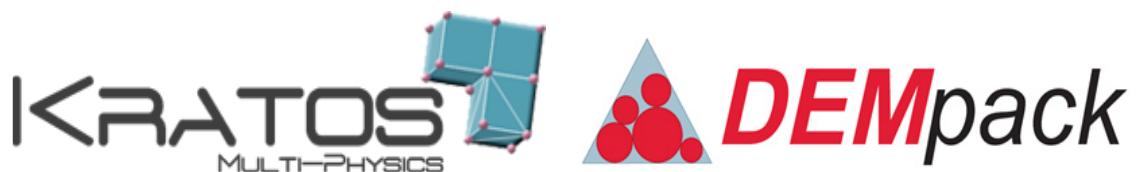


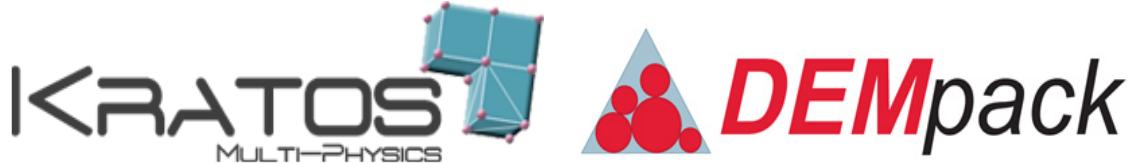
An overview on the main features of



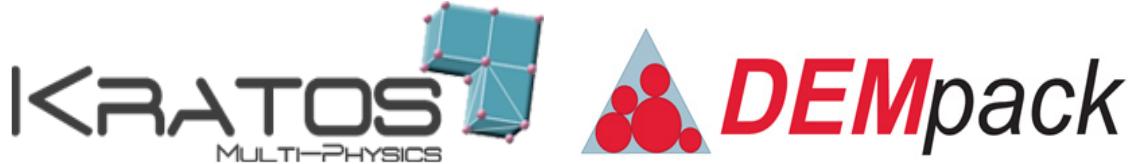
Guillermo Casas,
Miguel Angel Celigueta, Salvador Latorre,
Ferran Arrufat, Joaquín Irazábal,
Alessandro Franci, Eugenio Oñate

International Center for Numerical Methods in Engineering
Technical University of Catalonia (UPC). Barcelona. Spain

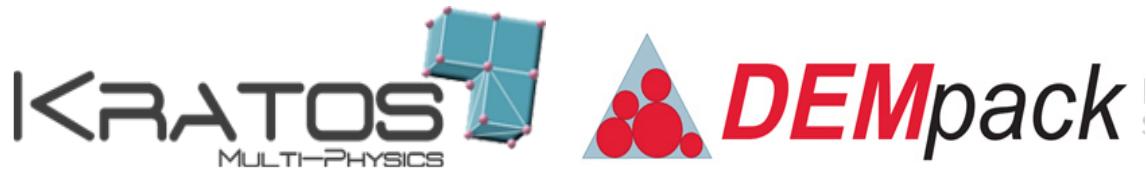




- What is Kratos - DEMpack?
- DEMpack – non-cohesive (granular materials, slightly cohesive soils)
- DEMpack – cohesive (rocks, concrete, fabrics)
- DEMpack – CFD (strong 2-way coupling)
- DEMpack – CSD (plasticity, damage)
- Wizards



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(framework)

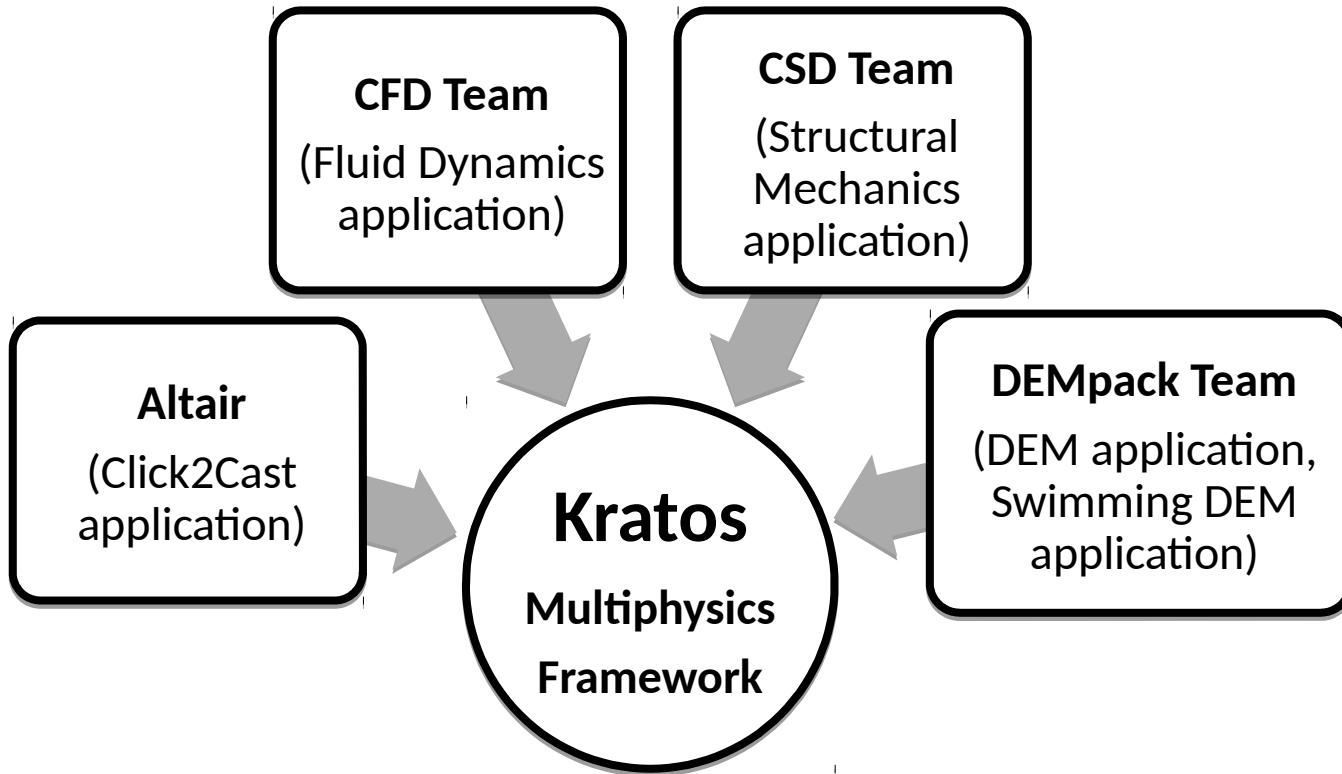
(application)

