Do you know your A,B,C's and V's?

CCC-ParaSolS Code Benchmarking Progress Update

J.P. Morrissey

Abingdon: 13–15 October 2025

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Schedule for this Network Event

- **Monday 13 October — Garden Room, the Cosener's House**
  - 09:30–10:30 Arrival & tea/coffee
  - 10:30–10:45 Introduction
  - 10:45–11:30 'Flash' research presentations
  - 11:30–12:00 Introducing the new CCC-ParaSolS online forum
  - **12:00–12:30 Progress on development of code benchmarking cases**
  - 12:30–14:00 Lunch
  - … …

https://www.ccc-parasols.ed.ac.uk/events/upcoming/networking-event-2/

Important Terminology: Calibration

- **What is calibration?**
- According to the ASME's Guide for verification and validation in computational solid mechanics: *"the process of adjusting physical modelling parameters in the computational model to improve agreement with experimental data"*
- This isn't a bad thing as we often need to fit model parameters that we cannot measure
- However, as with most things, the choice of calibration experiment is very important and can have a significant effect on your results
  - Simple rule: use a calibration experiment *representative* of your regime of interest
    - Don't use a static angle of repose test for a dynamic or stress dependent system

What is Verification and Validation?

- These are terms well defined in *other* fields
- **Verification** is the process of determining if the computational model accurately represents the underlying **mathematical model** and its solution
- **Validation** is the process of determining the degree to which a model is an accurate representation of the **real world** from the perspective of the intended use of the model
- **Accreditation** is the formal process where a model is judged to have sufficient credibility for a specific application after a peer review

Guide for the verification and validation of computational fluid dynamics simulations, AIAA – G – 077 – 1998, Reston VA 1988.

'Terminology for model credibility' (1979) *SIMULATION*, 32(3), pp. 103–104. Available at: https://doi.org/10.1177/003754977903200304.

Thacker, B.H. *et al.* (2004) *Concepts of Model Verification and Validation*, *Concepts of Model Verification and Validation*. Los Alamos National Laboratory, p. 41.

American Society of Mechanical Engineers. (2006) *Guide for verification and validation in computational solid mechanics.* American Society of Mechanical Engineers. Available at: https://www.asme.org/products/codes-standards/v-v-10-2006-guide-verification-validation (Accessed: 13 July 2015).

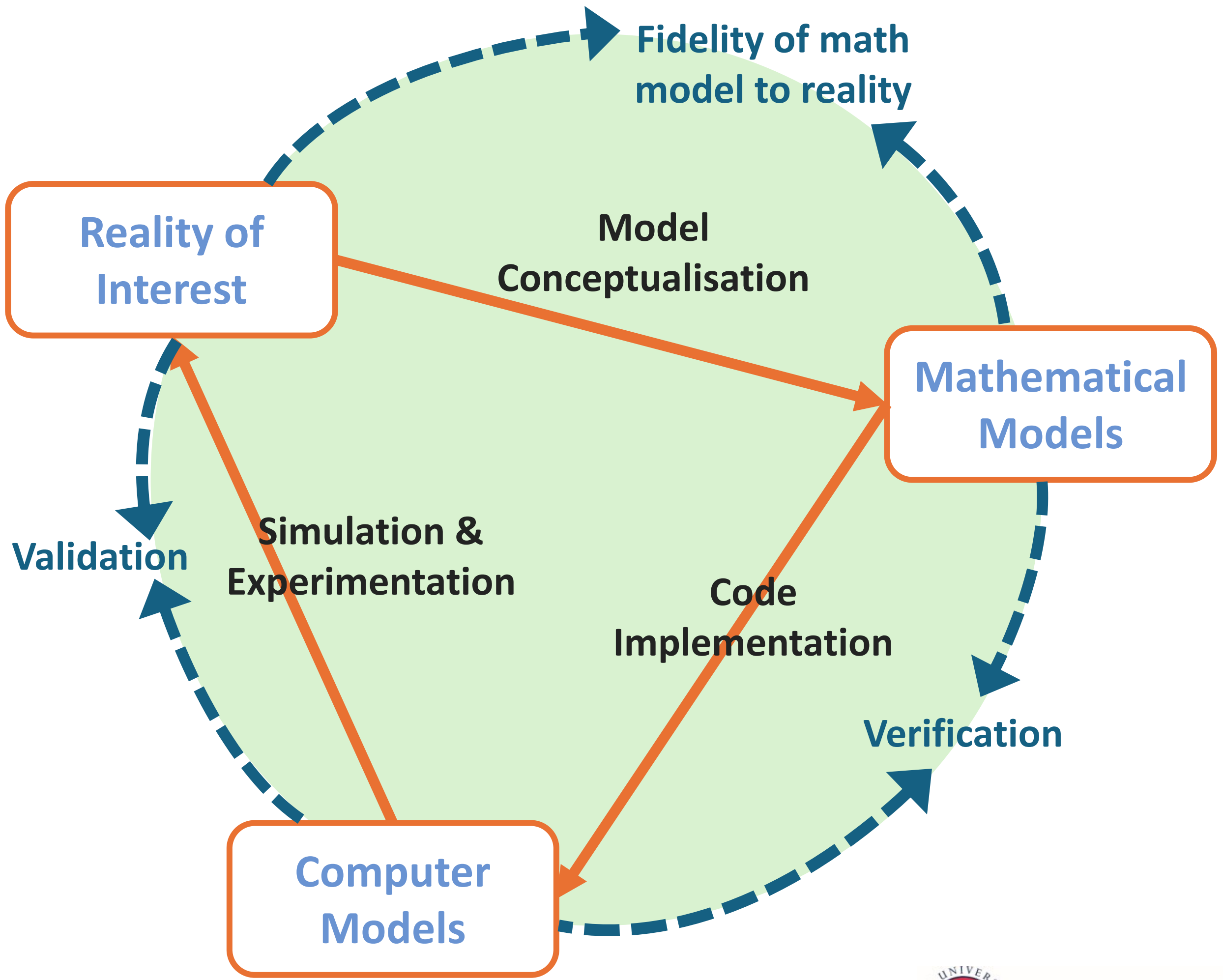
Oberkampf, W.L. and Roy, C.J. (2010) *Verification and Validation in Scientific Computing*. Cambridge: Cambridge University Press. Available at: https://doi.org/10.1017/CBO9780511760396.

More Simply …

- **Verification**
  - Are we **implementing** the model **correctly** ?
  - Mathematics, computational methods, code development
  - Multiple levels:
    - Code verification (e.g. bug free)
    - Calculation verification (e.g. grid or timestep convergence)
- **Validation**
  - Are we **implementing** the **correct model**?
  - Is the physics correct for your problem ?
  - Engineering knowledge and understanding

