Results

3.1 Micro - Testing

A work group discussed the options concerning testing on the particle scale. The group's results were reported by Roger Place , see Enclosure 5.3.1. A large number of different methods have been used to characterize particles with the purpose of using this information in DEM modeling. The paramount parameter is particle size. Here compromises are needed. Generally it seems to be more important to represent the width of the particle size distribution that the actual size. This is most significant in 2D – modeling. The next most significant parameter is shape which is most often represented by particles made up of overlapping spheres. Some efforts are made to represent very irregular particles by triangular sections.

Contact parameters can be measured using atomic force microscopy. The technique can handle particle - particle contacts for particles below 30µm. Similar tests are known for large granules (> 500 µm). In any case the experimental data does exhibit a huge amount of scatter. The correlation between particle and particle interface properties and the DEM contact parameters is know established yet.

3.2 Small Bulk Testing

A work group discussed the options concerning testing on the small bulk scale. The group's results were reported by Jörg Theuerkauf , see Enclosure 5.3.2. The group discussed the various testers available in the community. Testers generally fall into two groups: a) more or less well instrumented shear testers and b) testers mimicking some particular process. The first can possibly be used to measure the response of the bulk material to contact friction dominated motion. Other tests will be needed to supplement them such that all modes of interaction of moving particles with each other and the confining equipment can be captured.

The second area of concern is the reproducibility of bulk tests. Bulk solids experiments generally suffer under a large variability with differences of 40% between runs being not uncommon.

3.3 Multi – Phase Flow

A work group discussed the options concerning multi phase flow. The group's results were reported by Avi Levy, see Enclosure 5.3.3. Multiphase flows may be observed in many industrial applications. Traditionally the two-fluid model is being used to simulate the fluid-solid interactions. In the last decade DEM has been developed and significantly improved to simulate granular flow where the influence of the fluid phase can be neglected. However, neglecting the interstitial fluid effect on the granular phase can't be justified especially when transitional granular flow is observed.

Combining CFD & DEM software is an important task; however, some questions about the phases' coupling, i.e., the physics coupling verses the software coupling, should be addressed. Points of concern are: grid, particle sizes and distribution, particle shape, phase coupling, coupling models, boundary conditions and validation.

4 Steps forward

To make the DEM validation effort viable, project funding from outside the participants organizations will be needed. Dr. te Kamp suggested that contacts to the project funding body at Jülich could be used. Jülich provides a 50% funding and traditionally has a lack of good project proposals. He will initiate contacts.

Dow and BASF have contact people for European Research funding. A meeting shall be organized (e.g. in Brussels or in Delft) to evaluate the possibilities of a European funded project with the subject of DEM validation. For this an experienced partner will be needed to be able to generate a successful project proposal.

A second workshop will be held during PARTEC 2007 in Nürnberg, Germany. Contacts between Prof. Peukert, the PARTEC 2007 chair and Prof. Luding have already been established.

5 Enclosures

5.1 List of Participants

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5.2 Workshop Announcement

EUROPÄISCHE FÖDERATION FÜR CHEMIE-INGENIEUR-WESEN
EUROPEAN FEDERATION OF CHEMICAL ENGINEERING
FEDERATION EUROPEENNE DU GENIE CHIMIQUE

EFCE

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Chairman of the EFCE Working
Party Mechanics of Particulate Solids

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2006-04-10 / Fe

EFCE Working Party Mechanics of Particulate Solids to run Workshop on Discrete Element Modeling at the *5th International Conference for Conveying and Handling of Particulate Solids*

Discrete Element Modeling (DEM) is currently been used extensively in bulk solids handling research. Therefore the EFCE Working Party Mechanics of Particulate Solids (WPMPS) has joined forces with ChoPS-05 to make DEM one special focus during the conference in Sorrento. ChoPS-05 will have two regular sessions, a poster session and a plenary lecture by *Prof. Stefan Luding, TU Delft* devoted to DEM. In addition WPMPS will run a workshop on DEM co-chaired by Profs. S. Luding (Delft), J. Ooi (Edinburgh) and U. Tuzun (Surrey) during the conference. Both the plenary lecture and the workshop will take place on Wednesday August 30th, 2006.

The WPMPS workshop endeavors to increase the acceptance of DEM codes for simulation of bulk solids behavior. This requires the codes to be validated, which in turn needs carefully selected problems with a good experimental database for test runs. The workshop is intended to help identify a suitable set of problems for the *quantitative validation and verification of DEM type models* in the area of bulk solids handling. The workshop will commence with introductory presentations on the issues and methods relating to validation currently used in chemical, mining and agricultural engineering and physics research, as well as in industry. This will be followed by a discussion session by all workshop participants.

The workshop shall produce a framework for engagement between academic researchers, professional software companies and potential industrial beneficiaries of DEM numerical simulations that will identify areas that need significant further development both in terms of computational methodologies as well as the experimental validation procedures. It is hoped that in the longer term, the group of researchers brought together for the event will form the nucleus of a wider project formation aimed at setting the European/International standards of "best practice" in DEM Simulation software development and implementation in a broad range of industry sectors.

The EFCE Working Party Mechanics of Particulate Solids invites the scientific community to join the Workshop on DEM simulation of bulk solids behavior and would encourage participation in ChoPS-05. The workshop chairmen and Dr. H. Feise (hermann.feise@basf.com), chair of EFCE working party Mechanics of Particulate Solids, welcome all further enquiries in connection with attendance at the DEM workshop.

More information on the congress is available at http://www.ortra.com/solids/. Information about the EFCE Working Party Mechanics of Particulate Solids can be found at http://www.efce.info/wpmps.html

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5.3 Work Group Results

5.3.1 Standard calibration methods – Micro Properties (Roger Place)

Micro Testing – DEM Breakout Group (Rapporteur: Roger Place)
Micro = Particle scale

Bulk powder model parameters need to be accessed / developed from individual particle characteristic measurements

- Contact parameters
  - Both particle/particle and particle/wall
  - stiffness
    - Plastic/Elastic/Viscoplastic
  - Damping/Restitution
  - Interparticle forces
- Roughness
- Size/Distribution
- Shape/Distributionn (need to know how this will be used)
    - ie what properties will be derived
    - collisions
    - moment of inertia
- Density

Techniques available to measure individual particle characteristics (In increasing order of difficulty)

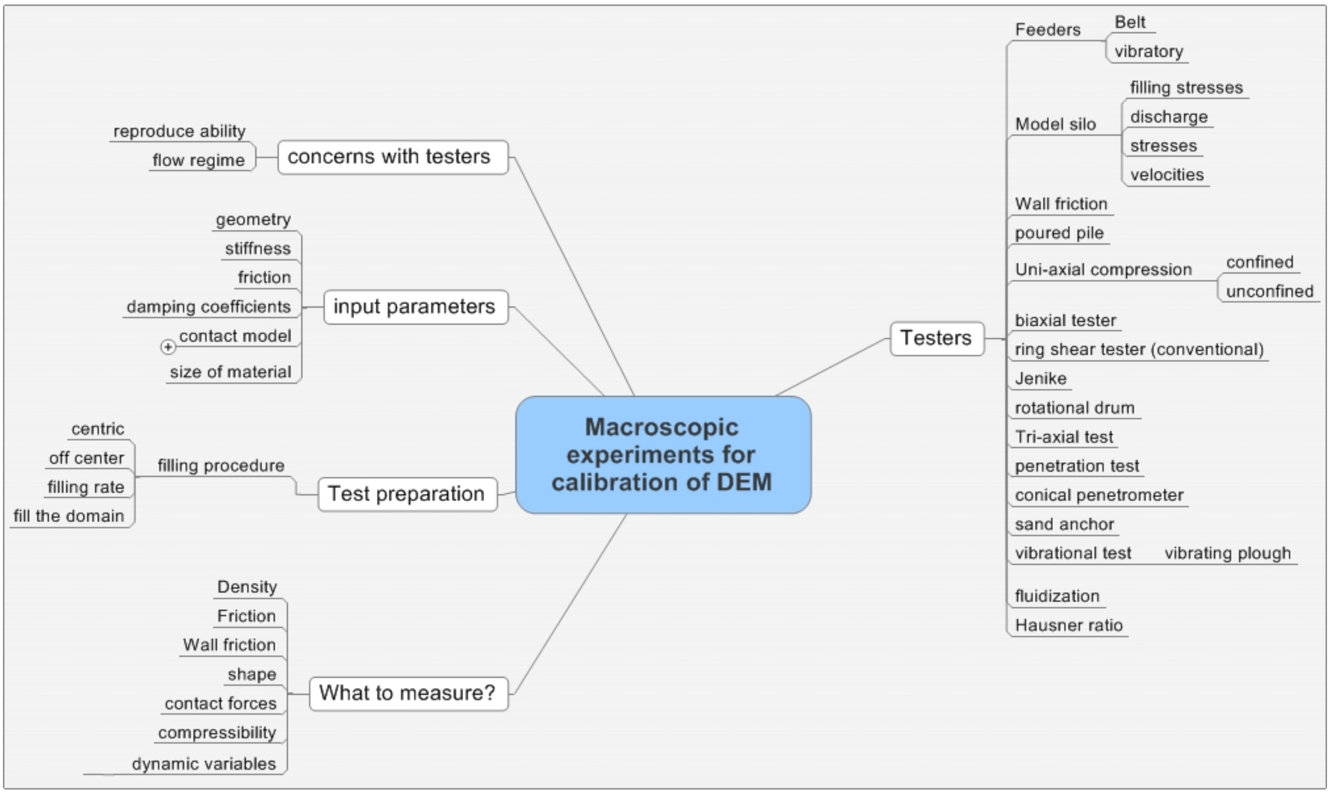
- Densities – OK
  - May need to account for distribution of densities and e.g. porous particles
- Size / size distribution
  - Many techniques
  - If very wide distribution when can fines be neglected
    - with volume diameter they have little mass but present in large numbers
- Shape / distribution
  - can be measured – both 2D & 3D
  - how to represent in models
  - can already handle sphere/sphere and sphere/plane collisions
  - can track position and orientation of all particles
  - should therefore be able to model particle shape through clumped spheres
    - BUT what if multiple contact sites?
  - handle distribution with radius frequencies function
    - OR library of individual particles?
  - what level of detail required
    - surface asperities (effect on interparticle force)
    - roughness – effect on friction

Contact parameter

  - Friction
    - Use AFM in lateral surface measurements
    - Scatter in results very large even making repeat measurements at same point.
  - Roughness
    - Can measure but do not know how to relate to friction
  - Adhésive forces – (AFM in vertical mode)
    - non reproductible
  - Damping /Coefficient of Restitution
    - Can measure by dropping spherical particle (> 1 mm) on to plane surface
    - Non spherical particles???
  - Stiffness
    - micro indentation or compression tests can be used to characterise particles down to ca. 1 mm.
    - Need to check if properties are isotropic.
- Conclusion
  - There are big gaps in the ability to
    - measure and represent relevant individual particle characteristics
    - relate micro properties to bulk powder flow parameters

Afterthoughts
The group did not include fluid particle interactions.
Peukert plenary indicates understanding in micro to macroscales is developing.

5.3.2 Standard calibration methods – Bulk Properties (Jörg Theuerkauf)



5.3.3 Multi phase systems (Avi Levy)

Comments on CFD-DEM coupling that rose during the DEM workshop in CHoPS 2006, Sorrento Italy.

Multiphase flows may be observed in many industrial applications. Traditionally the two-fluid model is being used to simulate the fluid-solid interactions. In the last decade DEM has been developed and significantly improved to simulate granular flow where the influence of the fluid phase can be neglected. This simplifies the modeling and simulations of many processes. However, neglecting the interstitial fluid effect on the granular phase can't be justified especially when transitional granular flow is observed.

Combining CFD & DEM software is an important task; however, some questions about the phases' coupling, i.e., the physics coupling verses the software coupling, should be addressed. In the following sections, some of the questions, which were raised by the multiphase subgroup, are presented.

- Grid

The mesh size of the computational domain has a very important role in CFD software. Coarse grid usually engulfs some physic's phenomena and the code convergence might become questionable. Therefore, in many CFD applications very fine grid is used especially to describe boundary layers and flow areas with large gradients. This contradicts the basic DEM assumption, where each computational cell should include at least few particles. This question needs, yet, to be answered. How coarse the computational grid can be without altering the characteristics of the flow fields, i.e., fluid & solid flows behaviors.

- Particle sizes and distribution.

Particle sizes and distribution might be an important parameter for choosing the optimal grid size, and modeling interaction terms between the particles and the fluid phase (e.g., mass, momentum and heat transfer).

- Particle shapes.

Particle shapes have a major effect of the flow characteristics and the interaction between the different phases. How can one calculate a drag force, or particle rotation for non-spherical particle in a specified grid? Using various shape factors, as it is often used in the two-fluid model, is simple but it is also questionable. Doesn't it alter the flow behavior?

- Phases coupling.