- Density



Kratos Framework

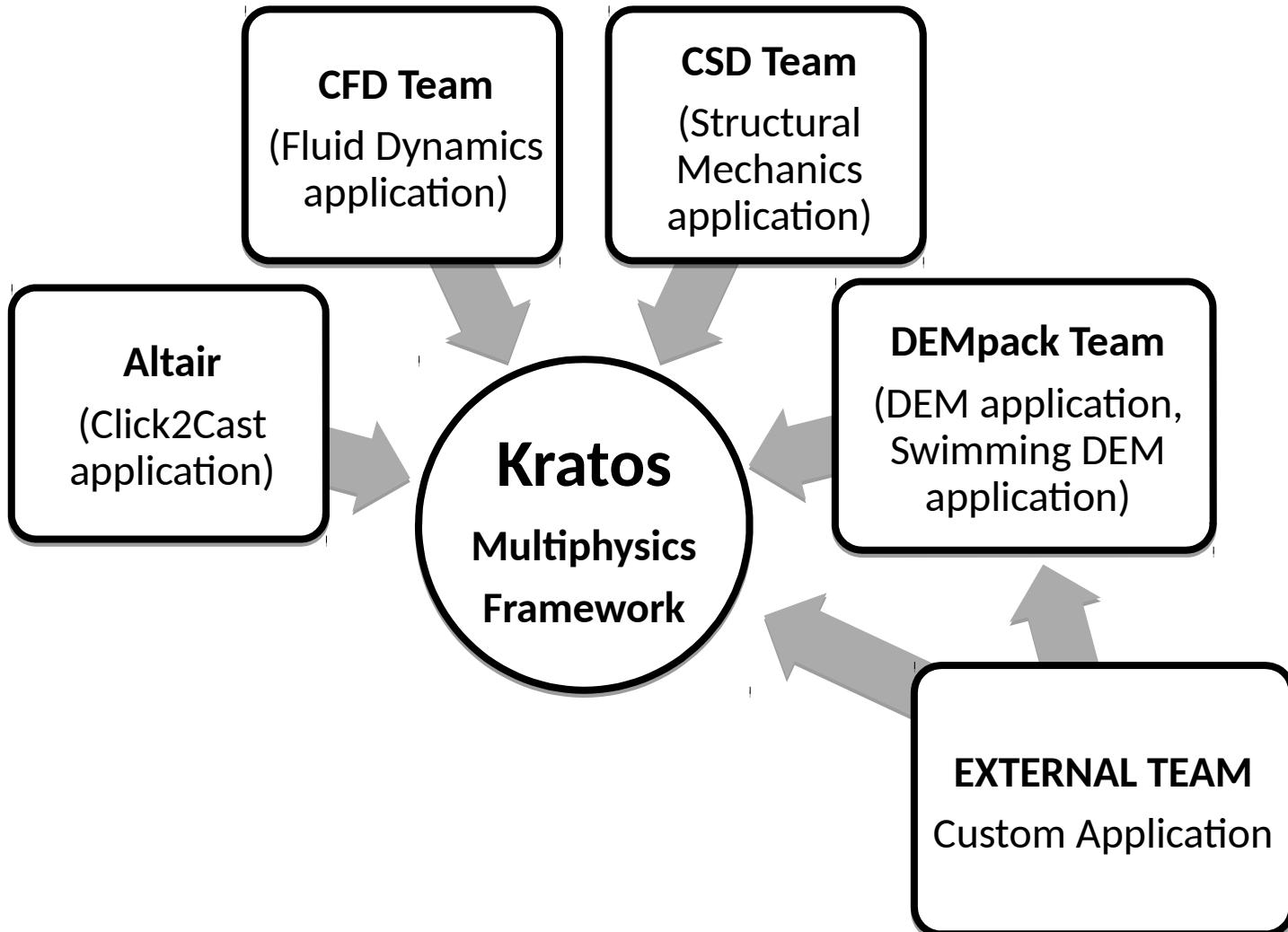
Team Working

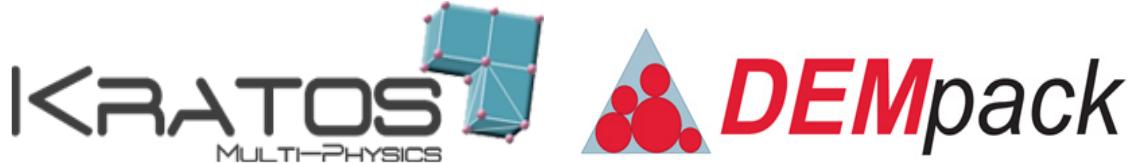


In Kratos each developer focus on his/her application and usually “talks” with Kratos or via Kratos to others

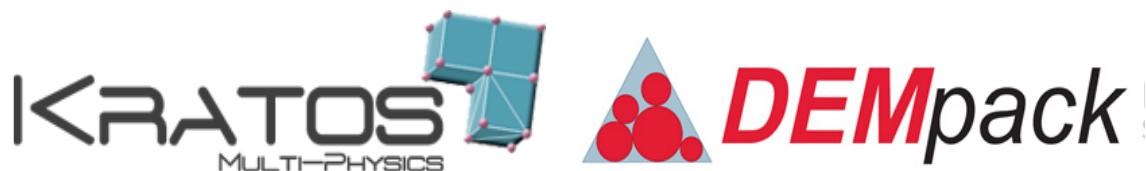
Kratos Framework

Team Working





- What is Kratos - DEMpack?
- **DEMpack – non-cohesive (granular materials, slightly cohesive soils)**
- DEMpack – cohesive (rocks, concrete, fabrics)
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- DEMpack – CSD (plasticity, damage)
- Wizards



(framework)

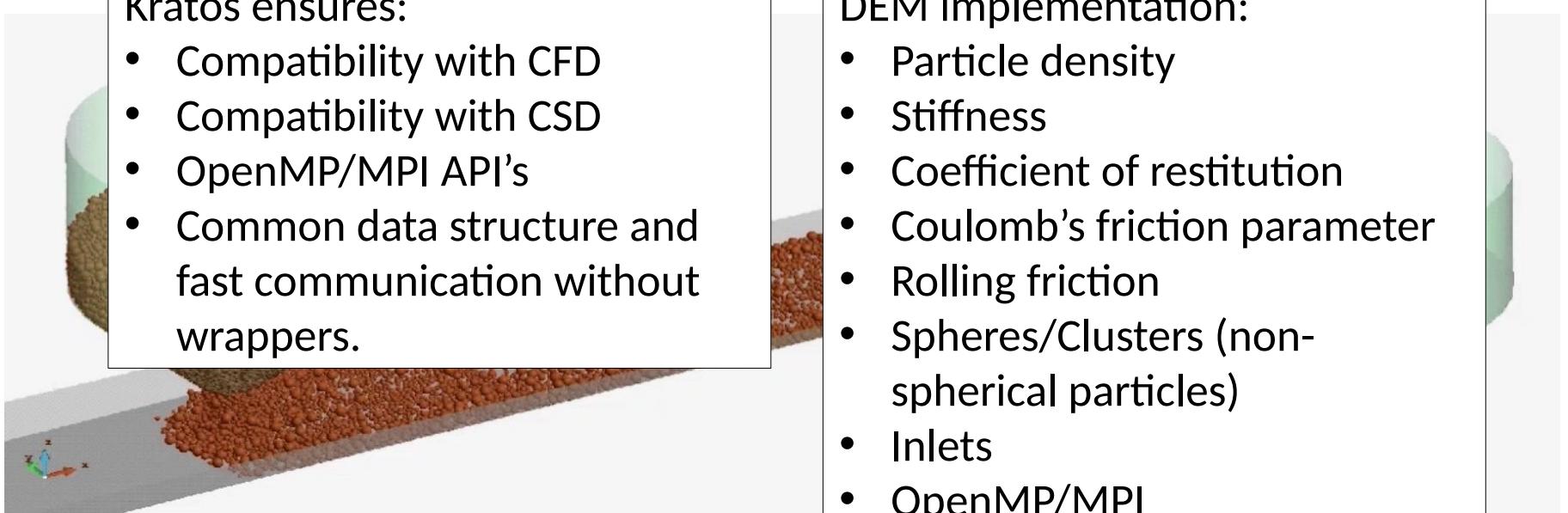
Kratos ensures:

- Compatibility with CFD
- Compatibility with CSD
- OpenMP/MPI API's
- Common data structure and fast communication without wrappers.