Parts of the Modelling & Simulation Cycle

- Assessment on the outer paths
- Tasks on the inner paths



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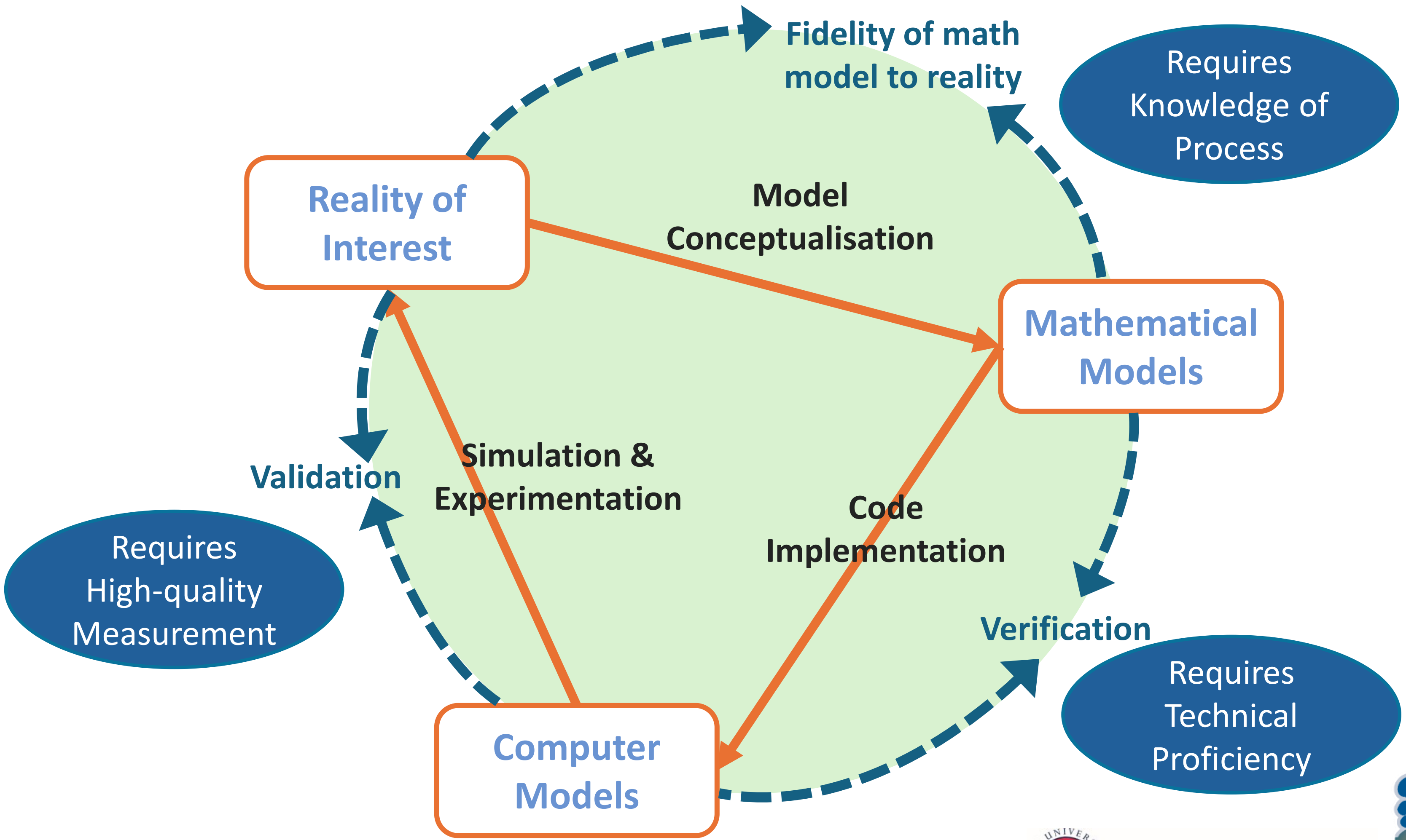


What is it for DEM and the community?

Verification Testing of Contact Models

- It is necessary to verify that the results that you get from any simulation are a correct and true representation of what is happening.
- Verification Testing will compare the known analytical solution with the results from the DEM simulation
- However, there are no "*standardised*" tests for verifying DEM codes
  - Problems involving particles only or particle & objects
  - Problems dealing with oblique impacts (varying angles & velocities) have been proposed
- 8 "*benchmark*" cases adopted here for checking P-P & P-G Interaction
  - Chung & Ooi, 2011

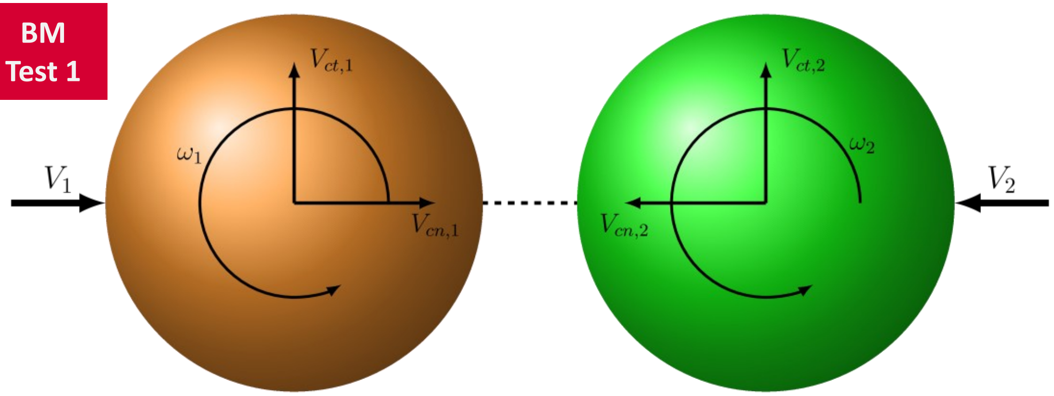
Chung, Y. C., & Ooi, J. Y. (2011). Benchmark tests for verifying discrete element modelling codes at particle impact level. *Granular Matter*, *13*(5), 643–656. https://doi.org/10.1007/s10035-011-0277-0

Verification of Elastic Contact Model

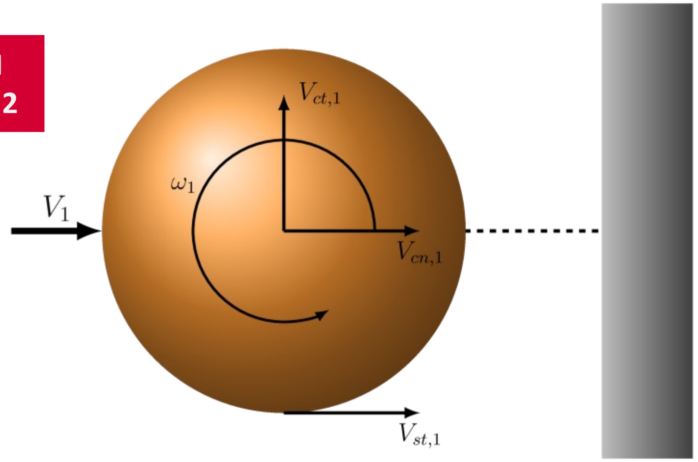
- Test 1 - Elastic Normal Contact of Two Identical Spheres
- Test 2 - Elastic Normal Contact of Sphere & Rigid Body
- Test 3 - Elastic Normal Contact of a Sphere & Rigid Body with varying Coefficients of Restitution
- Test 4 - Oblique Impact of a Sphere & Rigid Body with varying Coefficients of Restitution
- Test 5 - Oblique Impact of a Sphere & Rigid Body with varying tangential velocities
- Test 6 - Oblique Impact of 2 identical spheres with constant normal velocities and varying angular velocities
- Test 7 - Oblique Impact of 2 identical spheres with constant normal velocities and varying angular velocities
- Test 8 - Oblique Impact of 2 identical spheres with constant normal velocities and varying angular velocities