Coupling between the phases, in addition to the particle-particle & particle-wall interactions, results in higher computational efforts. This should be considered while developing software.
What is the right order for solving the conservation equations and implying the transfer terms?

- Coupling models.

What is considered to be the right or the best way to describe the forces between the phases? Which forces, except drag, should be considered? How does it influence the turbulence? Can it be neglected? How to overcome the influences of the coarse grid on the turbulence models? How to implement heat and mass transfer between the phases?

- Boundary conditions.

What are considered to be the proper boundary conditions for CFD-DEM simulations?

- Validation.

Validating the predictions of a numerical simulation is a very hard task. The simulation always produces more data then any one can get out of an experimental study. Standard test cases should be defined for validating multiphase flow problems. These cases should be validated experimentally, and later on, they should be used as a testing point for all the developed software.

In conclusion, the multiphase discussion group believes that the open questions mentioned above, together with many others questions, should be addressed and might be used as a starting point for many investigations in the near future.

Noted by: Avi Levy

5.4 Introduction by S. Luding, TU Delft

CHOPS-05 DEM talks

Contact models (III3):

- sticky contacts (I2,I3)
- frictional contacts (I2,I3)
- rolling- and torsion (I2,I3)
- long-range forces

FEM/CFD macro-models (III1):

- an-isotropy (...)
- micro-polar (rotations)

CHOPS-05 DEM talks

Parameter Calibration (III2,III3)

Elementary tests (I1,II1,II3,III3)
Applications (II2,II4,III1,III4)

Various particle shapes (III2)

Wide size distributions

WPMPS Workshop (Wednesday 10:40) Discrete Element Modeling/Validation

- Introduction to the workshop

A) Generic sim. of quasi-static shear, compression/tension

B) Large scale storage, conveying and handling applications

C) Multiphase processing of powders and particles

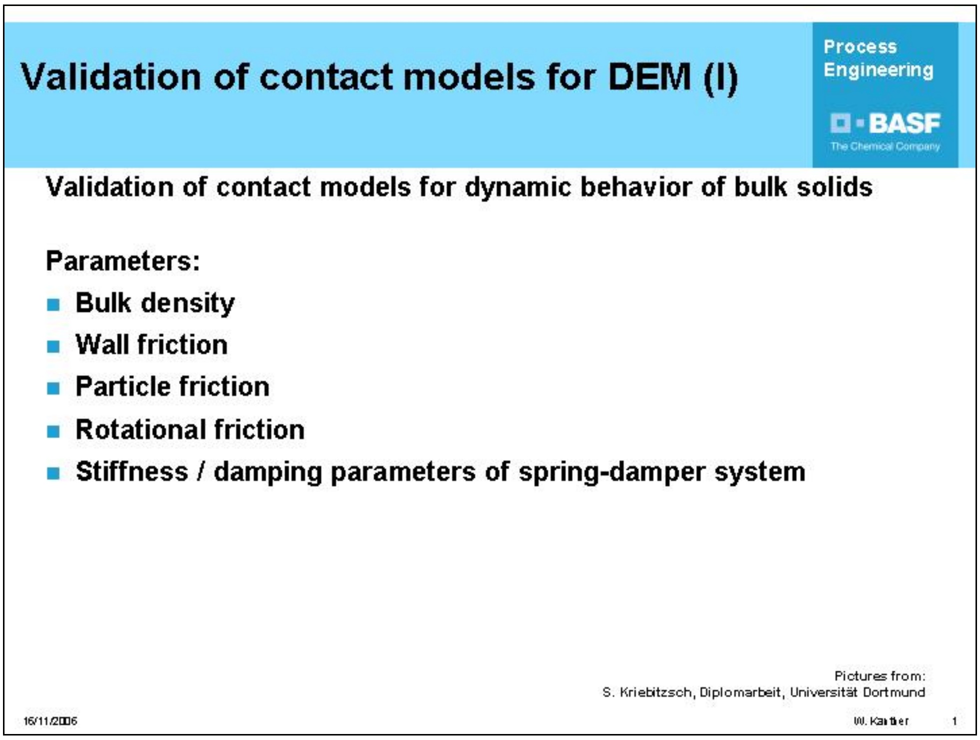
- Compilation/Conclusion/Further Steps

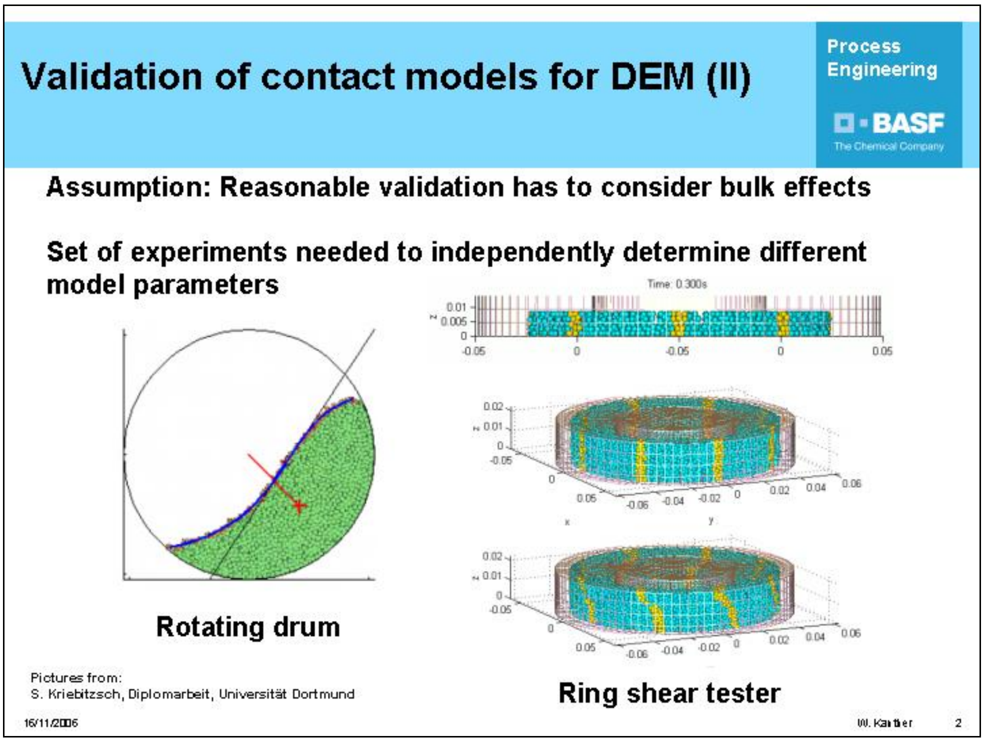
WPMPS Workshop (Wednesday 10:40)

- Hermann Feise, BASF
- Joerg Theuerkauf, DOW
- Jin Ooi (representing NESTLE)
- Lothar de Kamp, ITASCA
- John Favier, EDEM Solutions
- Torsten Gröger, Consultants
- …

5.5 Short Presentations

5.5.1 H.J. Feise, BASF





CFD/DEM for multiphase flows (I)

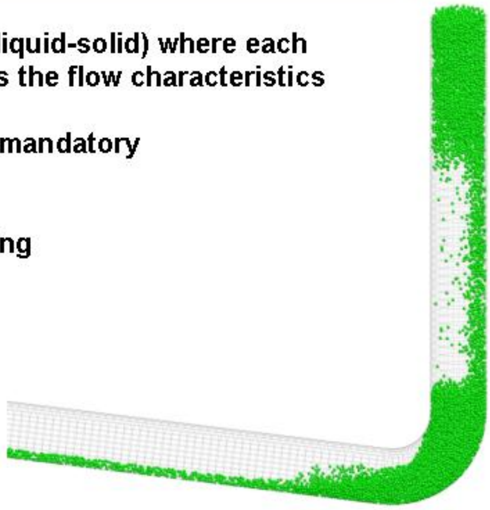
Process Engineering

BASF The Chemical Company

Scope:
Multiphase flows (gas-solid, liquid-solid) where each phase significantly influences the flow characteristics of all other phases
Two-way (4-way) coupling is mandatory

Example: Pneumatic conveying
Subjects of interest:

- **Product flux**
- **Pressure drop**
- **Prediction of flowability**
- **Prediction of flow regime**



Calculation: S. Götz, Universität Dortmund

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CFD/DEM for multiphase flows (II)

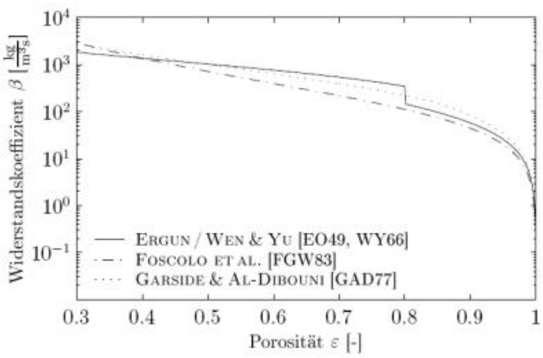
Process Engineering

BASF The Chemical Company

Validation procedure for drag models needed

Critical aspects:

- **Nonspherical particles**
- **Size distribution**
- **Swarm effects**
- **Cohesion**



Diss: S. Götz, Universität Dortmund

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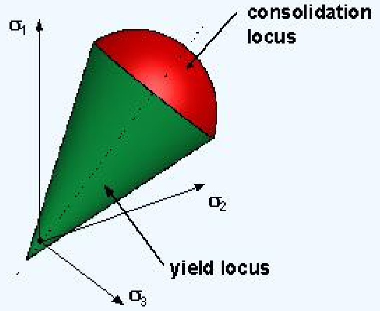
FEM for Bulk Research (I)

Process Engineering

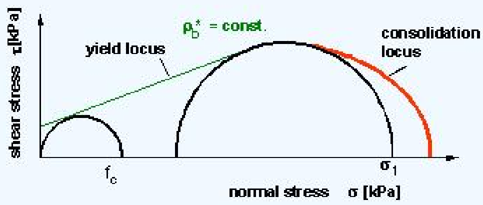
BASF The Chemical Company

The Drucker - Prager - Model as basis for the FEM-simulation



Drucker - Prager - Model with contractive flow on yield cap

- dilatant flow on yield cone
- contractive flow on yield cap
- tensile strength



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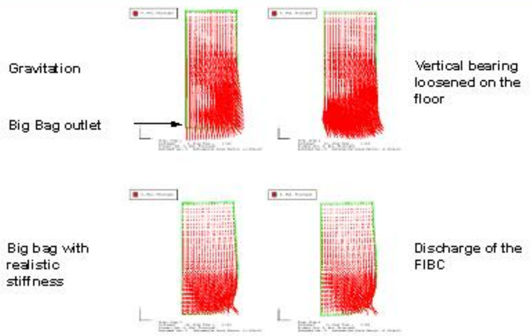
FEM for Bulk Storage Research (II)

Process Engineering

BASF The Chemical Company



- **Lab tests with Fine Dolomite**
- **First simulations**
- **Lab tests with additional cohesive products**
- **Verification in large scale tests**
- **Constitutive models suitable for bulk solids, preferably in a multi-phase setup**
- **Models using parameters that can be measured at reasonable expenditure of time and money**