(application)

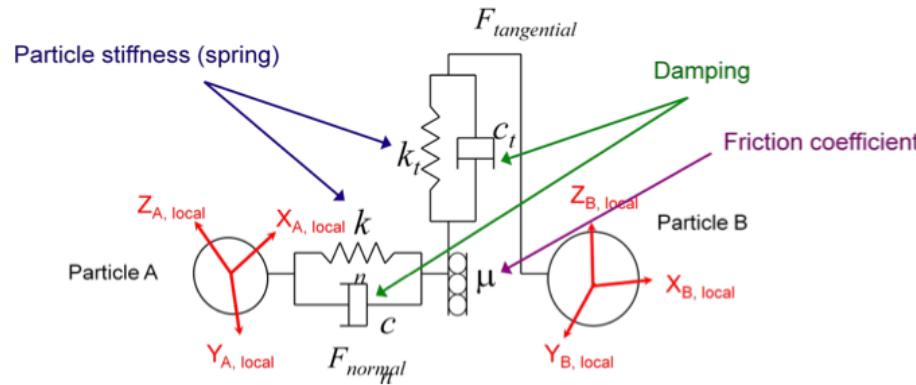
DEM implementation:

- Particle density
- Stiffness
- Coefficient of restitution
- Coulomb's friction parameter
- Rolling friction
- Spheres/Clusters (non-spherical particles)
- Inlets
- OpenMP/MPI



Contact force models: Linear Spring Dashpot, Hertz Mindlin Dashpot

C. Thornton, S. J. Cummins, and P. W. Cleary. *An investigation of the comparative behaviour of alternative contact force models during inelastic collisions*. Powder Technology, 233:30-46, 2013.



$$\text{HMD: } F_n = \frac{4}{3} E^* R^{1/2} \alpha^{3/2} + 2\gamma \sqrt{mk_n} v_n$$

$$F_{te}^n = F_{te}^{n-1} + k_t^n \Delta \delta \quad \text{for } \Delta F_n \geq 0$$

$$F_{te}^n = F_{te}^{n-1} \left(\frac{k_t^n}{k_t^{n-1}} \right) + k_t^n \Delta \delta \quad \text{for } \Delta F_n < 0$$

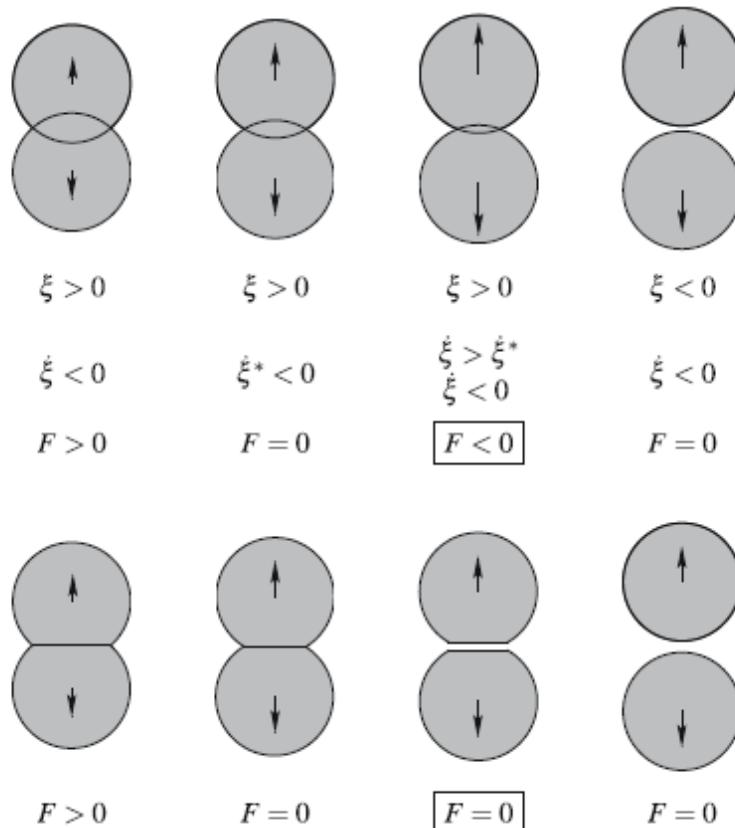
$$F_t = F_{te}^n + 2\gamma \sqrt{mk_t} v_t \quad \text{except if } F_t \geq \mu F_n \text{ then } F_t = \mu F_n$$

where R is the radius of the sphere and the variable stiffnesses are given by

$$k_n = 2E^* \sqrt{R\alpha} \quad \text{and} \quad k_t = 8G^* \sqrt{R\alpha}.$$

Contact force models: Linear Spring Dashpot, Hertz Mindlin Dashpot

C. Thornton, S. J. Cummins, and P. W. Cleary. *An investigation of the comparative behaviour of alternative contact force models during inelastic collisions*. Powder Technology, 233:30-46, 2013.