Verification Tests 1-4

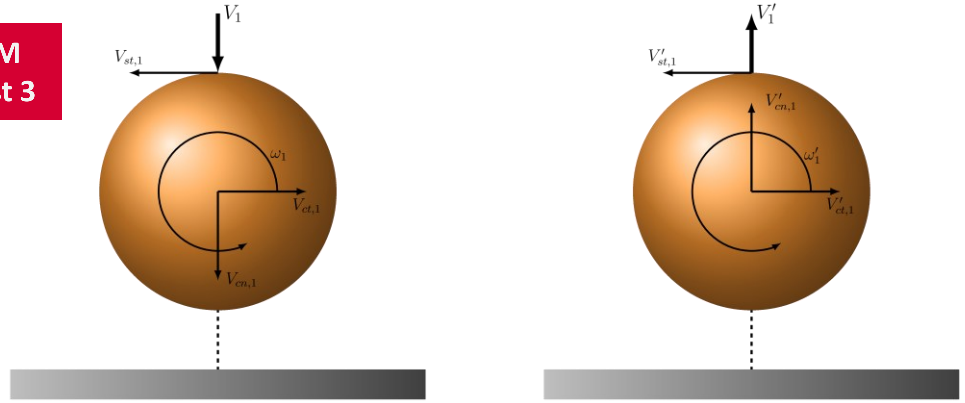
BM Test 1



BM Test 2

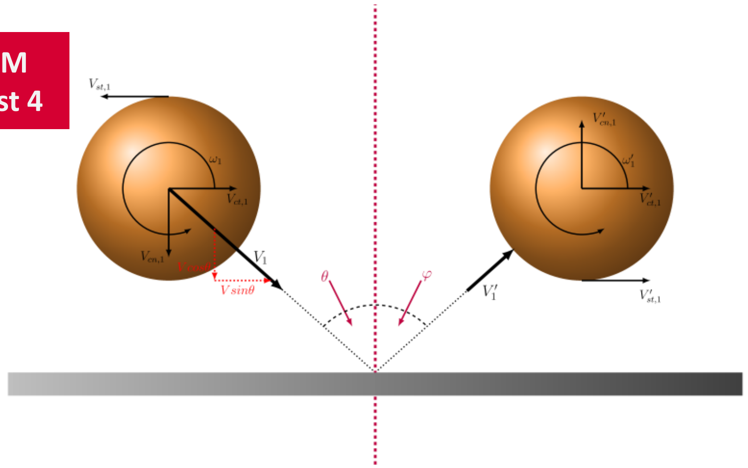


BM Test 3



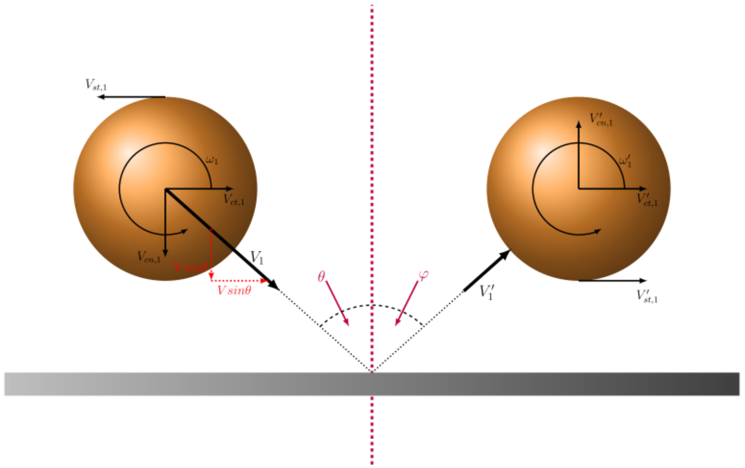
Before Impact — After Impact

BM Test 4

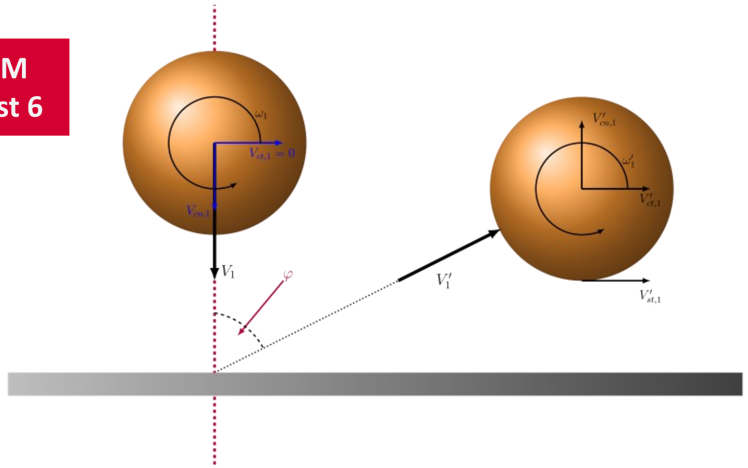


Verification Tests 5-8

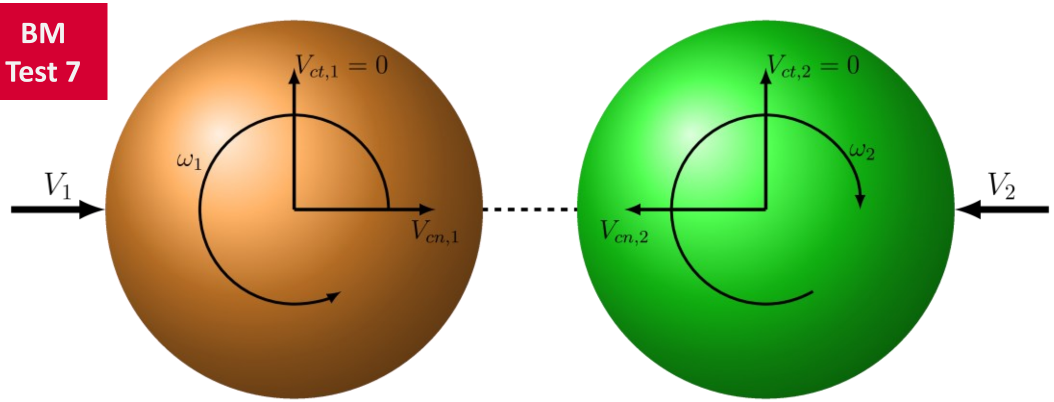
BM Test 5



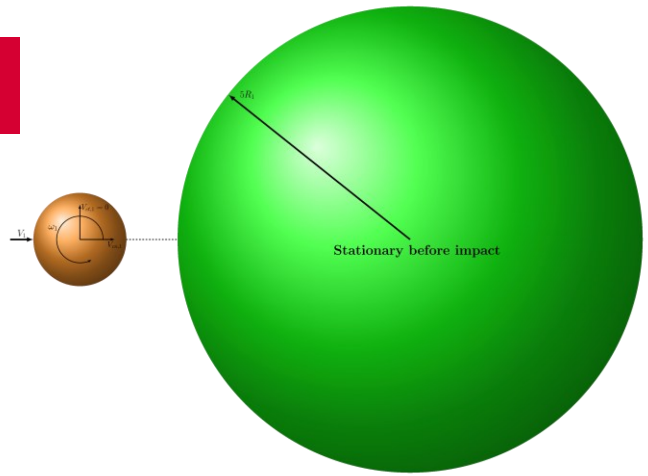
BM Test 6



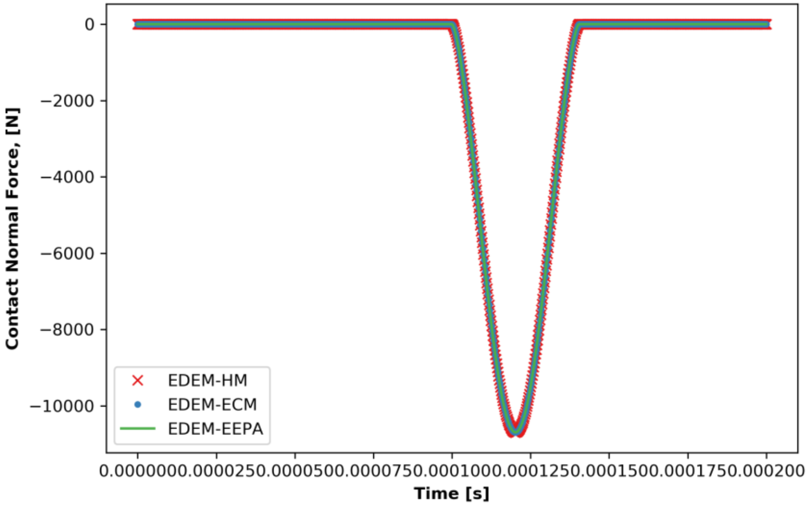
BM Test 7

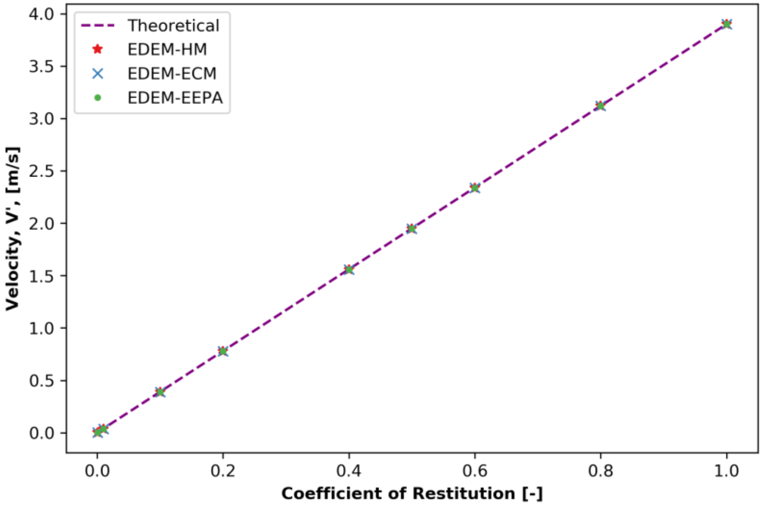


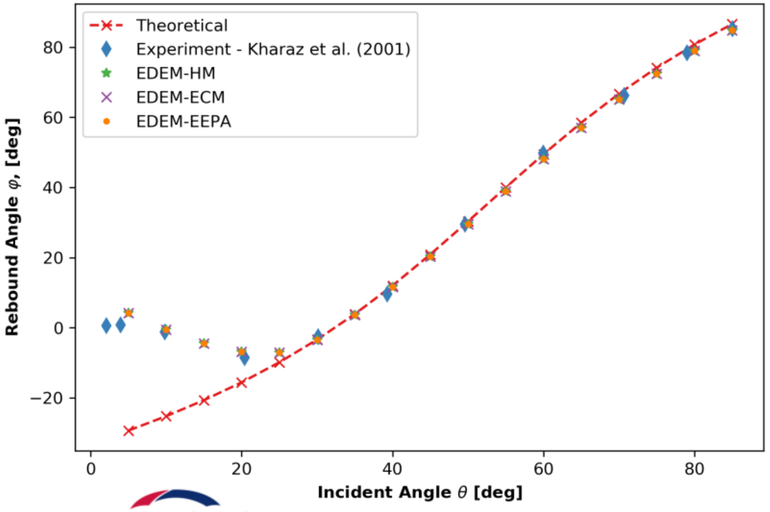
BM Test 8

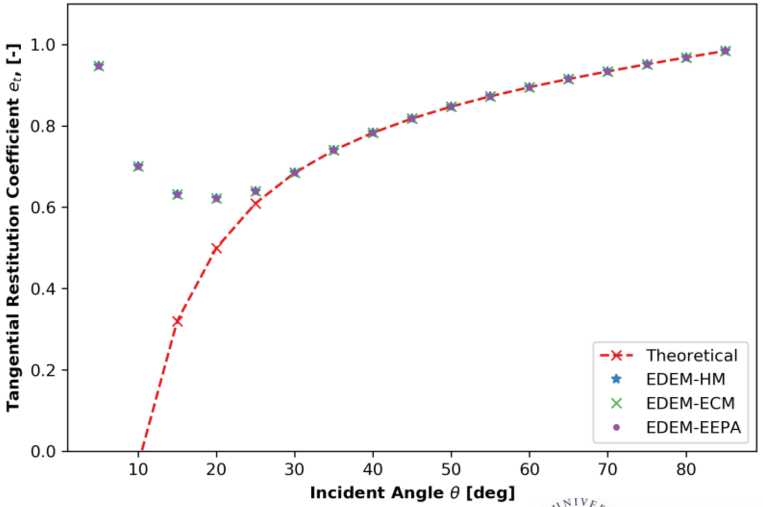


Selected Verification Results









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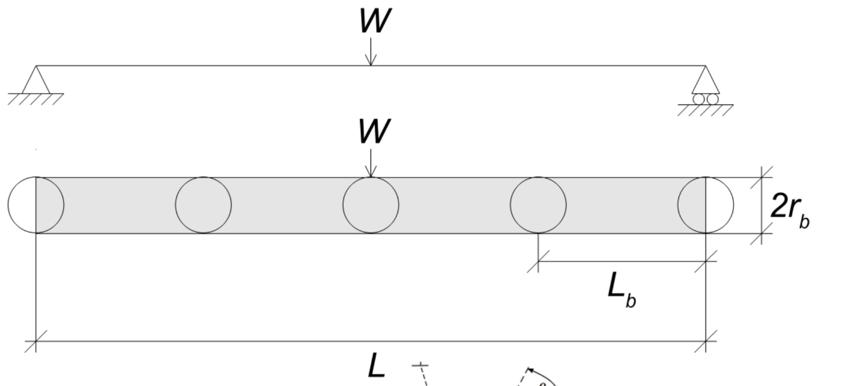
Extending for Other Model Types

- This type of verification testing can typically be carried out for most types of contact models
  - Rolling friction tests to measure torque on slope
  - Sliding friction on inclined plane
  - Bond models are often verified using 3-point bending tests and cantilever displacement tests
  - Known solution for JKR/DMT model
  - Known solution for liquid bridge model



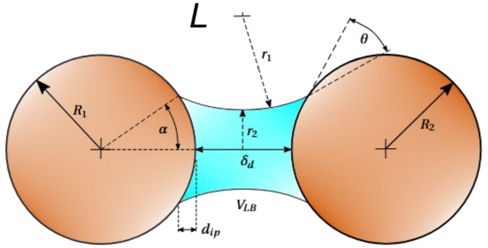


Figure 1: Liquid-bridge between two particles

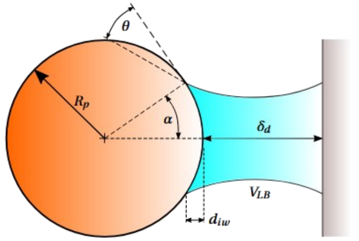