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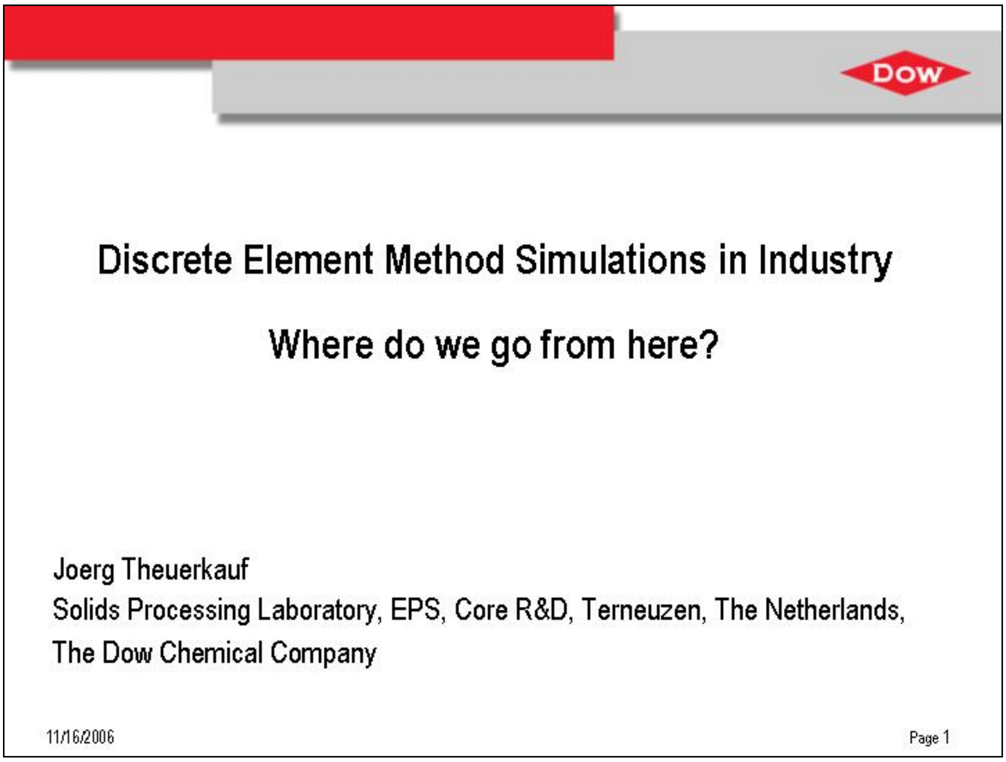
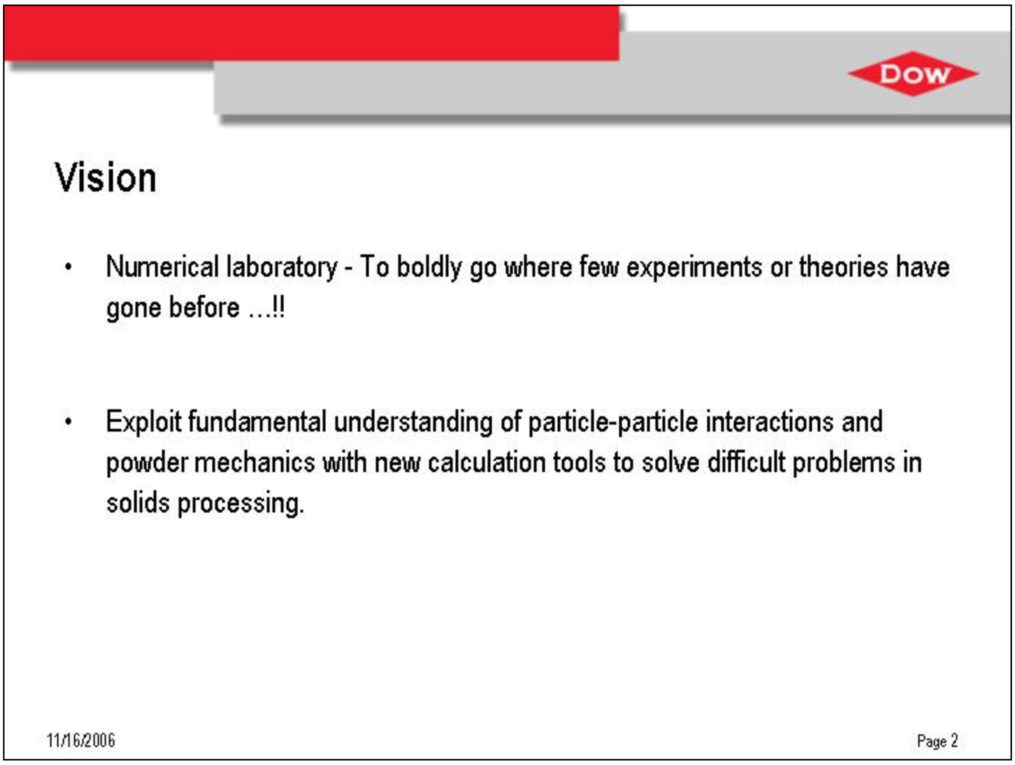
5.5.2 J. Theuerkauf, Dow Chemicals



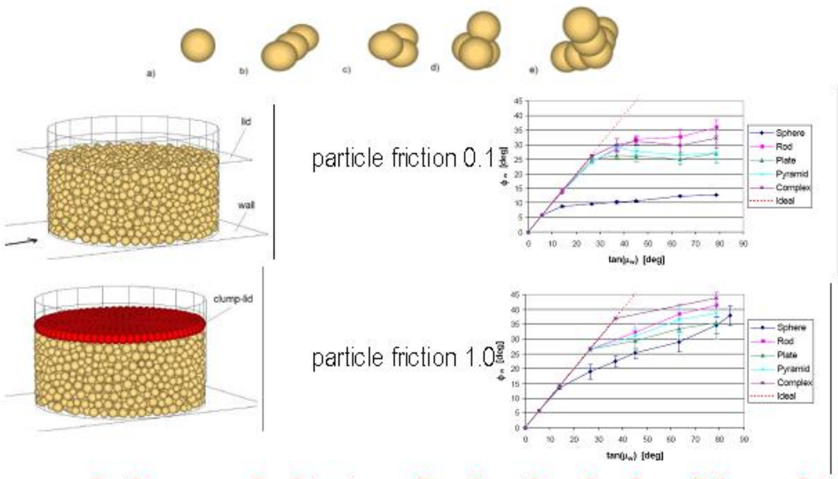


What was done so far?

- Selected examples of DEM applications
  - shear testers
  - storage in silos
  - screw conveyers
  - mixers
  - packing structure
  - material testing
  - pneumatic conveying/fluidized beds

New insights and agreement with theories.
Models have been calibrated for the systems under investigation.

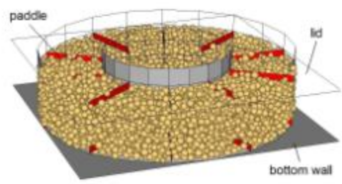
Wall friction calibration for storage problems

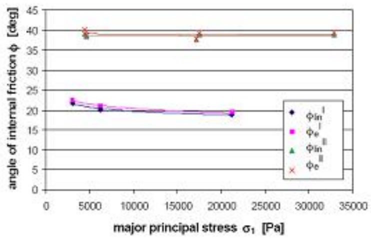


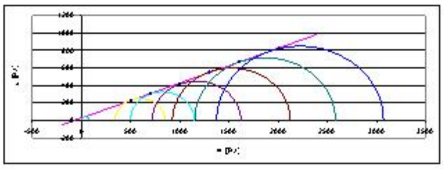
Is the numerical tester reflecting the physics of the real tester?

DOW

Determining particle-particle friction -rotational ring shear tester-







Flow properties:

ϕ_{lin} = 21.8 deg

ϕ_e = 22.5 deg

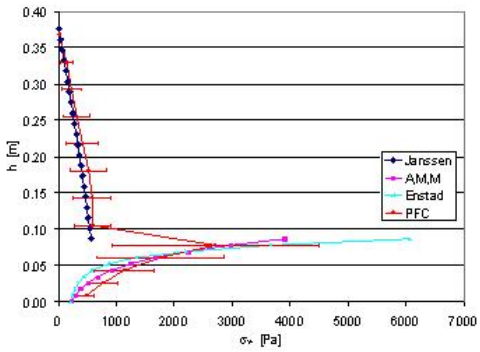
c = 27 Pa

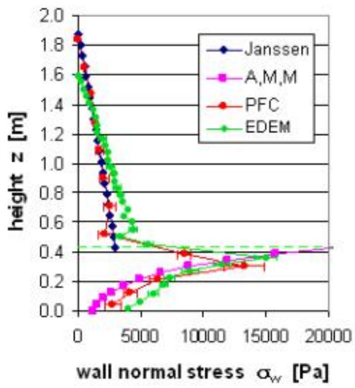
f_c = 80 Pa

ρ_b = 589.5 kg/m^3

DOW

Time averaged wall normal stresses during discharge





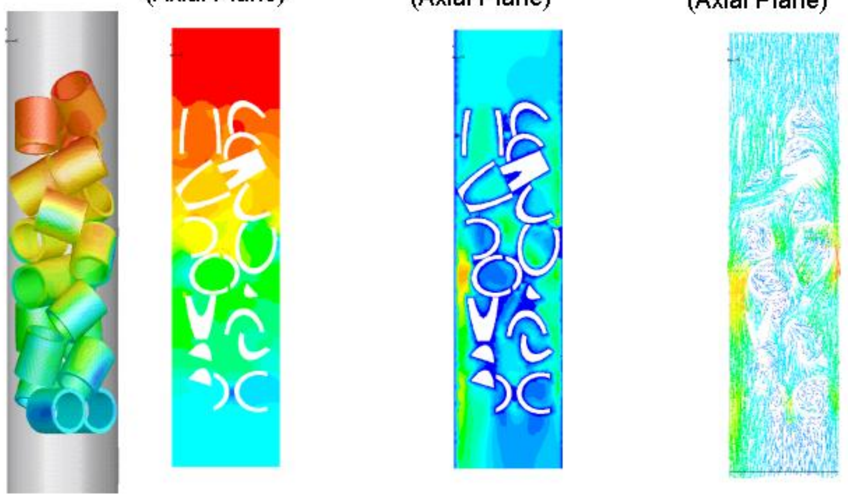
What is needed?

- good understanding of the right contact models and their calibration for the specific materials
  - LSD, Hertz, Burgers, liquid bridges, Ludings, etc **How complicated do we have to get?**
  - contact bonds, parallel bonds
    - » Do we need to study the particle-particle contact or is a system response good enough?
    - » Experimental validation on a particle-particle level or for the assembley? –It depends.
- Calibration techniques for micro parameters
  - choose the **right one** - depending on granular flow situation
    - » particle-particle contacts dominate (shear)
    - » particles bouncing around (dilute flow)
- Multi phase flow
  - coarse grid for fluid
  - Dem particles the fluid phase
  - coupling with flow simulation software
    - » particle induced or dampened turbulence
    - » shape and drag coefficent
- How many particles do we need for a realistic system response? scale up of particle size
- Coupling of continuum approach and DEM

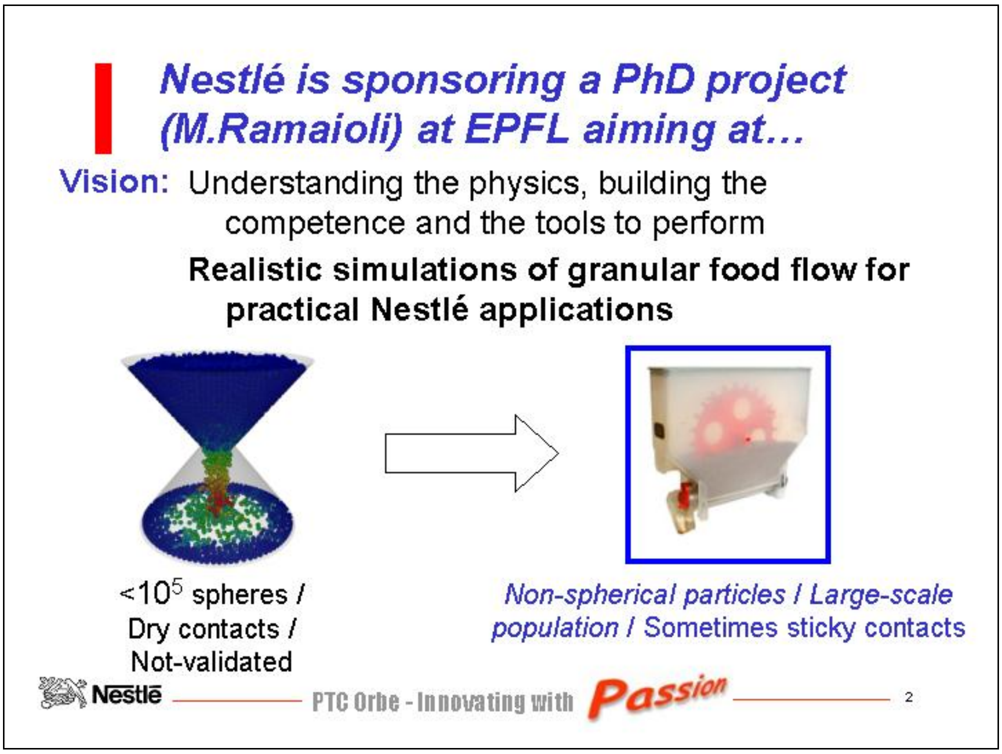
User norm/guide "DEM101" the unique calibration parameters and procedure

Process optimization: DEM-Fluent/CFX- reaction

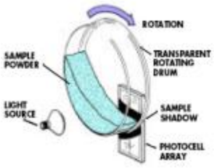
Pressure Field (Axial Plane) | Velocity contours (Axial Plane) | Velocity vectors (Axial Plane)



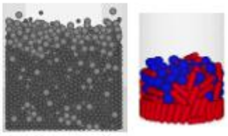
5.5.3 M. Ramaioli, Nestlé



DEM is compared with experiments to characterize powders and for validation



- Impact tests and rotating drum tests to gather restitution and friction coefficients