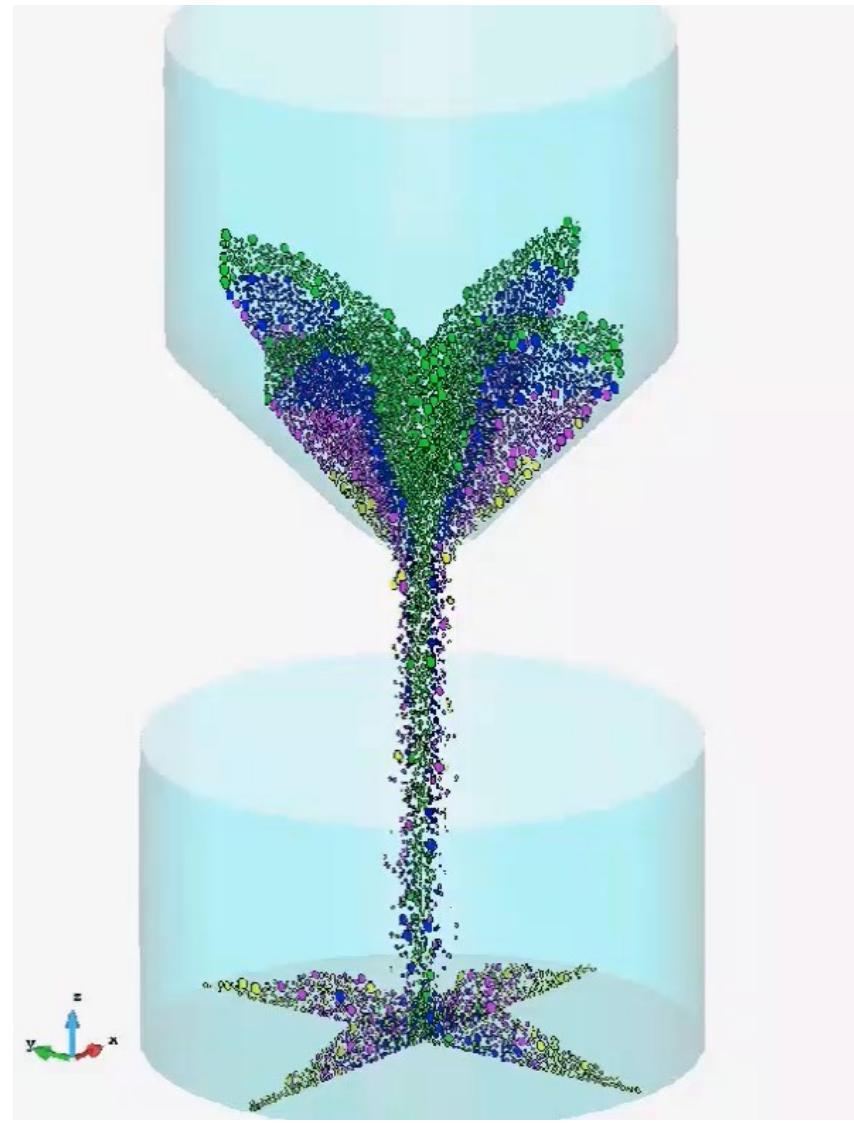
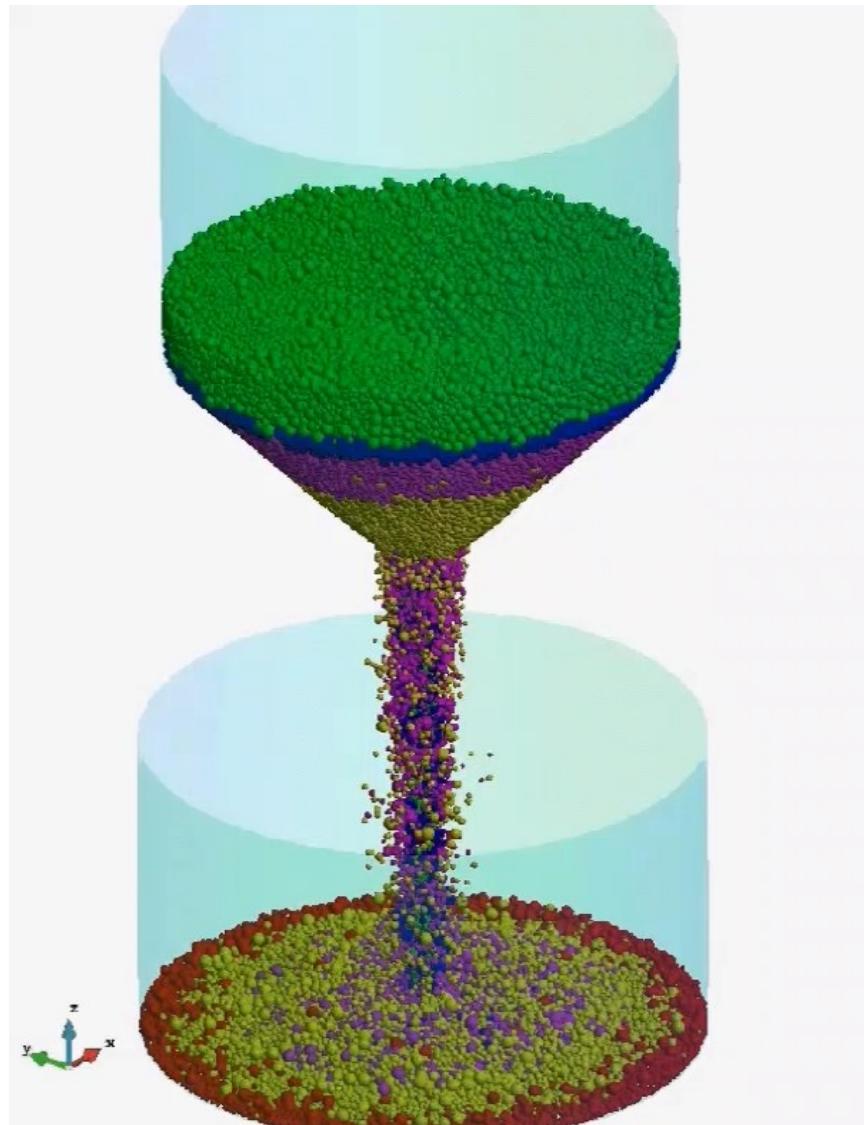
**shorter contact time, so
stronger damping to ensure fulfilment of
the Coefficient of Restitution.**

Other features:

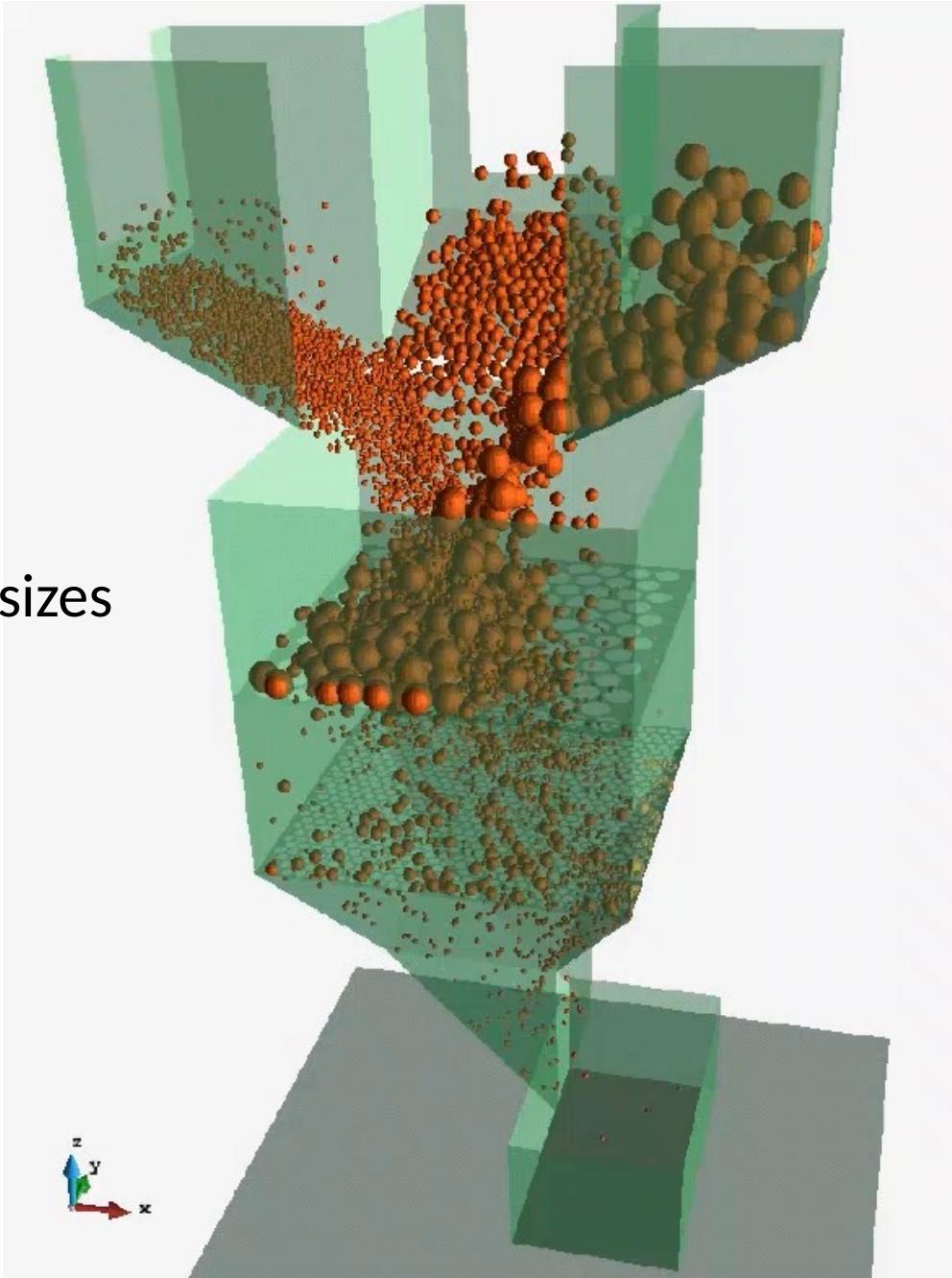
- All contact models ('constitutive laws') can be plugged or unplugged to the sphere
- JKR and MDT cohesion
- Several integration schemes

No traction allowed and abrasion wear for walls

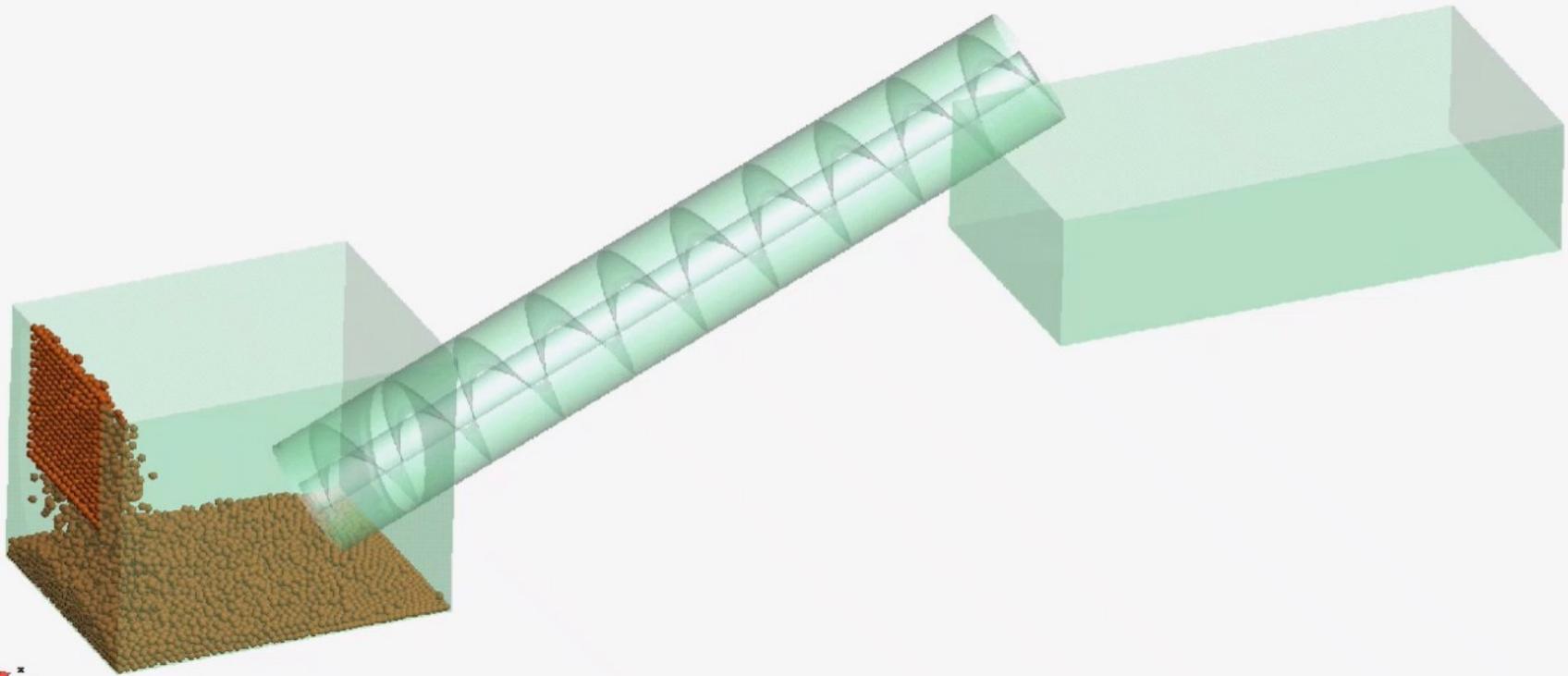
DISCONTINUUM METHODS (PARTICLES) FOR GRANULAR FLOWS