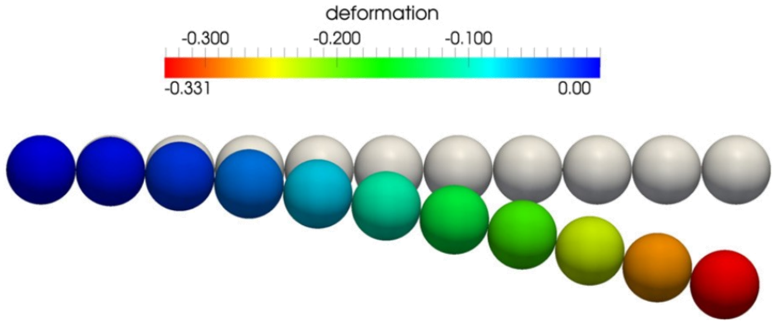


Figure 2: Liquid-bridge between a particle and a wall

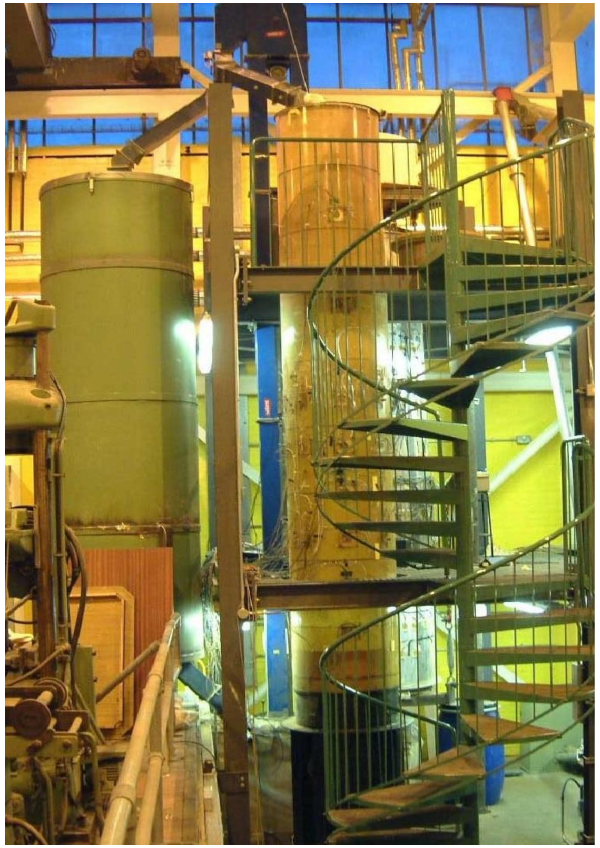


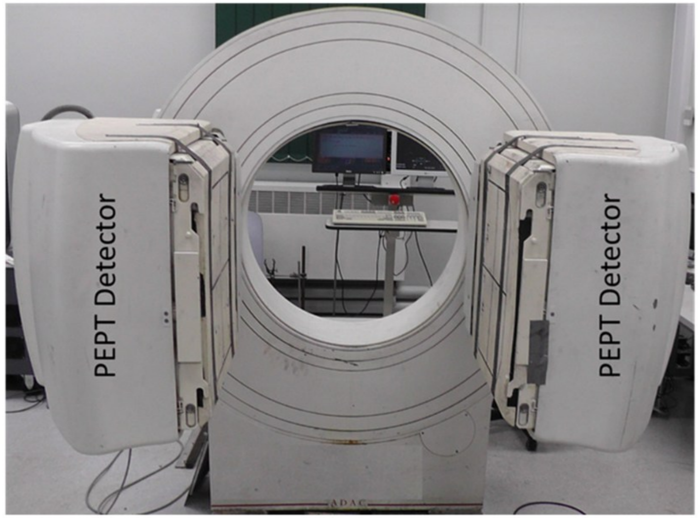
A secondary role...

- These simple problems serve as excellent introductory problems to DEM and any DEM code
- As a training exercise they:
  - Ensure the user has an understanding of the basic mechanics being tested in order for them to set up the problem correctly
  - Ensure the user knows how to use the features of a code to set up a very specific, well controlled problem with well defined boundary conditions
  - Learn about the DEM method and the importance of aspects such as calculation timestep
  - Learn to interrogate the DEM data to make a rigorous comparison with a theoretical solution
- Ideally users should be able to replicate such tests before moving on to more complex industrial or research problems

Validation is More Challenging

- The goal of validation is to quantify confidence in the predictive capability of the model by comparison with experimental data
  - Requires high quality measurement data which can be difficult to come by
  - Uncertainty quantification of the experimental data
  - Quantitative comparison
  - ££££££





What is Benchmarking Anyway?