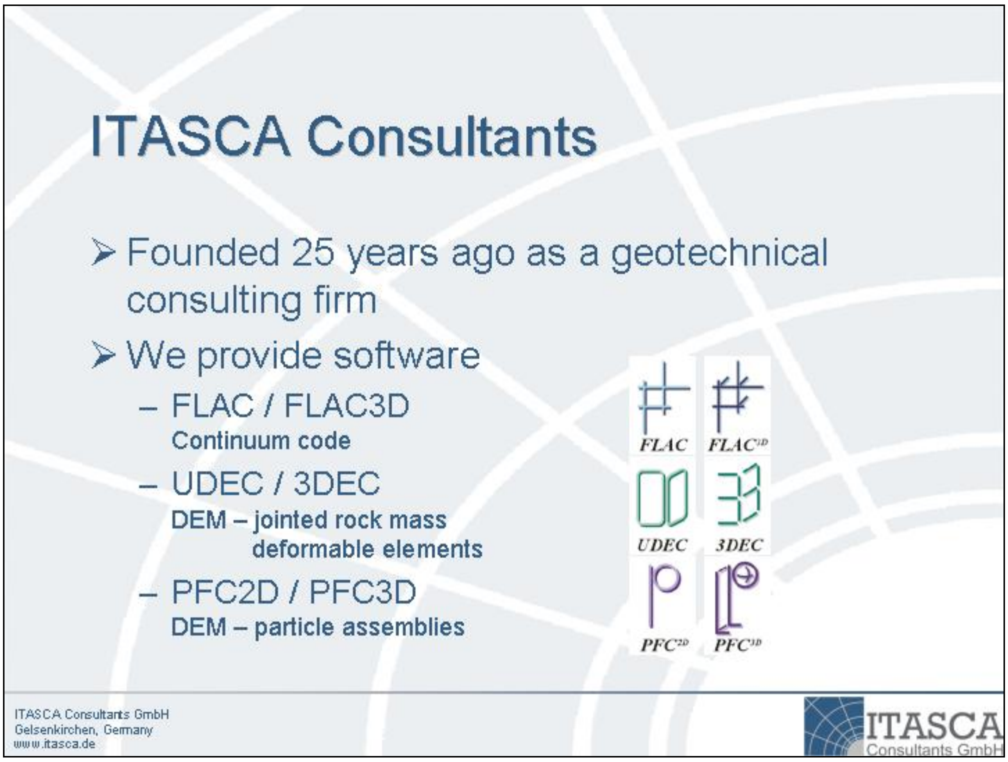
- Vibration-induced segregation of spherical and elongated particles

- Flow of powder beverages in dispensers

But still many limitations prevent DEM from being an industrial modelling tool…

- Still too few validations
- No established procedure to gather grain properties
- Populations are too limited for most industrial applications
- Granular physics is not yet mastered sufficiently to rely on approximated "reductions" of the real system: e.g. softer particles, bigger grains, subdomains, 2D.

5.5.4 L. te Kamp, ITASCA Consultants



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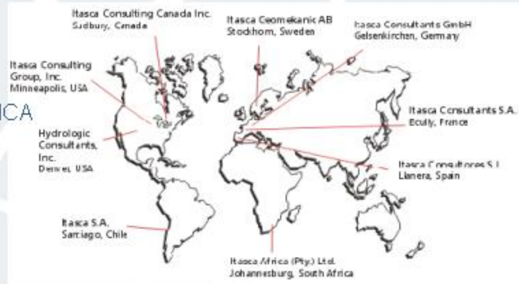

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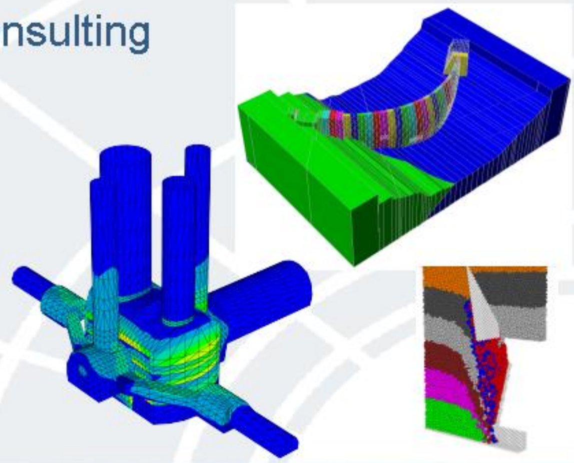

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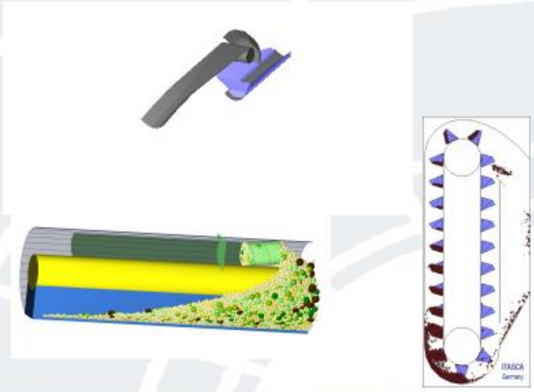

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Planning the future

- Application
  - More acceptance from industry
  - New fields of application
- Development
  - Mechanics and Physics
  - Model size
  - Calculation speed

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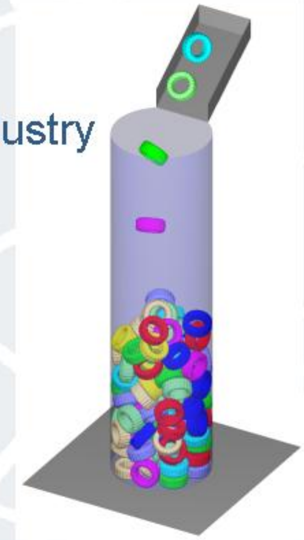
Application

- More acceptance from industry
  - Prove that DEM can
    - Solve their problems
    - Reduce costs
    - Replace costly experiments
    - Support the design
    - Prove concepts



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Application

- More acceptance from industry
  - Validation of the DEM
    - Run selected problems with good experimental backup
    - Numerical prove of concepts
  - Definition of standards
    - E.g., influence of model setup

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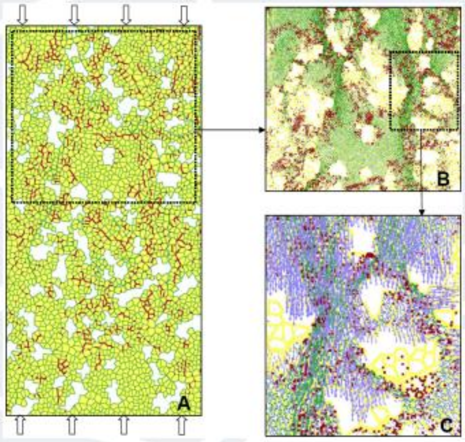
Application

- New fields
  - Loading and damage of mineral structures



Application

- New fields
  - Masonry and buildings under static and dynamic load

Development

- **Mechanics and Physics**
  - Material behavior
    - Contact models
    - Particle shape
  - Other effects
    - e.g. electrostatic charge
  - Coupling
    - Fluid
    - Thermal

Development

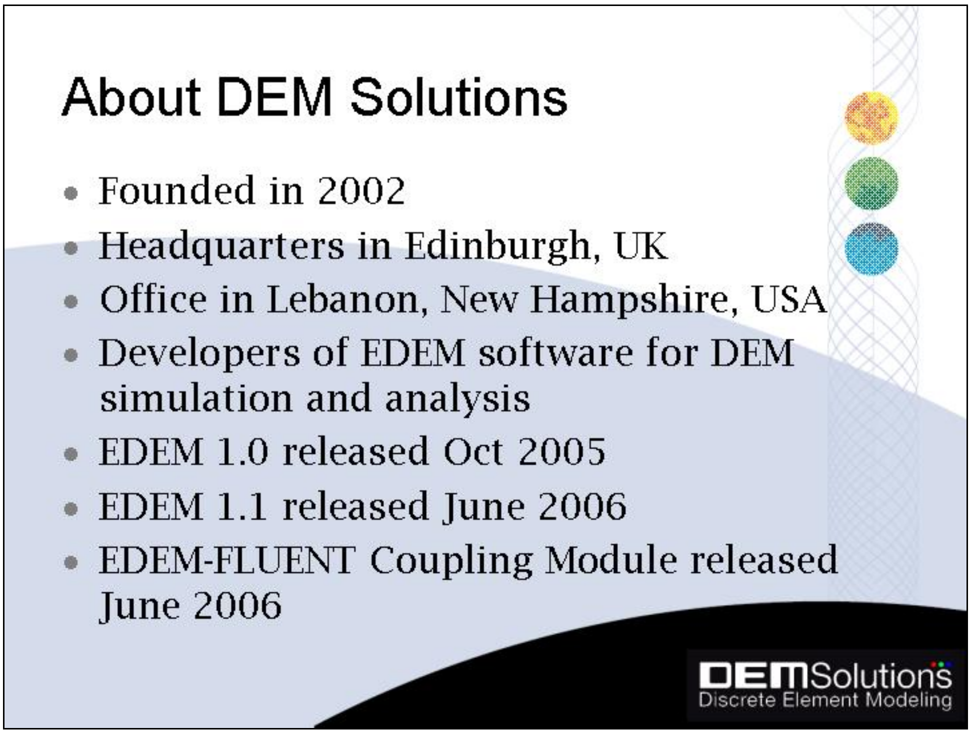
- **Model size / computation time**
  - Scaling laws
  - Different algorithms
  - Different hardware
  - Different compilers

Remarks

- Researcher and software vendors strongly depend on the input from industry
- Identify a few selected problems and validate DEM
- Set up a strategy for future development
  - Identify the needs
  - Identify potential fields of application
  - Questionnaire ?
- More cooperation of universities and the software vendors

Thank you for your attention !