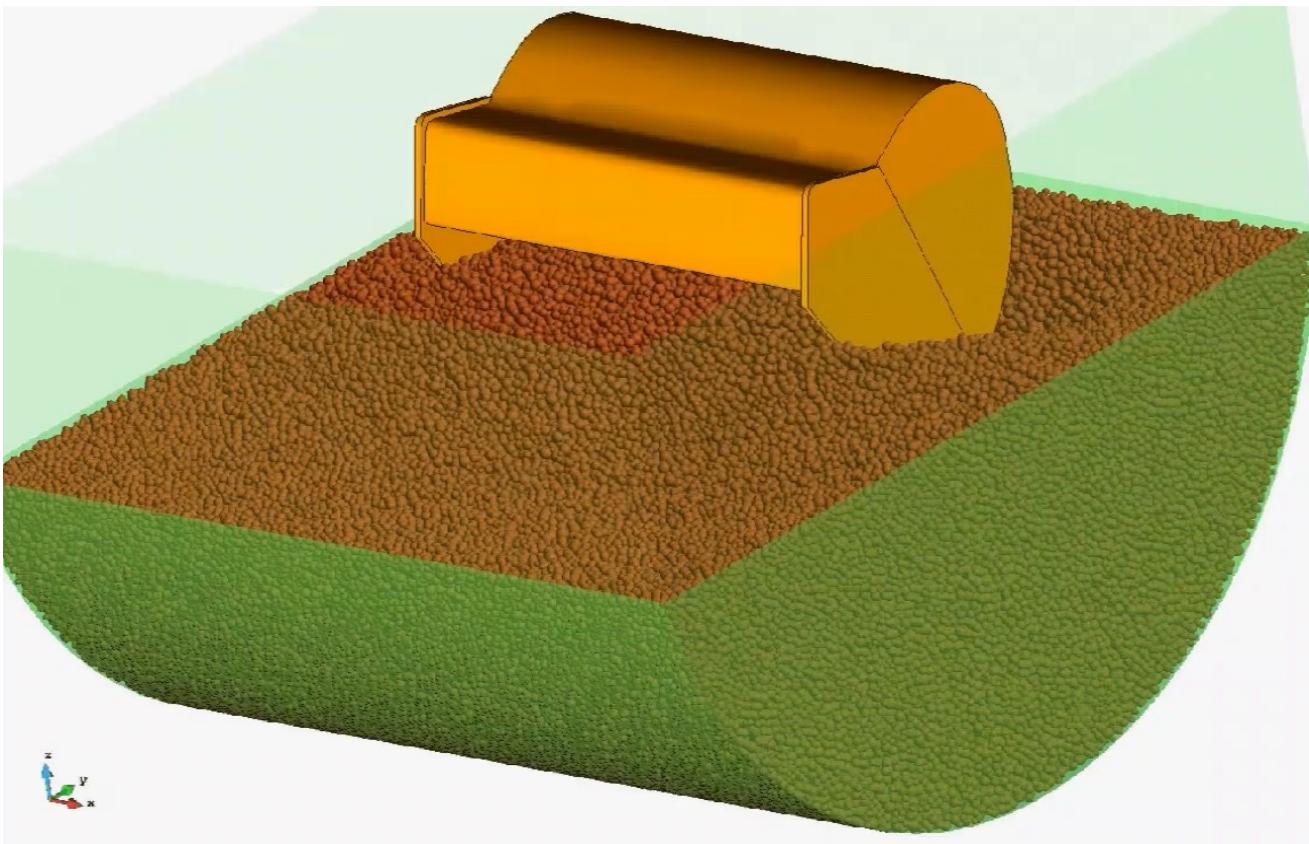
Sieve, 3 different sizes



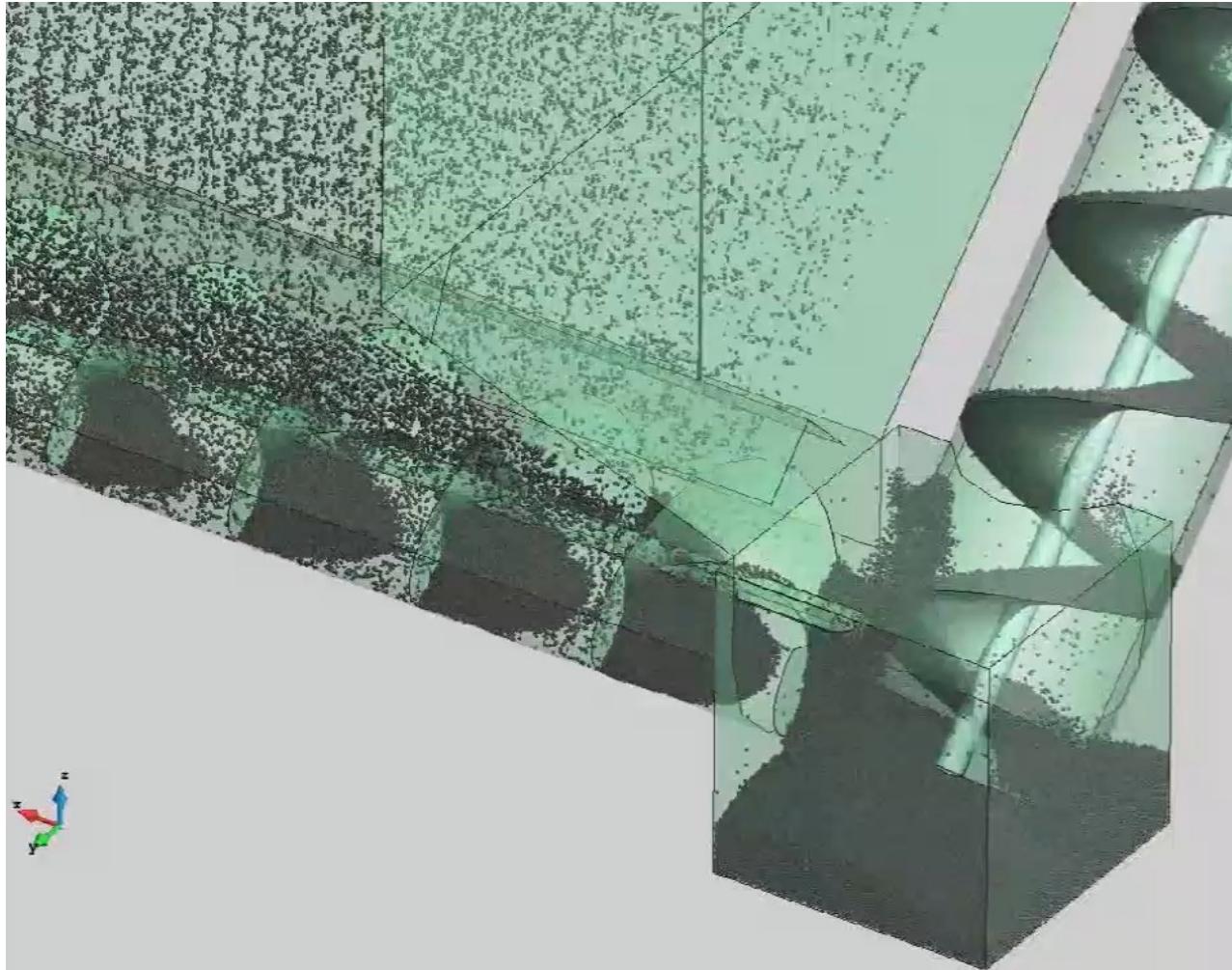
Archimedes screw for granular matter