- Typically described as *"the process of measuring or comparing a product or service against another to identify areas of weakness or for improvement"*
  - Process benchmarking
  - Performance benchmarking
  - Strategic benchmarking
  - Common business practice
- In computer science Benchmarking is the process of measuring and comparing the performance of a computer system, its hardware (like CPUs and GPUs), or software (like databases) using standardised tests
  - We often do this to compare performance between DEM codes and/or HPC resources
  - The outcome of the simulation is irrelevant, the size of the problem is of concern

Capturing Key Physics

- There is a need for proving that models capture the correct physics before using to study a problem
- A qualitative verification that a complex model can capture the key physics of a real system
  - A DEM Benchmark Suite

- **ON-DEM WG4** is looking at best practices and has begun the process of developing a series of DEM problems for benchmarking, verification & validation
  - Particle level dynamics
  - Granular shear flow between rough walls
  - Triaxial monotonic compression
  - Masonry blocks
  - Rotating drums
  - Tabletting

Silo Discharge Benchmark Problem

- Silo discharge is a very common industrial use case
- It is still very difficult to design a silo that is sufficiently strong

Silo Discharge Benchmark Problem

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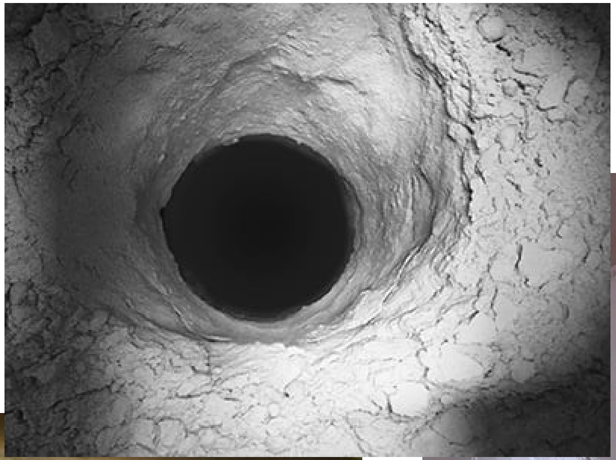
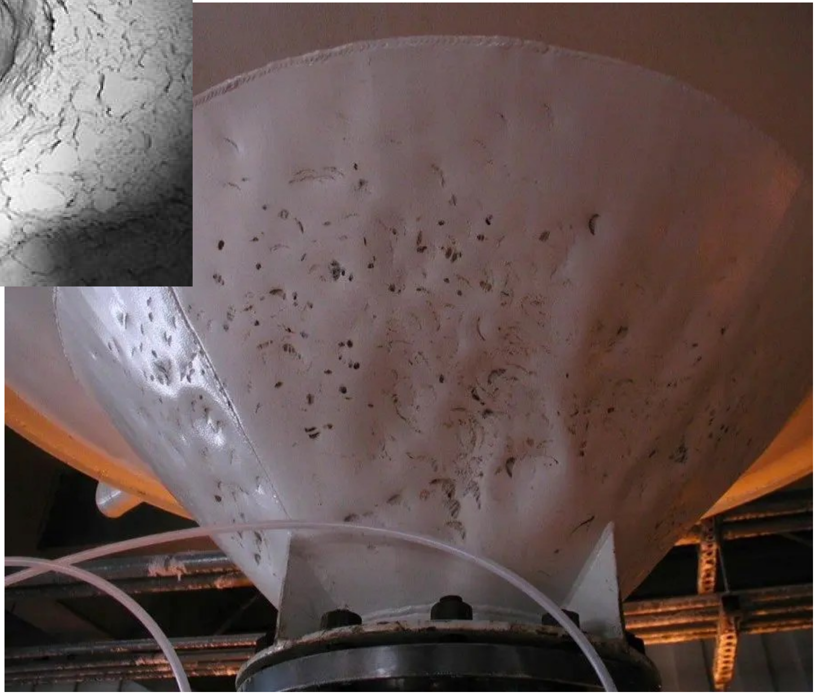
Silo Discharge Benchmark Problem

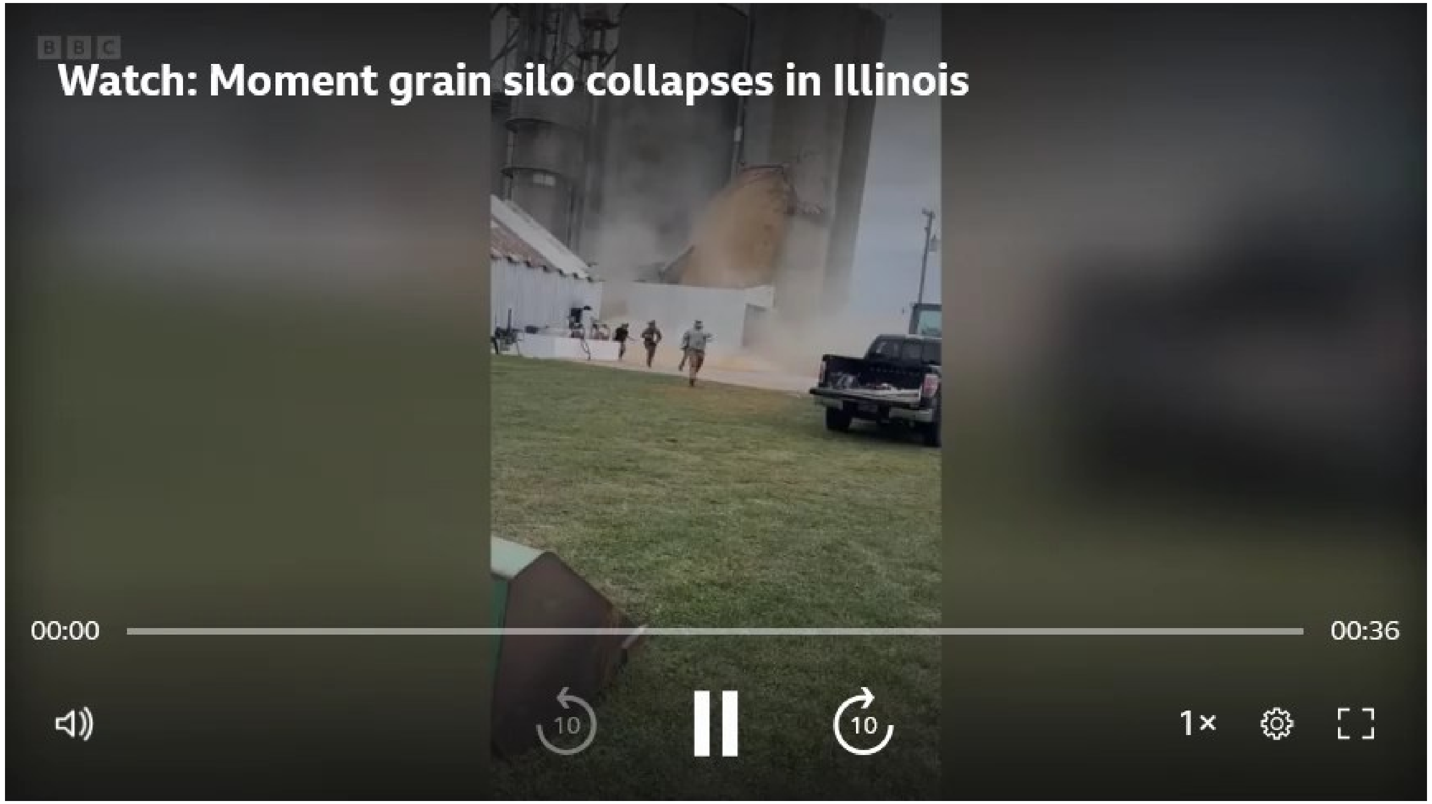
- Silo discharge is a very common industrial use case
- It is still very difficult to design a silo that material will flow from