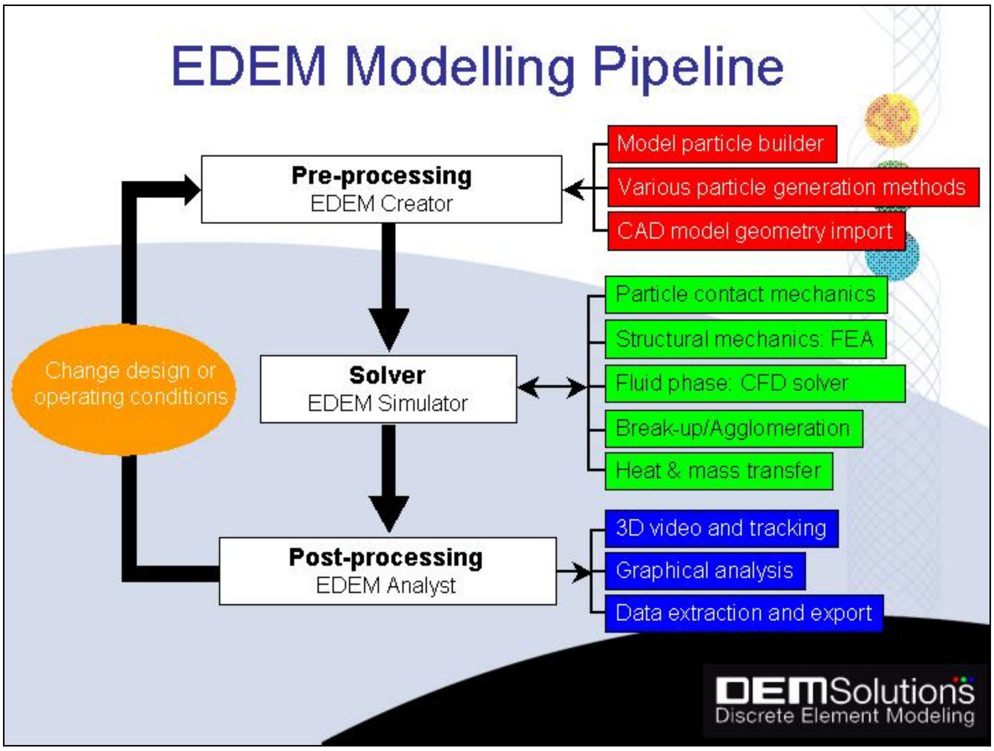
5.5.5 J. Favier, DEM Solutions

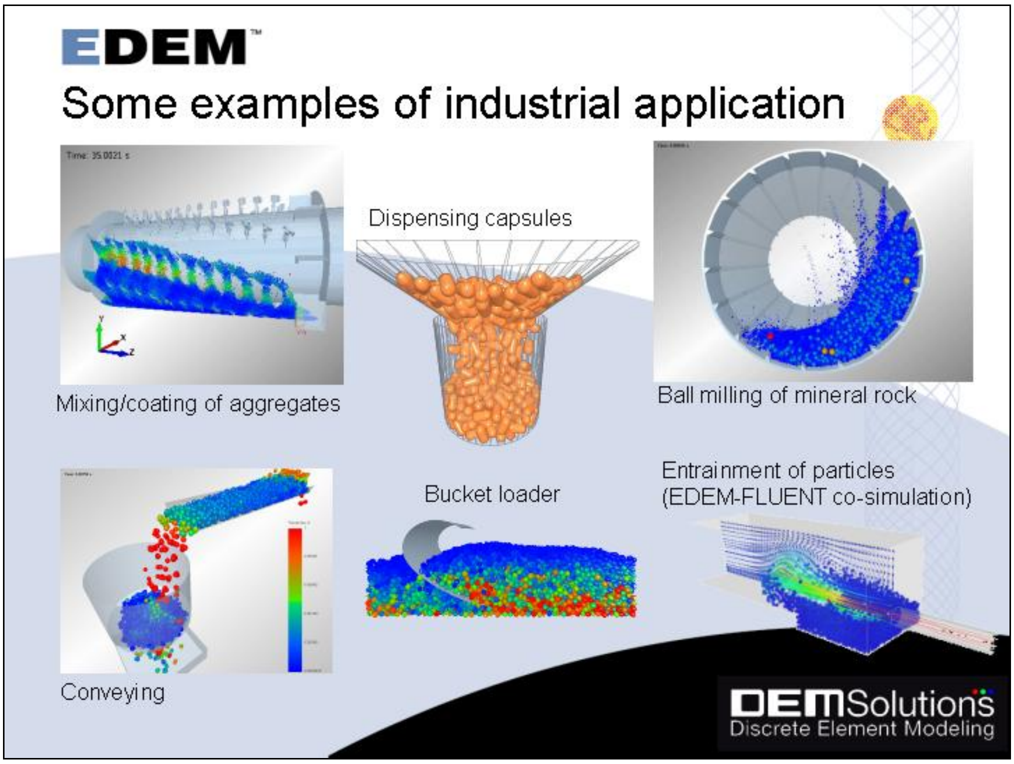


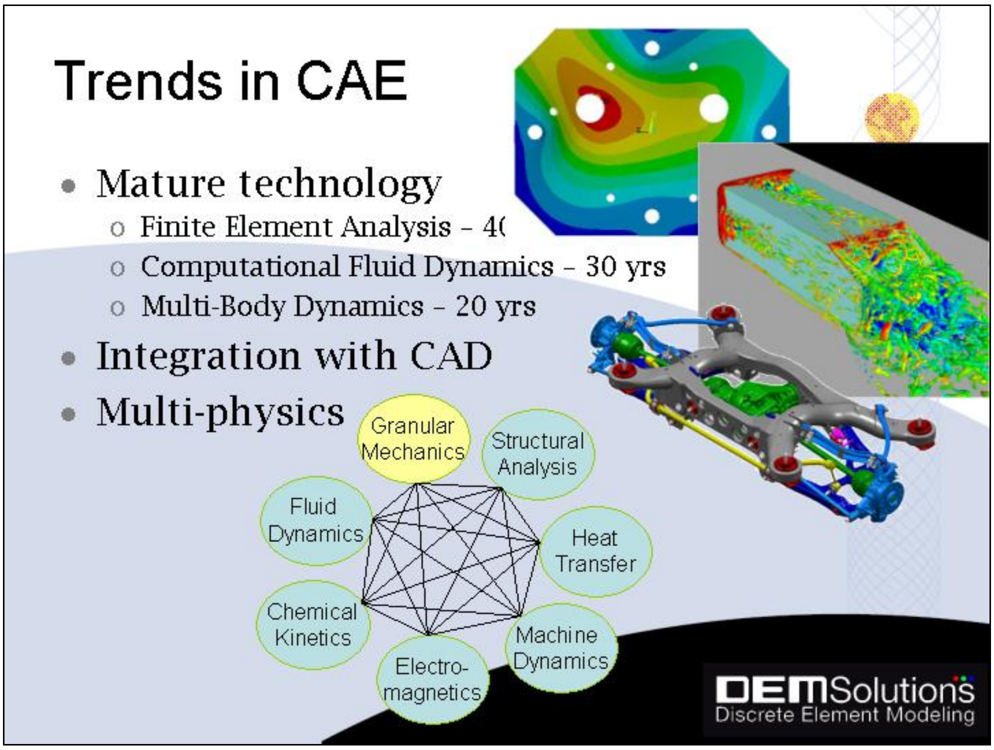
EDEM™

- 3D DEM simulation and analysis tool
- Fully functional GUI for pre- and post-processing
- CAD compatible for import of particle and equipment geometry
- Applications interface for user programmable control of particle initialisation, contact physics, body forces
- Suite of tools for data visualisation, analysis and extraction
- Couples with other ... MBD, ...

DEMSolutions
Discrete Element Modeling




EDEM™
Some examples of industrial application
Dispensing capsules
Mixing/coating of aggregates
Ball milling of mineral rock
Bucket loader
Entrainment of particles
(EDEM-FLUENT co-simulation)
Conveying
DEMSolutions
Discrete Element Modeling


Trends in CAE
Mature technology
Finite Element Analysis – 4
Computational Fluid Dynamics – 30 yrs
Multi-Body Dynamics – 20 yrs
Integration with CAD
Multi-physics
Granular Mechanics
Structural Analysis
Fluid Dynamics
Heat Transfer
Chemical Kinetics
Machine Dynamics
Electro-magnetics
DEMSolutions
Discrete Element Modeling

Drivers for application of CAE

- Engineering
  - o Higher and more consistent quality product
  - o Faster production
  - o Lower energy usage
  - o Design of new products and processes
- Business
  - o Better return on investment
  - o Shorter time to market
  - o Technical advant

DEMSolutions
Discrete Element Modeling

Drivers for application of DEM

- Engineering
  - o Provides information about internal bulk behaviour
  - o Expanding range of industrial applications and application know-how
  - o Discrete methods required to advance quality of predictive simulation of granular systems
- Computational
  - o Faster computing
  - o Improving performance/cost of hardware
  - o Coupling of DEM with other nu methods

DEMSolutions
Discrete Element Modeling

Characteristics of particulate solids handling and processing operations

Range of particle shape and size
- Usually non-spherical particles

Complex machine geometry
- Moving machine components

May have interactions which involve mass, momentum, and heat transfer
- Between particles
- Between particles and machinery
- Between particles and fluids

DEMSolutions
Discrete Element Modeling

What information can DEM provide?

Particle

Particle kinematics
Particle size/mass/temperature
Particle-particle contact forces
Particle-boundary contact forces
Particle body forces: gravitational, fluid, electro-magnetic
New particle formation

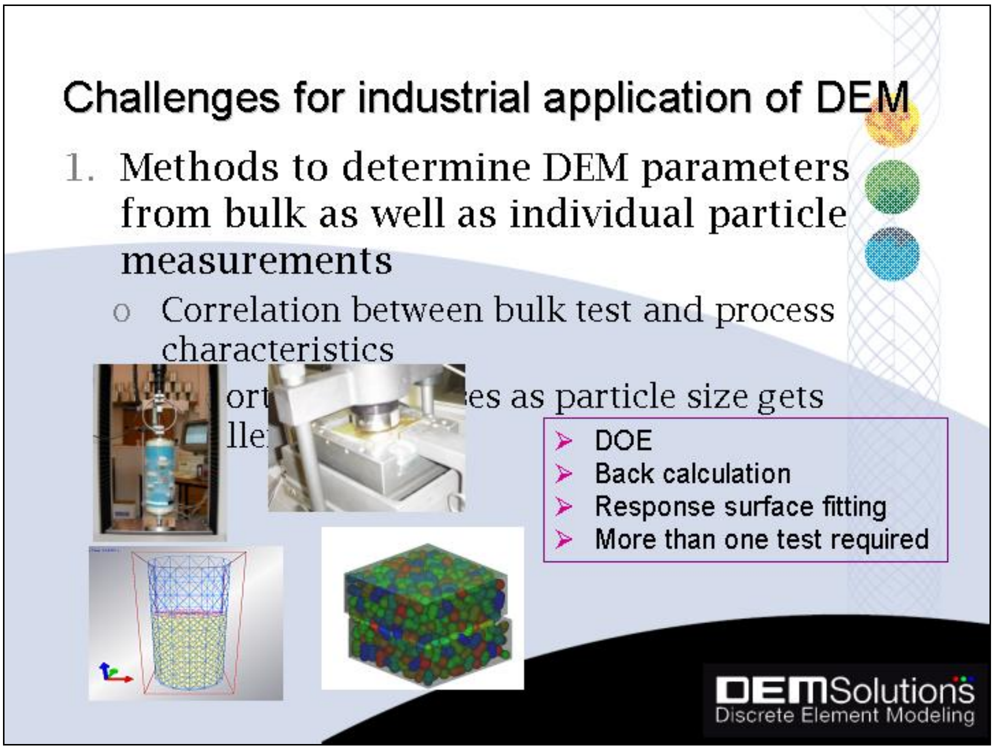
DEM results

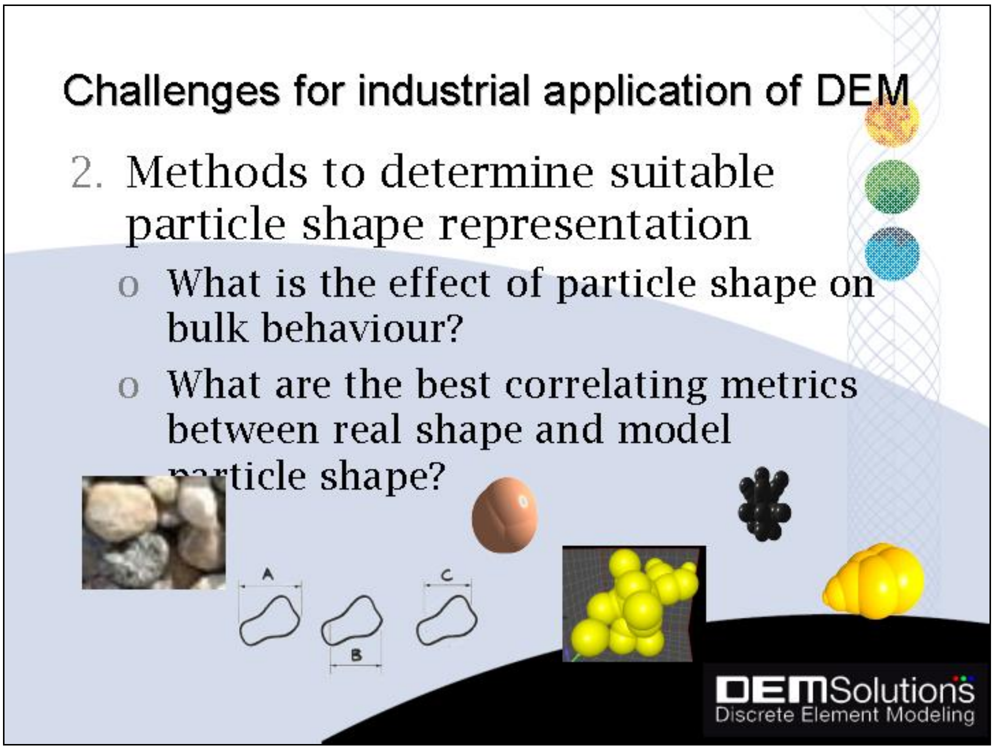
Bulk

Mixing dynamics
Uniformity of flow
Bridging
Granulation
Agglomeration
Mechanical energy consumption
Particle-machine interaction
Pneumatic transport

Segregation
Residence time/ hold-up
Damage/attrition
Breakage
Surface coating
Erosion
Heat transfer
Fluidization

DEMSolutions
Discrete Element Modeling


Challenges for industrial application of DEM
1. Methods to determine DEM parameters from bulk as well as individual particle measurements
o Correlation between bulk test and process characteristics
es as particle size gets
DOE
Back calculation
Response surface fitting
More than one test required
DEMSolutions
Discrete Element Modeling


Challenges for industrial application of DEM
2. Methods to determine suitable particle shape representation
o What is the effect of particle shape on bulk behaviour?
o What are the best correlating metrics between real shape and model particle shape?
A
B
C
DEMSolutions
Discrete Element Modeling

Challenges for industrial application of DEM

3. Parametric studies of DEM contact algorithms
   - Sensitivity
   - Scaling

→ Optimisation procedures

DEMSolutions Discrete Element Modeling

Challenges for industrial application of DEM

4. Establishment of benchmarking for DEM codes
   - Validation against standard tests
   - Relate DEM model to continuum model benchmarks
   - Relate DEM simulation to alternative techniques
   - Reference point for the “layman”