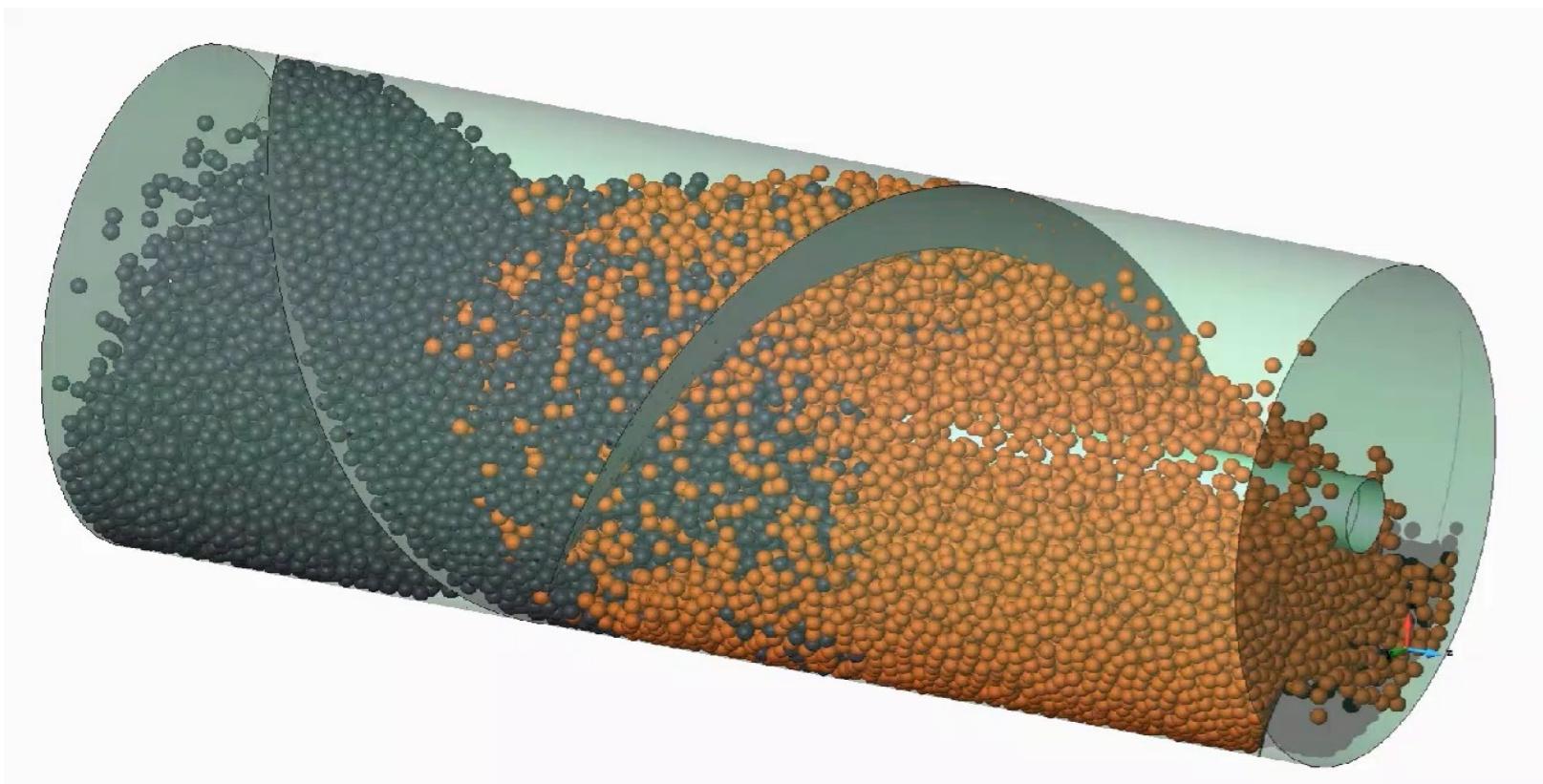
Mining bucket



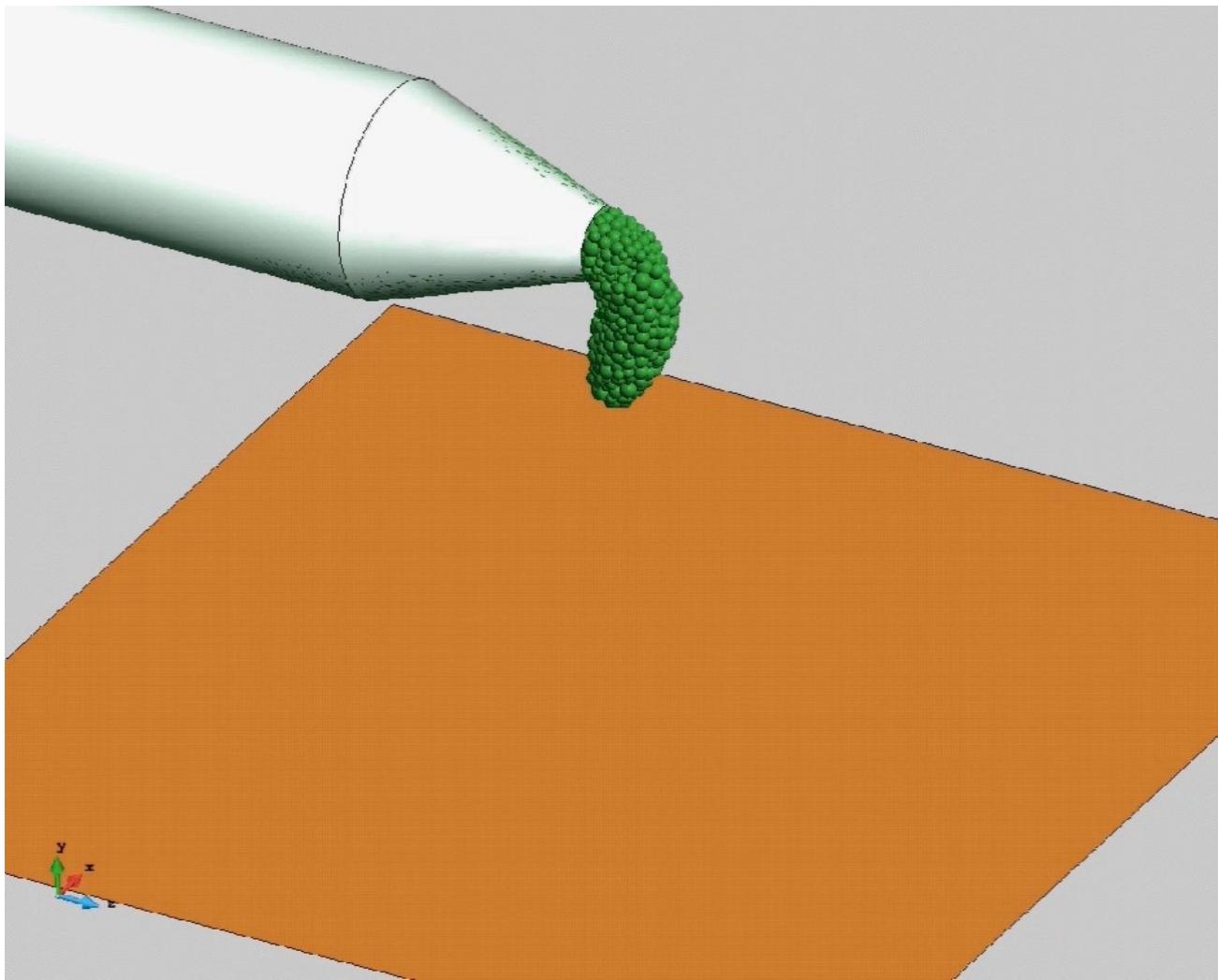
Feeding and conveying