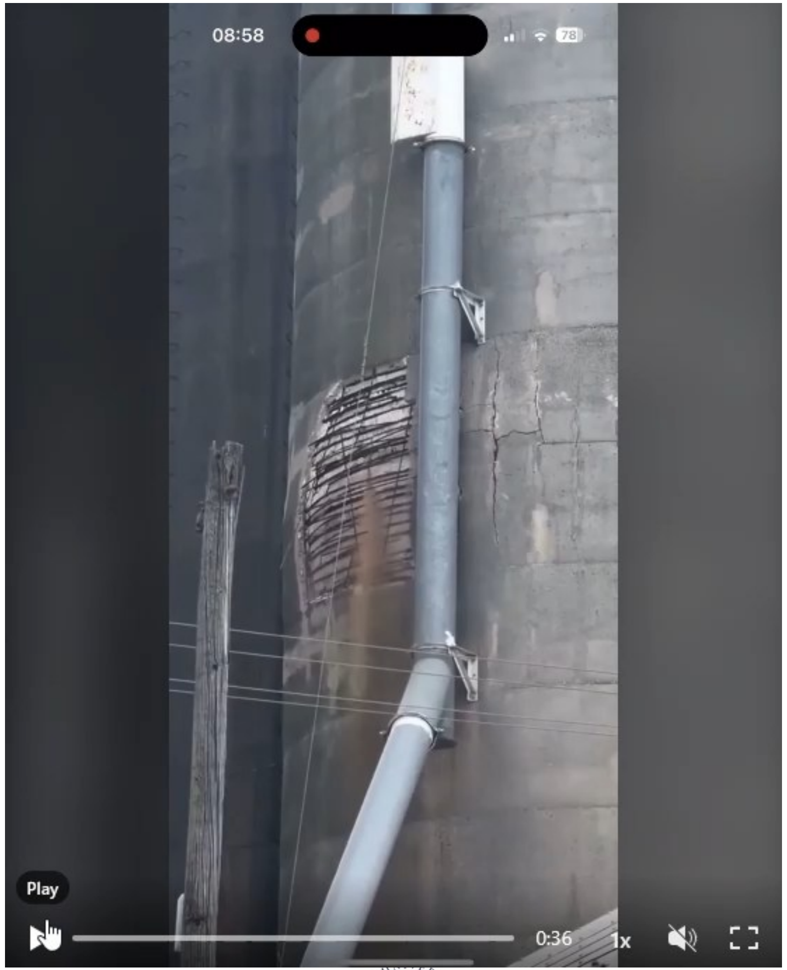


Grain Silo Collapse

- Grain silo in Illinois, USA
  - https://www.bbc.co.uk/news/videos/cwy75we8nnlo





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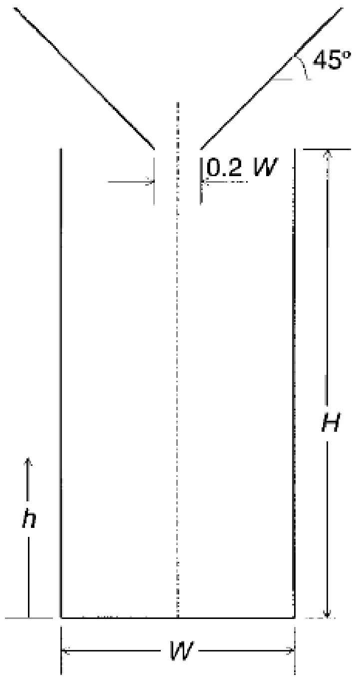
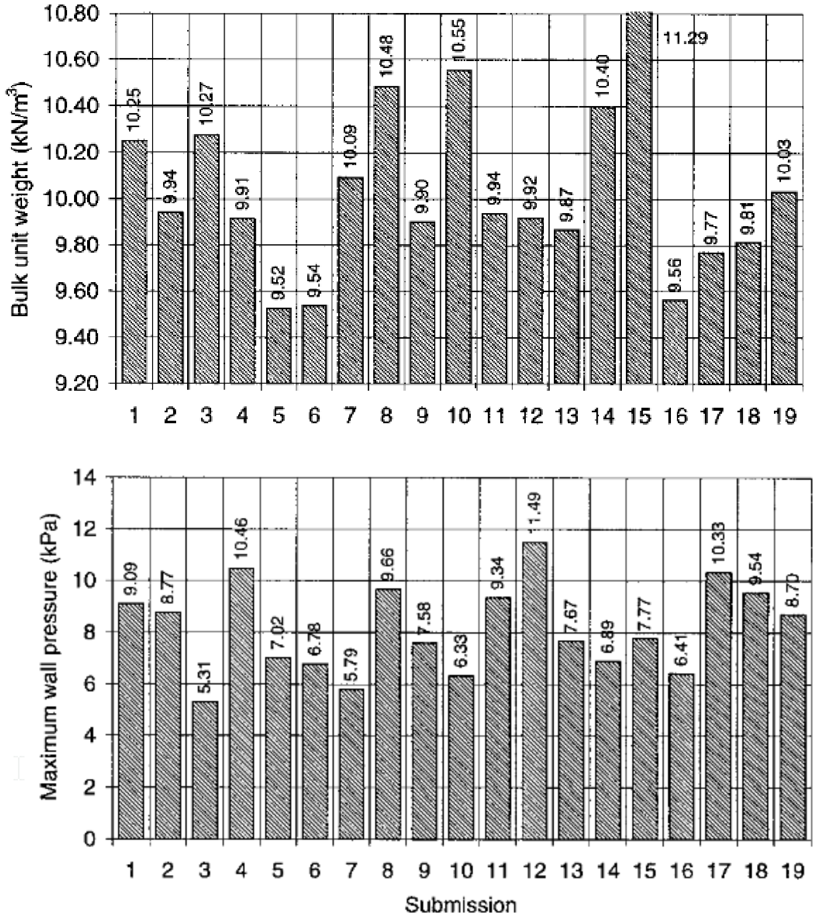
DEM Silo Benchmark Tests

- An excellent test case for DEM
  - Analytical predictions for silo wall pressures and discharge rates through an orifice
  - Eurocode EN 1991-4:2006 describes the uses of simple Janssen Theory for calculating wall pressures during the design of silos
  - Beverloo provided the prediction of discharge of discharge rate for a given opening width and particle size combination
- Not the first time tried in DEM!





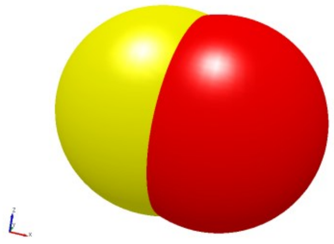
Holst, J.M.F.G., Rotter, J.M., Ooi, J.Y., Rong, G.H., 1999. Numerical Modeling of Silo Filling. II: Discrete Element Analyses. J. Engrg. Mech. 125, 104–110.

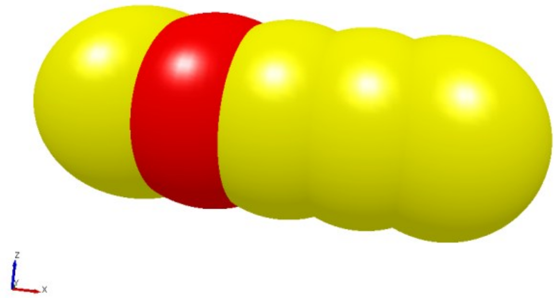
Rotter, J.M., Holst, J.M.F.G., Ooi, J.Y., Sanad, A.M., 1998. Silo pressure predictions using discrete–element and finite–element analyses. Philosophical Transactions of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences 356, 2685–2712.

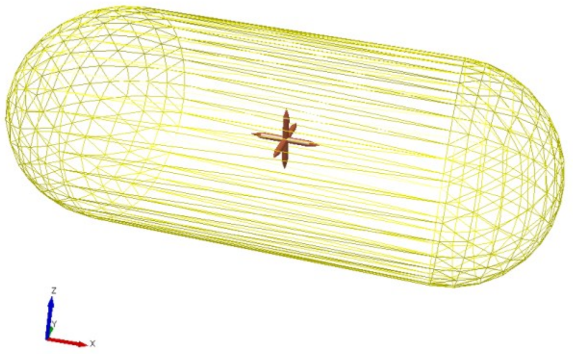
Developing a Silo DEM Benchmark

- Several items of interest:
  - Predicted fill level (and resulting bulk density)
  - Predicted wall pressure distribution (Eurocode)
  - Predicted discharge rate (Beverloo)

- Consider several particle shapes:
  - ~~Sphere~~
  - Multi-sphere with very low aspect ratio (AR=1.25)
    - Sphere radius = 1mm
    - 80K particles
  - Multi-sphere with high aspect ratio (AR=2.5)
  - Sphero-cylinder with high aspect ratio (AR=2.5)
    - 40K particles
  - Interparticle friction = 0.4
  - EPSD / Type C rolling friction model (0.01)