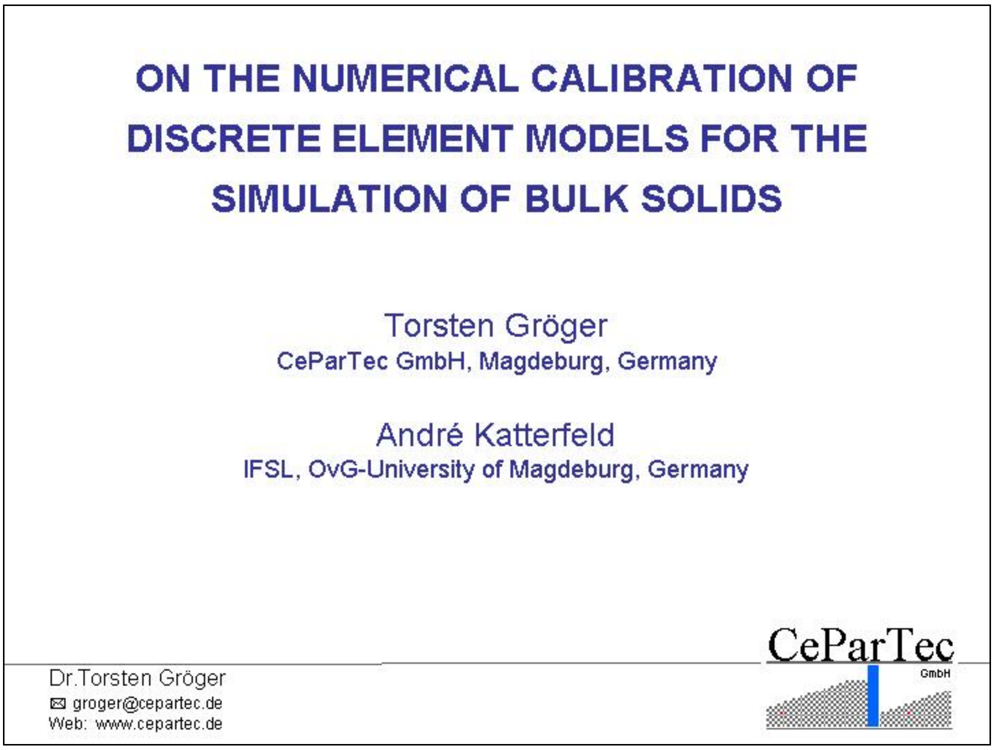
DEMSolutions Discrete Element Modeling

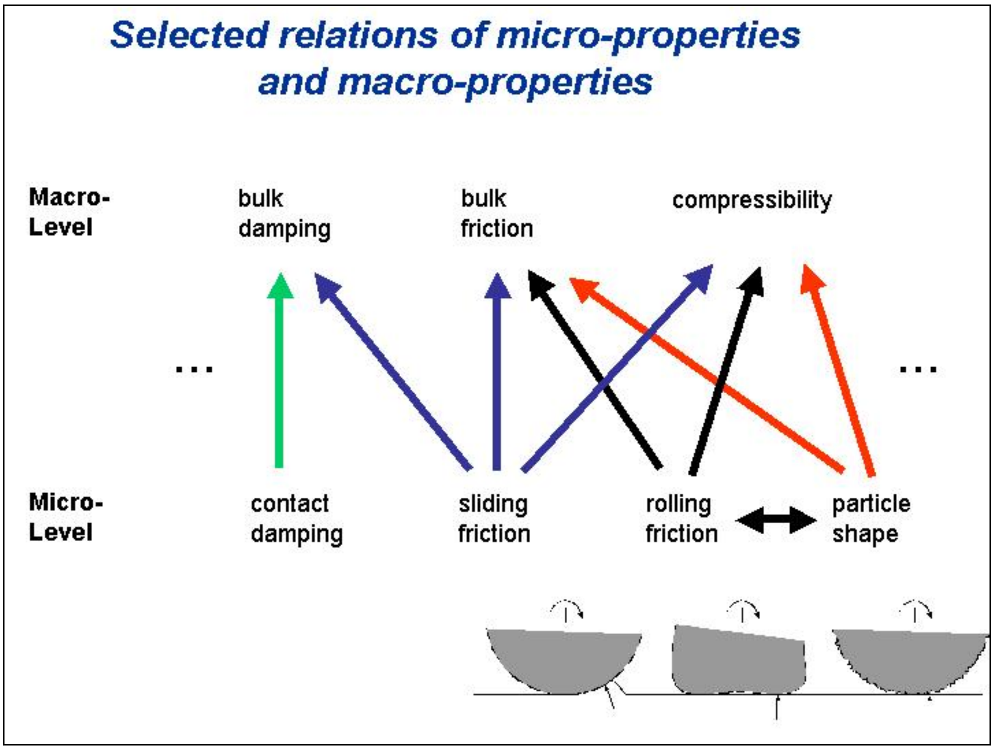
Conclusions

- DEM is now a viable simulation tool for industrial particulate processes
- More DEM validation and benchmarking is required to increase acceptance by industry
- Integration with other CAE tools is advancing and will widen the use of DEM
- DEM is an valuable addition to the engineers toolkit which compliments experiment and physical testing

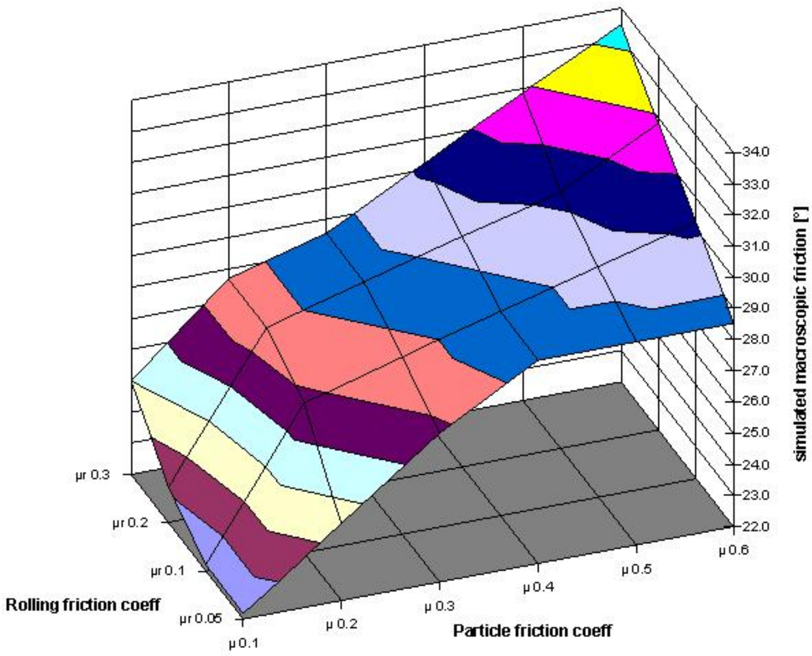
DEMSolutions
Discrete Element Modeling

5.5.6 T. Gröger, CeParTec

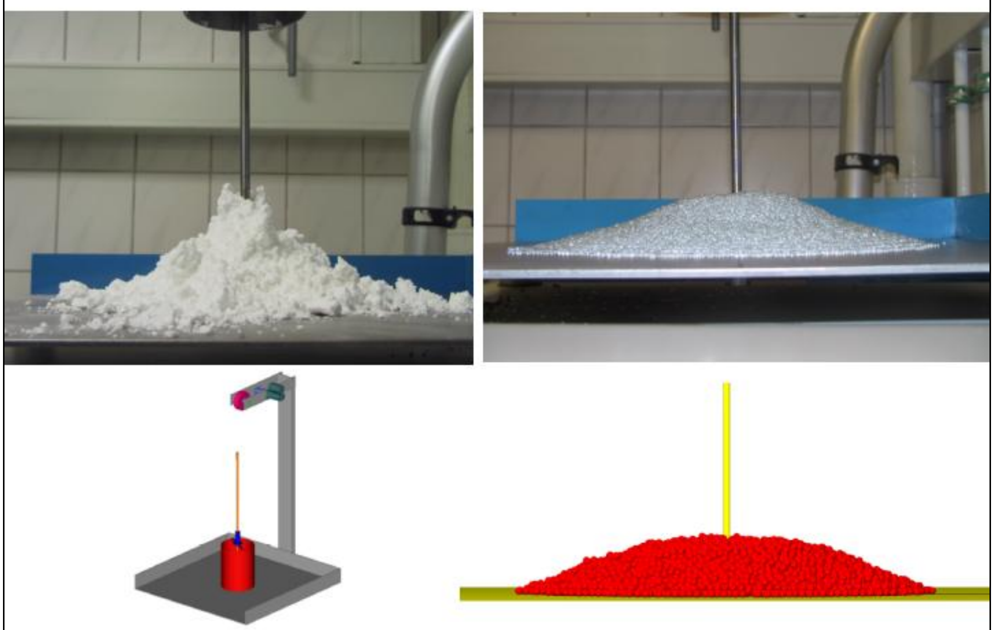




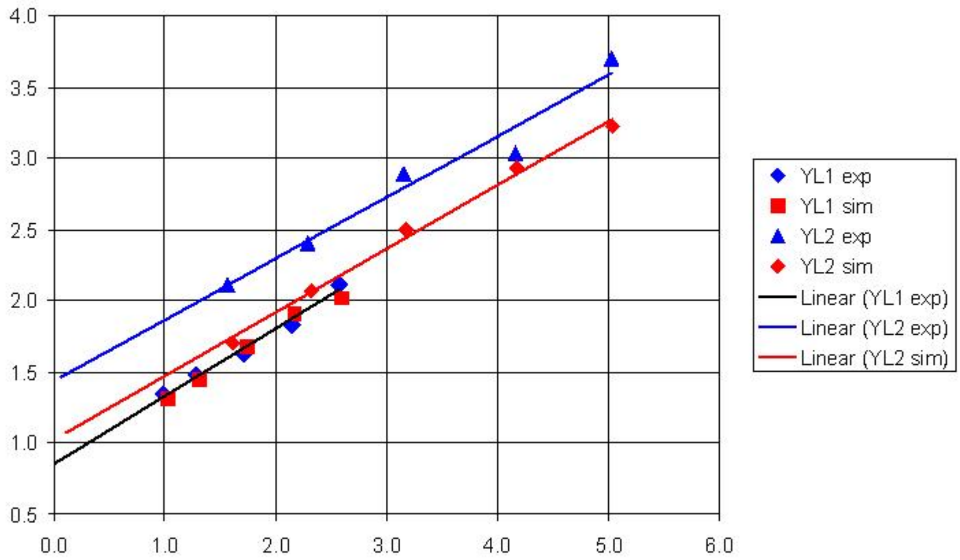
Macroscopic friction of a sphere assembly



Calibration of friction



Yield loci of a cohesive sphere assembly

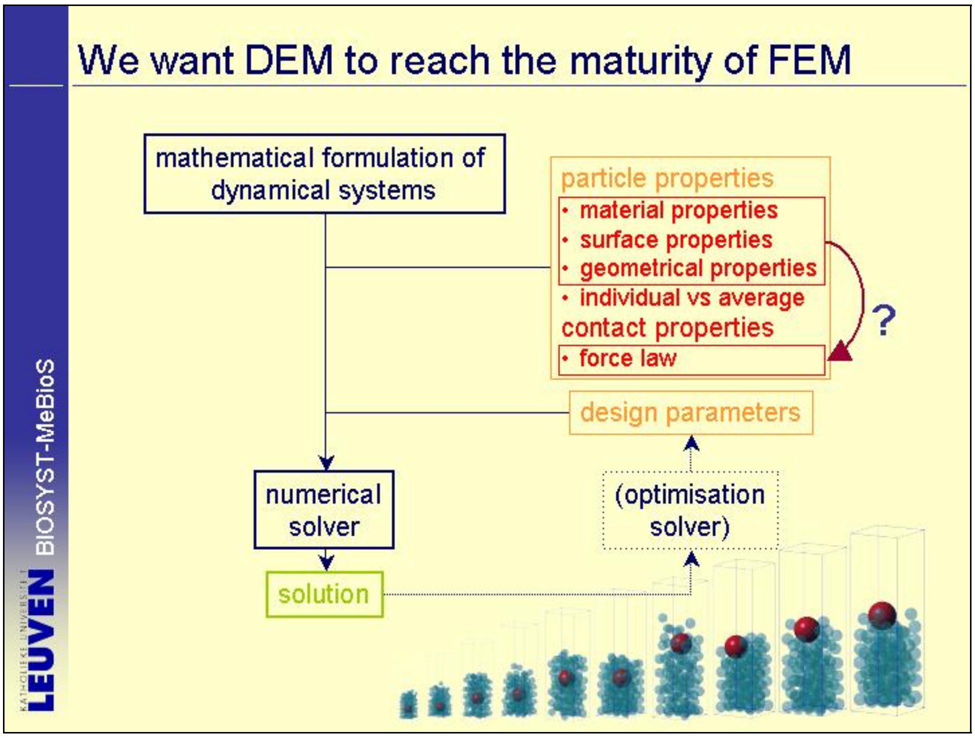


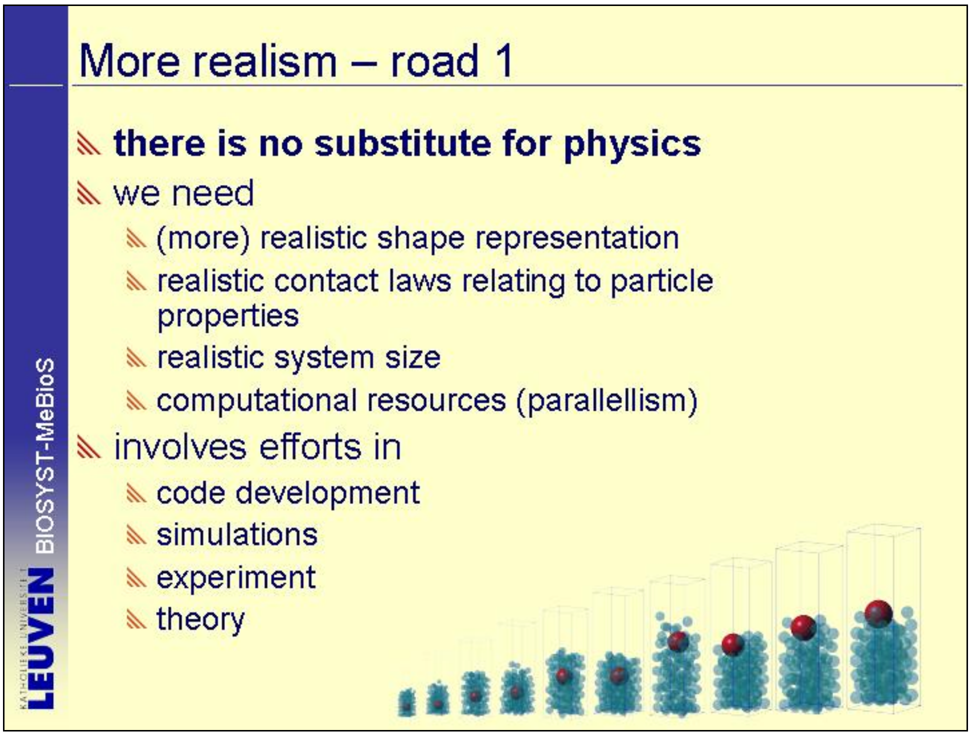
Group of experimental researchers and numerical researchers working on
Calibration of Granular Material

- identification of the influences of the micro-properties on macro-properties
- development of simple experiments that can easily be simulated

Standard Calibration Technique for DEM-Models

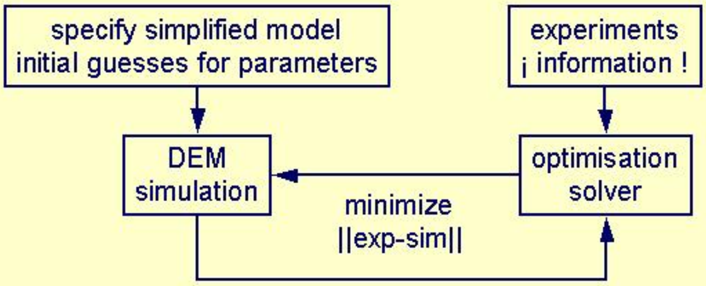
5.5.7 E. Tijskens, KU Leuven



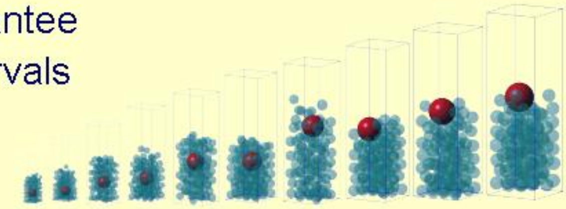


More realism – road 2

- **model calibration → model optimisation**

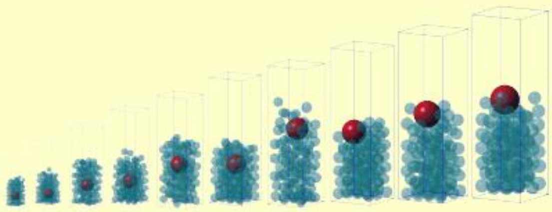


- optimality guarantee
- confidence intervals

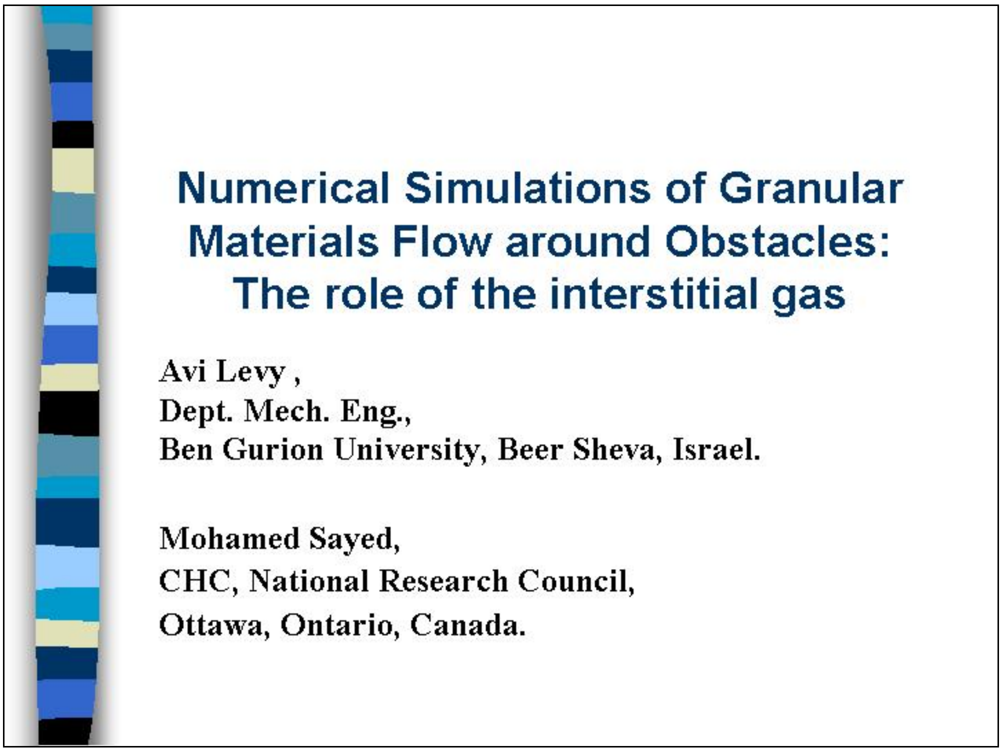


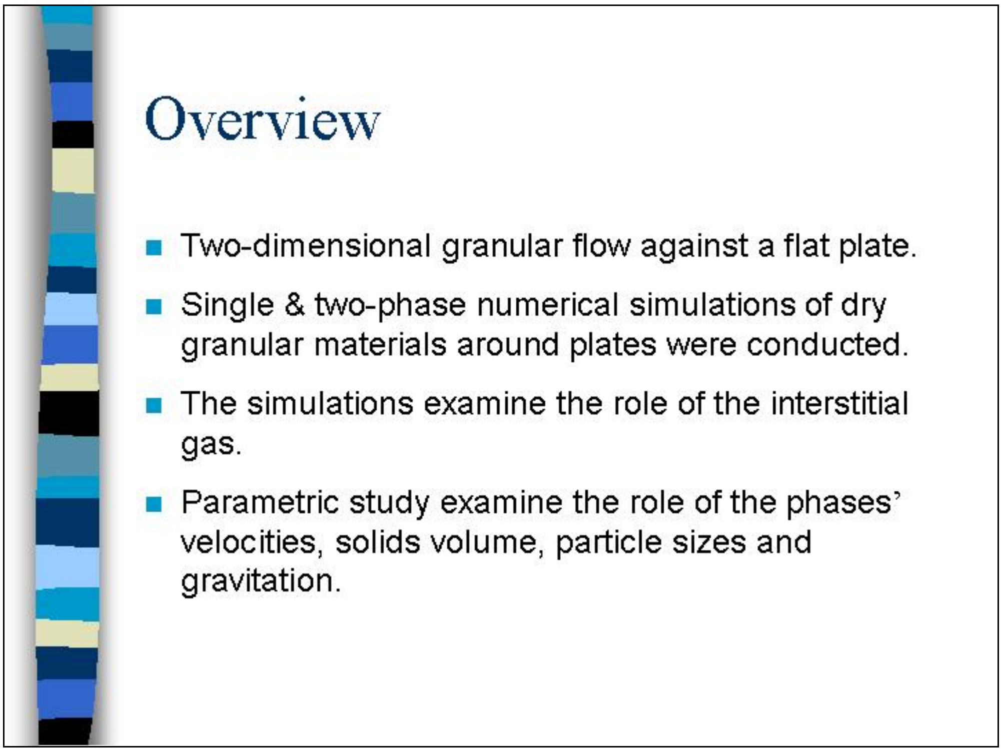
More realism – road 2

- danger ahead
  - "push the button" approach
  - interpolation vs extrapolation
  - information exposure of experiment
- need to be put on firm footing
- involves efforts in
  - code development
  - simulations
  - experiment
  - theory



5.5.8 Avi Levy, Ben Gurion University





Introduction

- Flow patterns are influenced by bulk material properties, flow rates and geometry of both the flow channel and the obstacle.
- Many experimental studies where conducted to determine the drag force of the granular flow on immersed objects, force fluctuations, the role of obstacle shape, and the jamming potential.
- Tuzun et al. (1985) examined the 2D dense flow in a vertical bin around various inserts.
- The formation of a distinct granular shock wave in front of an obstacle observed by Buchholtz and Poschel (1998). They carried out 2D molecular dynamics simulations of an unconfined stream of particles and determined the role of the force on the obstacle, obstacle size, and upstream velocity.

Introduction

- Amarouchene et al. (2001) experiments showed that such shock waves form in front of obstacles. Their measurements provide detailed geometry of the shocks and velocity profiles for flow around cylinders, wedges, and plane obstacles.
- Rericha et al. (2002) also observed shock waves in numerical and experimental investigation of dilute granular materials with wedge-shaped obstacles.
- Wassgren et al. (2003) conducted comprehensive molecular dynamics simulations of the interaction of dilute granular flows with cylinders. They observed granular shock waves and compared to those observed in compressible gas flow.

Introduction

- For dense flows, the experiments of Chehata et al. (2003) showed that no such shock waves took place.
- The effects of the interstitial gas on the granular flow interaction with obstacles have been traditionally neglected.
- Those effects have been examined in a number of situations such as hopper discharge (e.g. Srivastava & Sundaresan, 2003).
- However, the role that the interstitial gas plays as a granular stream impacts an obstacle, and in particular on shock wave characteristics, remains poorly understood (Levy & Sayed, 2006).

Approaches for modeling granular flow

Single-Phase Granular Flow Model

The Particle-In-Cell (PIC) Approach

•An ensemble of particles represents the bulk material.
•Each particle is given attributes such as density, position, and velocity.
•Particles are advected in a Lagragian manner.
•The momentum equations, however, are solved on a fixed Eulerian grid.
•Various variables are mapped between the particles and the grid.
•granular stress: Frictional (surface friction & interlocking) & Dynamic (collisions & momentum transfer).

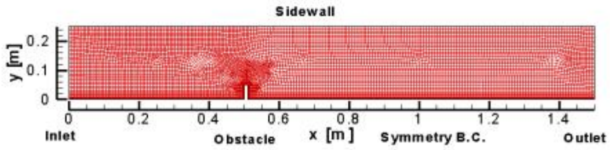
Two-Phase Gas-Solids Model

Two-Fluid Eulerian-Eulerian formulation.

•Numerical solution is obtained using the code FLUENT
•The granular phase follows the kinetic theory.
•The flow is isothermal.
•The influence of gas turbulence is neglected.
•Inter-Phase Forces: based on Ergun's equation for solids volume fraction >0.2 , otherwise the force is calculated using drag force on a single particle with Richardson-Zaki modification.

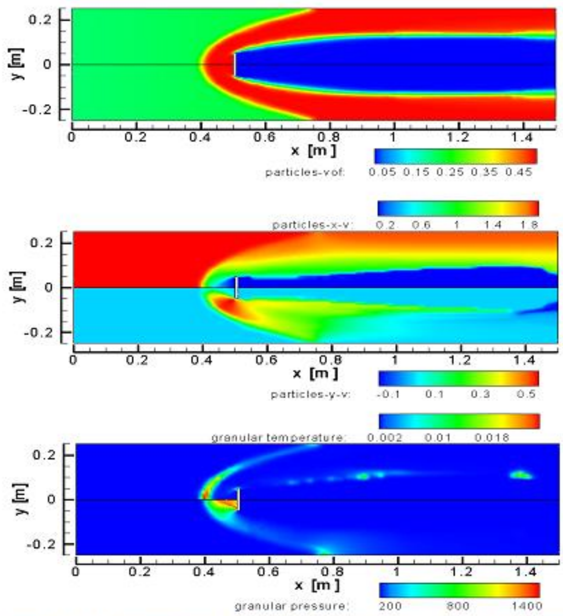
Single-Phase Granular Model

Initial and Boundary conditions

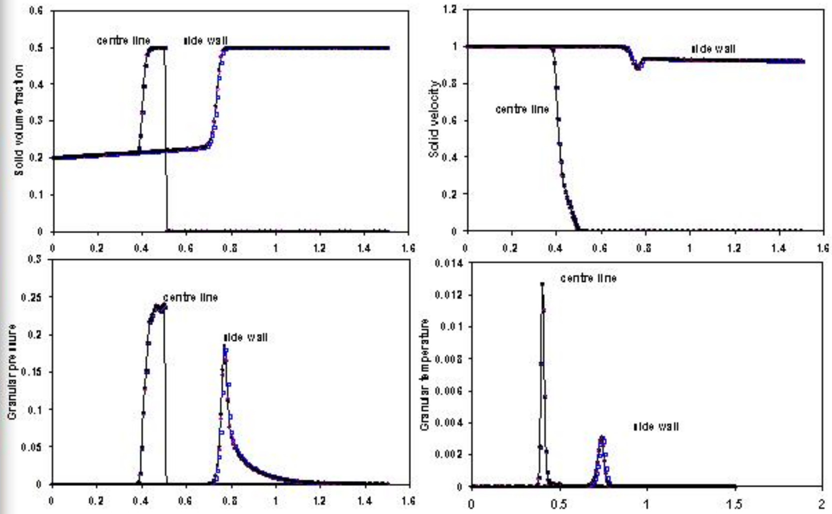


The *base* test case:
volume fraction = 0.2.
No Gravity.
No Fluid-Solid interaction.