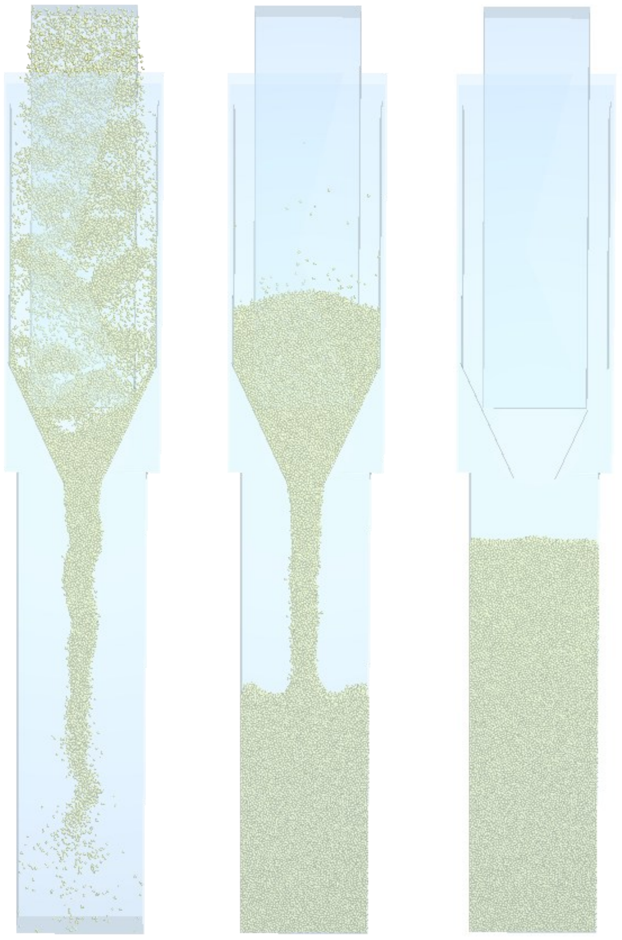




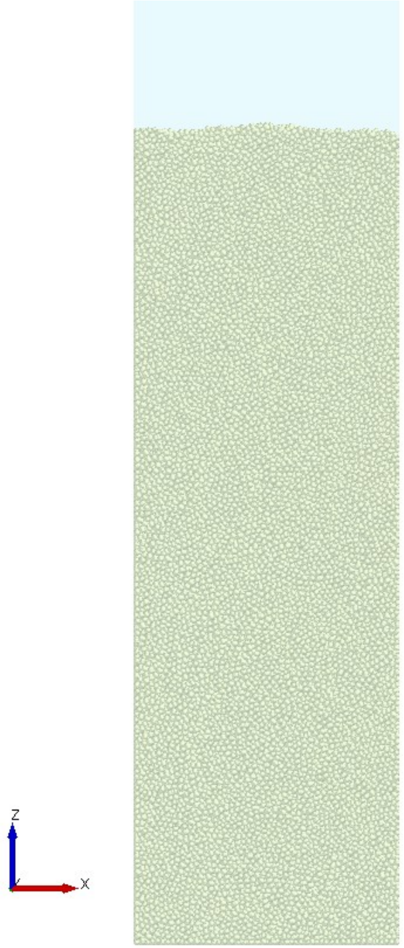


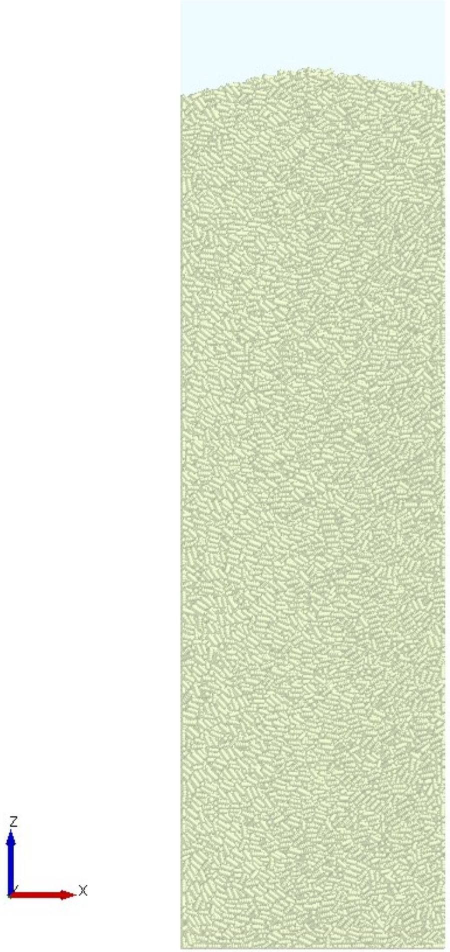
Silo Geometry

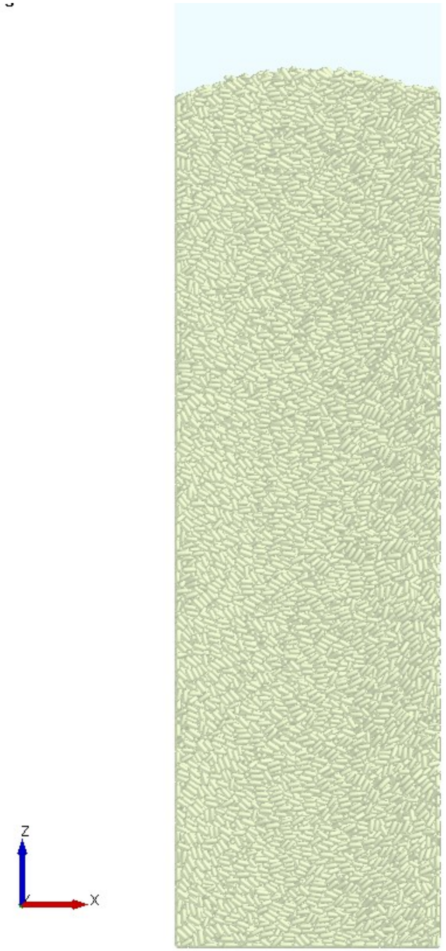
- Geometry
  - Width = 0.1m (40-50 particles of low AR)
  - Height = 0.4m
  - Depth = 0.025m
  - Non-periodic
    - Frictionless walls front and rear
    - Frictional walls elsewhere
  - 2 wall friction values: 0.1, 0.6
- Relatively tall silo
  - Aspect ratio when filled > 3
- 4 opening widths
  - 10, 20, 30, 40 (mm)



Filled Particle Silos







Why So Tall?

- The horizontal pressure p_h in the container can be described by Janssen equation for cylindrical silo (Eurocode 1) by:

$$p_{hf}(z) = \gamma K z_0 \left[1 - exp^{\frac{-z}{z_0}}\right]$$

$$z_0 = \frac{1}{\mu K}\frac{A}{U}$$

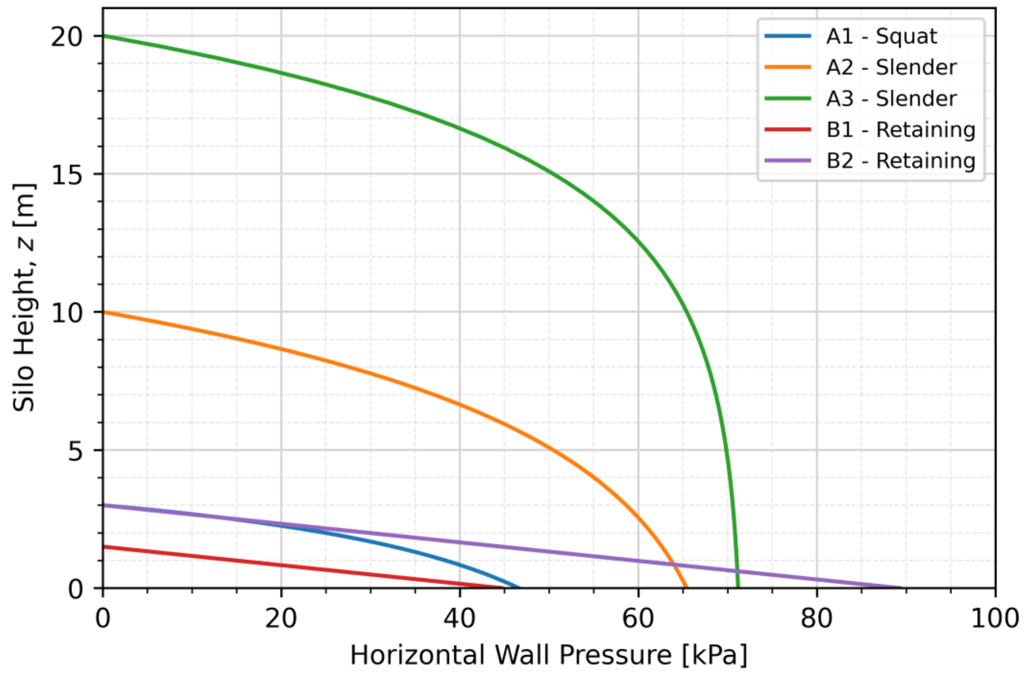
$$p_{vf}(z) = \frac{p_{hf}}{K}$$

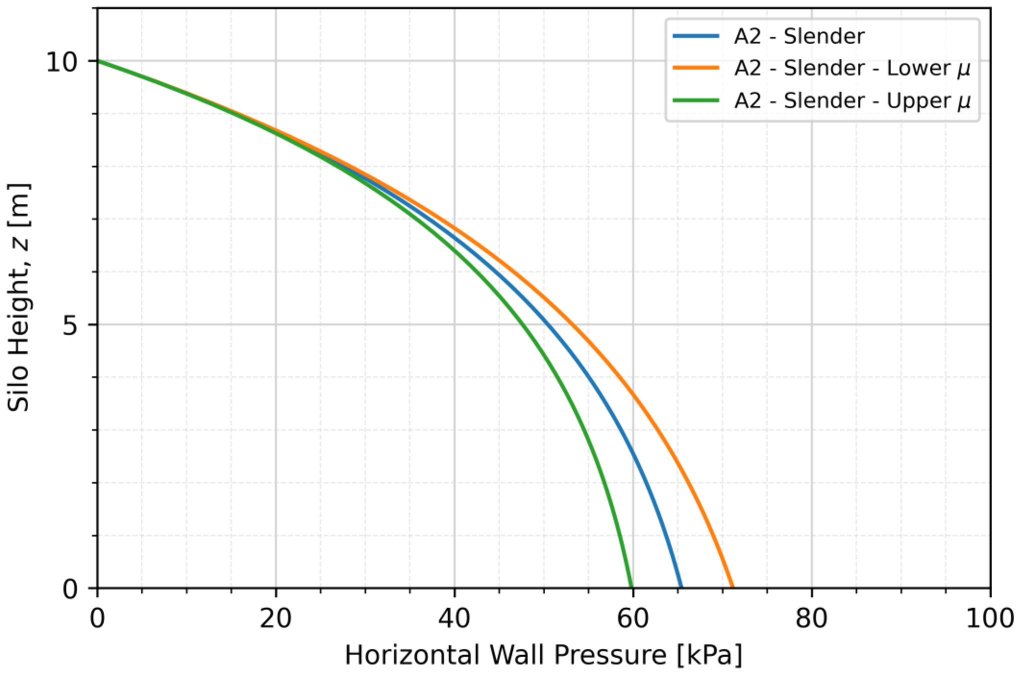
where γ, K, A, U, $\mu = \tan\phi_w$ are the characteristic unit weight, lateral pressure ratio, plan cross-sectional area, plan internal perimeter and the wall friction coefficient respectively

- Material Properties
  - Lateral pressure ratio, K = 0.2, 0.45, 0.7
  - Unit Weight 38.74 kN/m^3
  - Wall friction ≈30°

Diameter	Heights	Label
4m	3m, 10m, 20m	A1, A2, A3
7.5m	3m	B1
10m	1.5	B2

Silo Behaviour





Key observations:

1. The solid stresses reach maximum/asymptotic value of $p=\gamma D/4\mu$ and $\sigma_v=\gamma D/4\mu k$ at some depth
2. The magnitude of stress is proportional to container size times bulk density and inversely proportional to wall friction coefficient

Larger wall friction μ reduces the horizontal stress in the solid down the depth of the container

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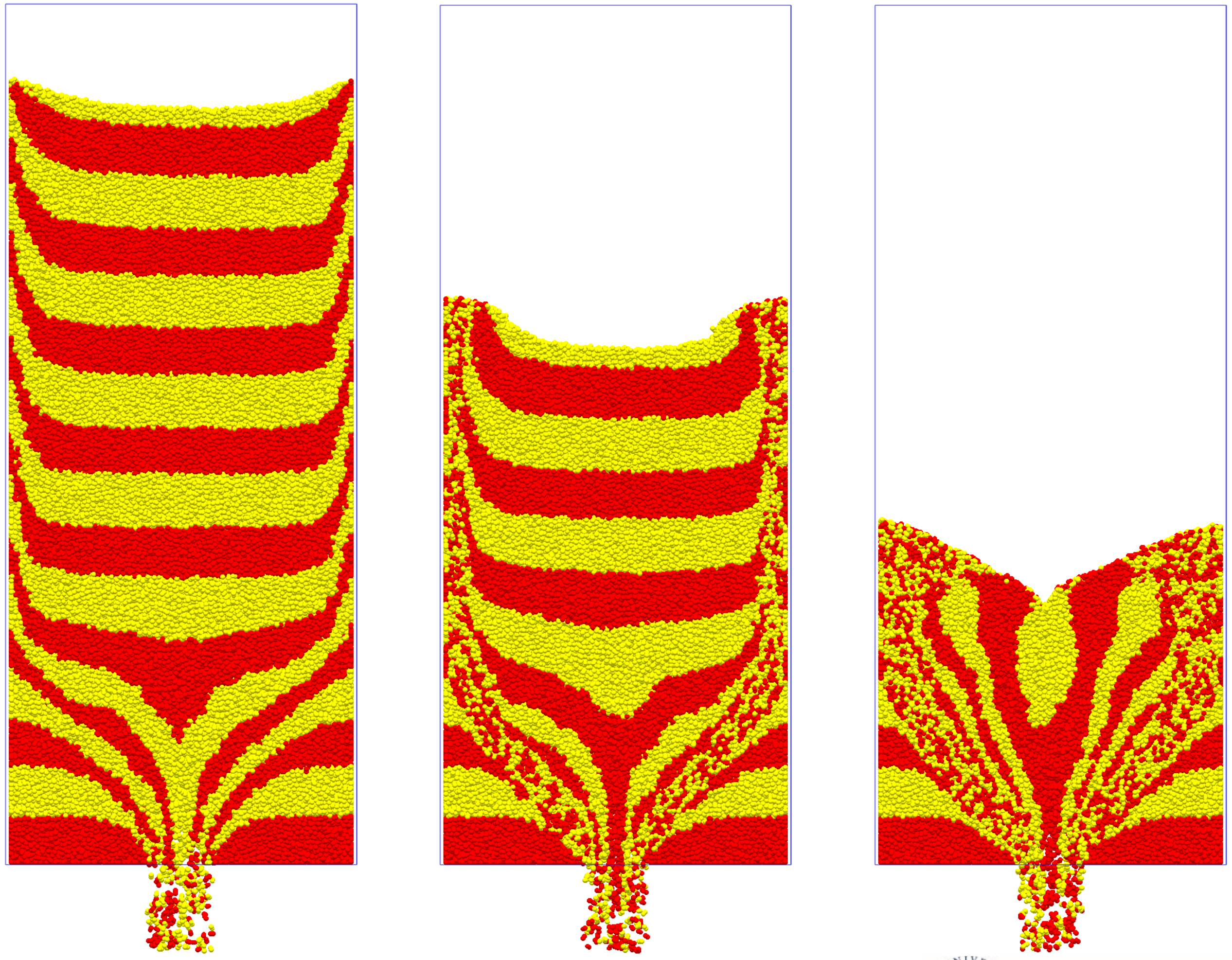
DEM Analysis Criterion

- Expected behaviour:
  - Mass flow above transition
  - Transition height
  - Shear layer at wall
  - Asymptotic wall pressure distribution
  - Asymmetric wall pressures
  - Mass flow rate variation
    - Per particle shape
    - Per opening width
    - Per wall friction value?



Results

- **Not today….**

- Initial runs completed in EDEM on GPU
  - CPU runs on EDEM, YADE, MercuryDPM and LAMMPS to be completed

- Guidance will be sought for implementations in other codes!
  - How to do dynamic factories with constant creation rate?
  - Multi-sphere (CLUMP?) and sphero-cylinder particle shapes

- Comment: Even with a few years DEM experience, switching codes is daunting!

Schedule for this Network Event

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Questions?

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Particulate Solids Simulations

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