Case No.	Inlet v_s	Inlet v_g
1	1.0	0.1
2	2.0	0.1
3	2.0	1.0
4	3.0	0.1



Particles flow field characteristics for case 3: a) Solid volume fraction; b) solid velocity components; and c) granular pressure and temperature.

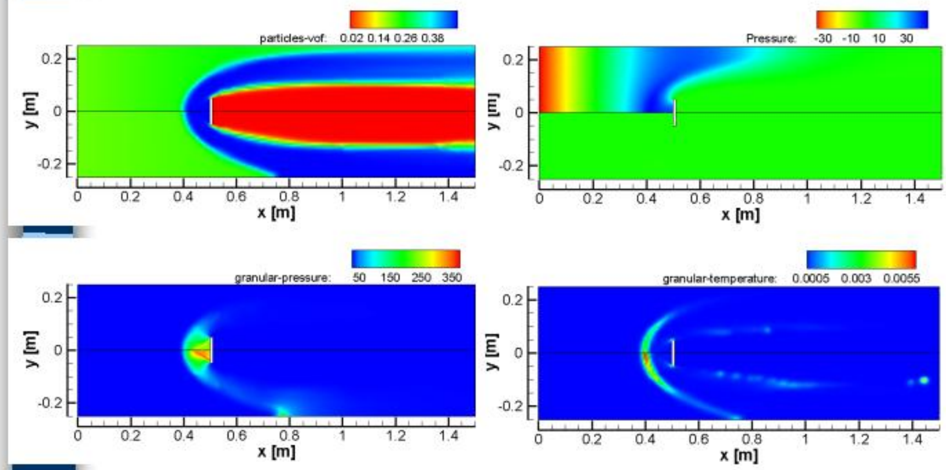


Prediction of the numerical simulations for the solid volume fraction, normalized velocity, granular pressure and temperature, (a) to (d), respectively, along the symmetry line and the side wall for cases 1-4

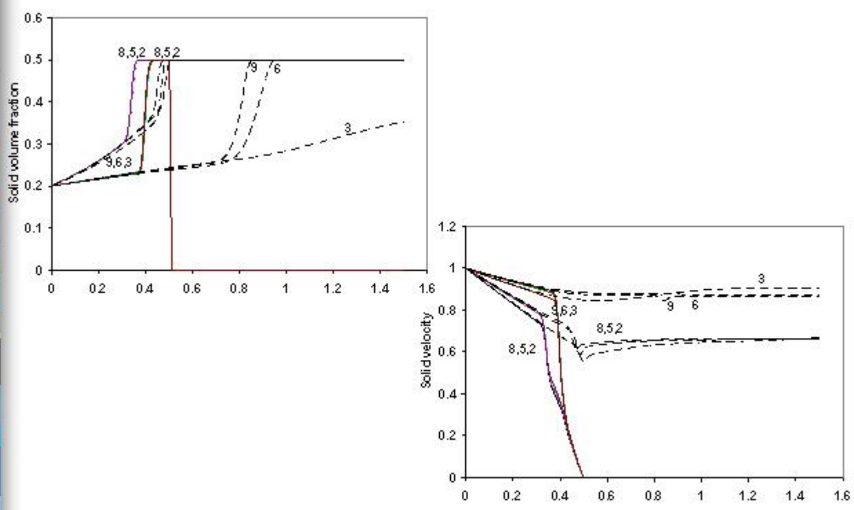
Two-Phase Granular Model

Initial and Boundary conditions
The *base* test case:
volume fraction = 0.2; No Gravity; Particle's dia. 1mm.

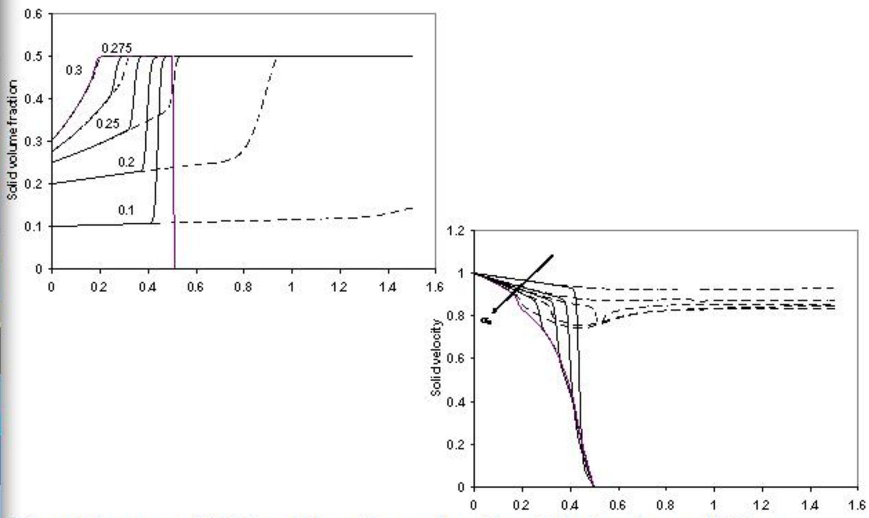
Case No.	Inlet $\mathbf{v}_s$	Inlet $\mathbf{v}_g$
1	1.0	0.10
2	1.0	0.25
3	1.0	0.50
4	2.0	0.20
5	2.0	0.50
6	2.0	1.00
7	3.0	0.30
8	3.0	0.75
9	3.0	1.50



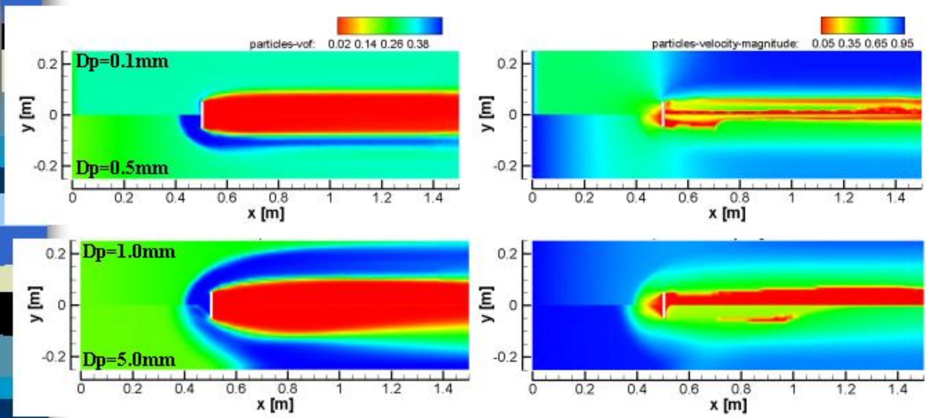
Comparison between flows with two-phase flow and single-phase granular flow, upper and bottom parts respectively, solids volume fraction, pressure and granular temperature and gas pressure for inlet solids and gas velocities of 1 and 0.5 m/s, respectively, and inlet solid volume fraction of 0.2.



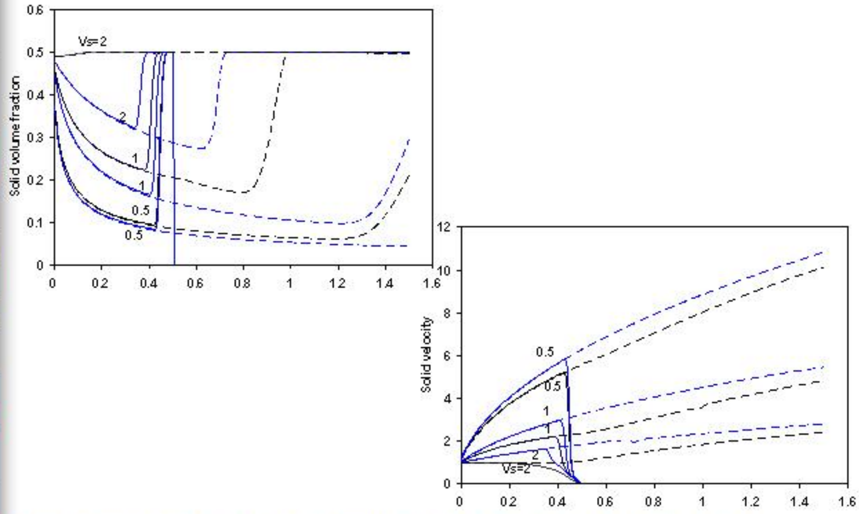
The influence of the inlet velocities (inlet α_s =0.2) on the profiles of solids volume fraction and velocity along the center line (solid lines) and the side wall (dashed lines) for cases 2, 5 and 8 (inlet vg / vs = 0.25) and 3, 6 and 9 (inlet vg / vs = 0.5)



The influence of inlet solids volume fraction (inlet vg / vs = 0.5) on the profiles of solids volume fraction and velocity along the center line (solid lines) and the side wall (dashed lines) for inlet α_s =0.1, 0.2, 0.25, 0.275 and 0.3, respectively.



The influence of particle sizes on the solids volume fraction and velocity for inlet α_s =0.2, and air and solids velocities 1 & 0.5 m/s, respectively.



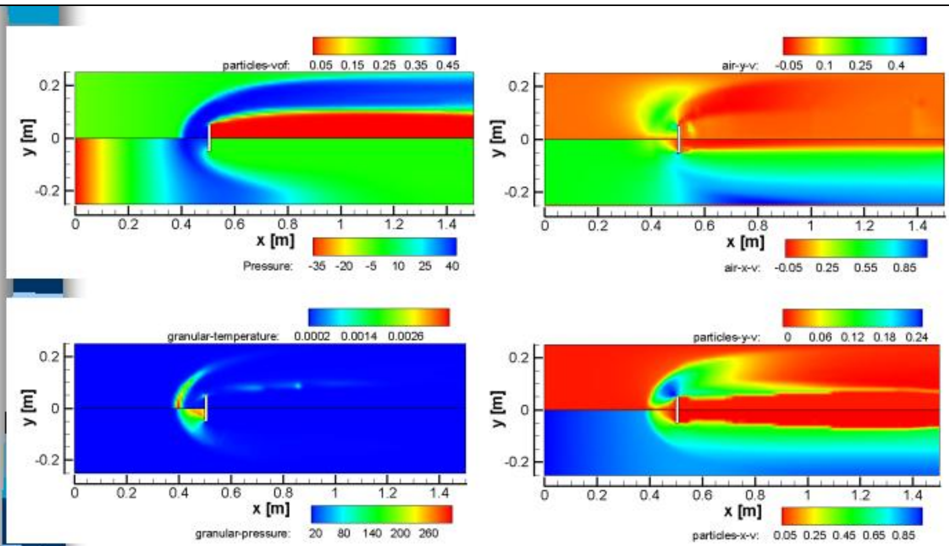
The influence of the inlet velocities (inlet vg /vs = 0.1 & α_s =0.49) with gravity on the profiles of solids volume fraction and velocity along the center line (solid lines) and the side wall (dashed lines) for single and two phase granular model, blue & black, respectively.

Conclusions

- The simulations based on two different rheological models and numerical methods gave very close results.
- By deducting the fluid-solid interaction term the influence of the interstitial fluid phase on the granular flow can be eliminated.
- By normalizing the properties of the granular phase, the predictions of the numerical simulations converged into the same solution for the non-interactive cases (i.e., the solution of the solid phase flow field is self-similar).
- A granular shock wave was observed in front of the obstacle, where velocities and solids volume fraction underwent a jump.
- The shock wave is forms when upstream solids fraction is relatively low, for a wide range of velocities.

Conclusions

- The shock has a parabolic-shaped front.
- A stagnant wedge forms inside the shock immediately in front of the obstacle.
- The formation and the shape of the bow granular shock wave are influenced by the presence of the gas phase, particle size, the interaction forces between the phases, and gravity.
- The role of the interstitial gas is too significant to ignore for the present problem.
- The effect of the gas flow was negligible only in the vicinity of the obstacle, where granular creeping flow is observed



Contour plots of solids volume fraction and gas static pressure, solids and gas velocities, and granular temperature and pressure for inlet solids and gas velocities of 1 and 0.5 m/s, respectively, and inlet solid volume fraction 0.2.