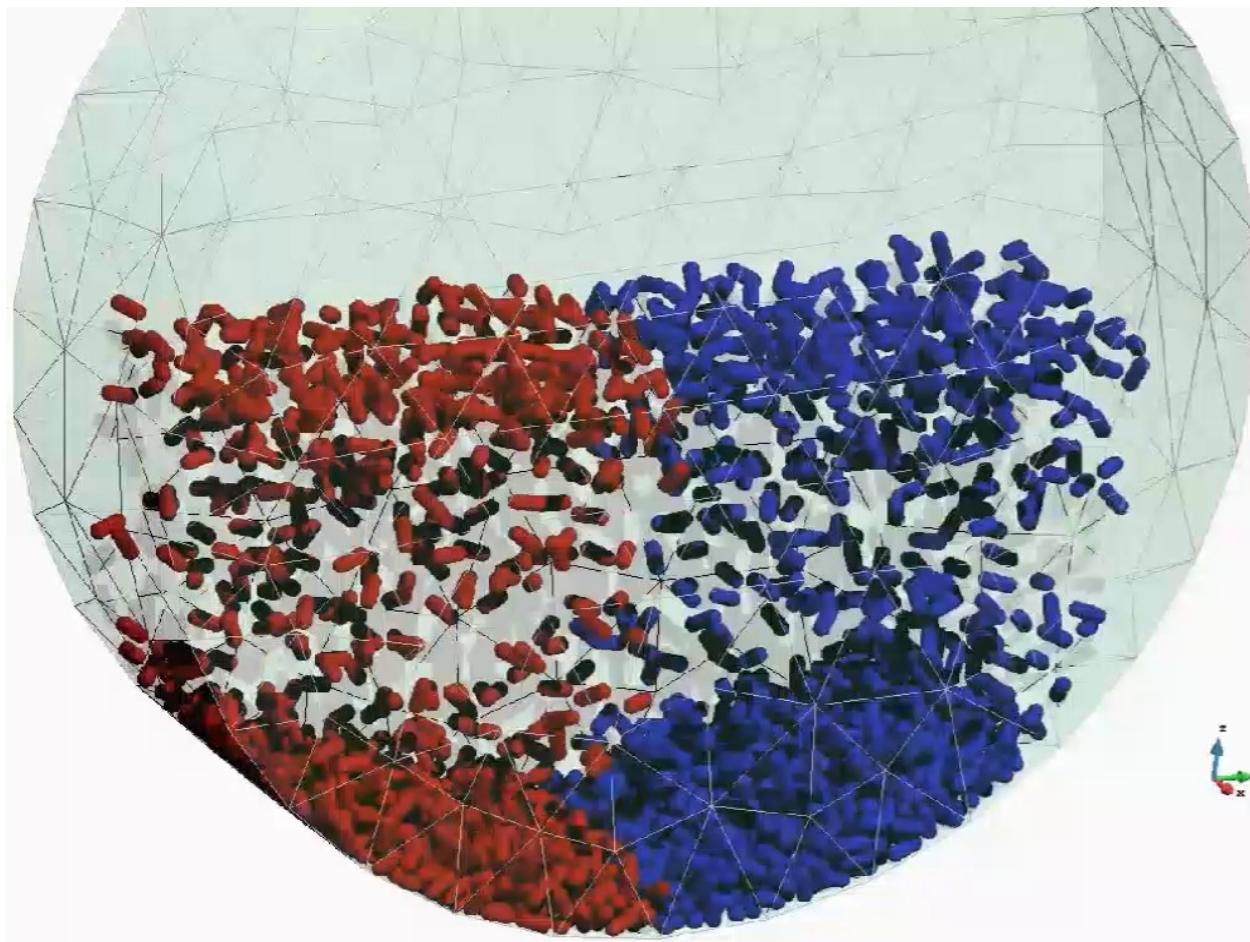
Mixing processes



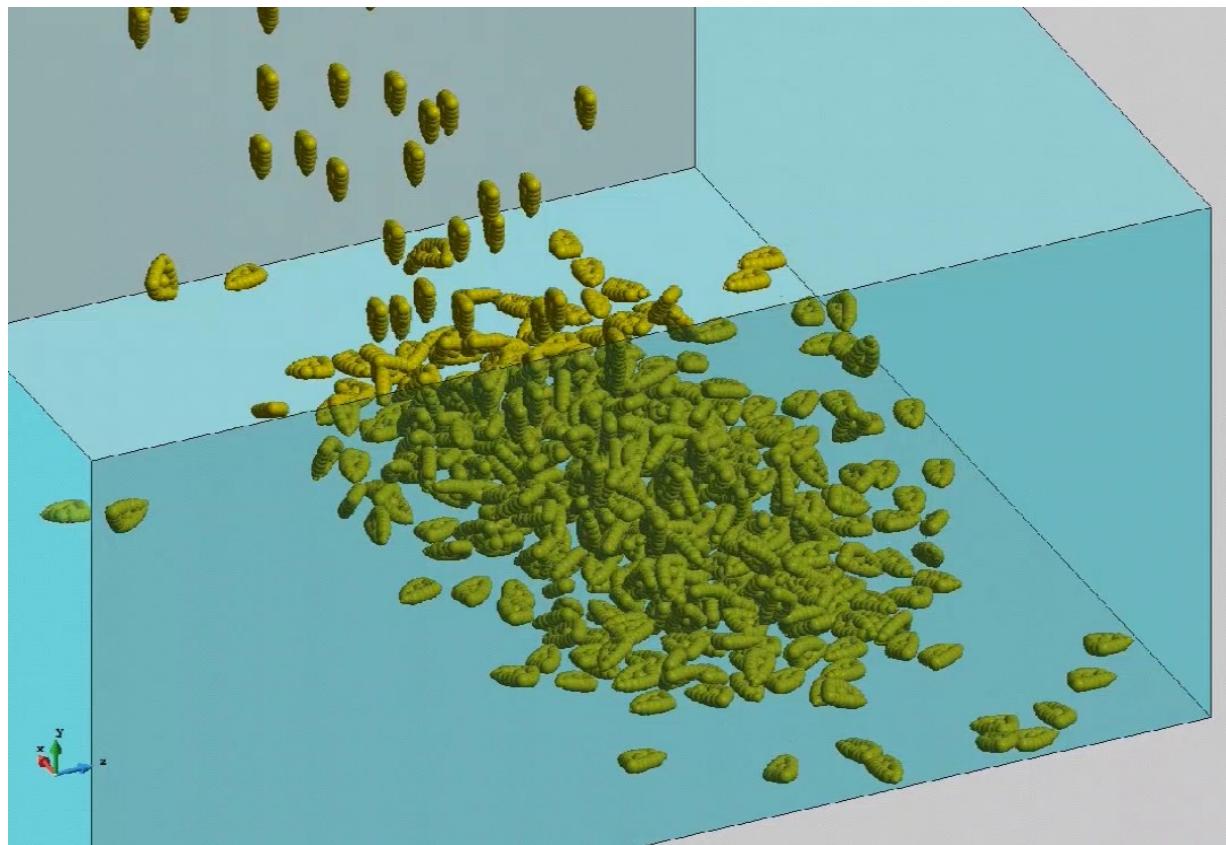
Cohesive materials (JKR, MDT models)



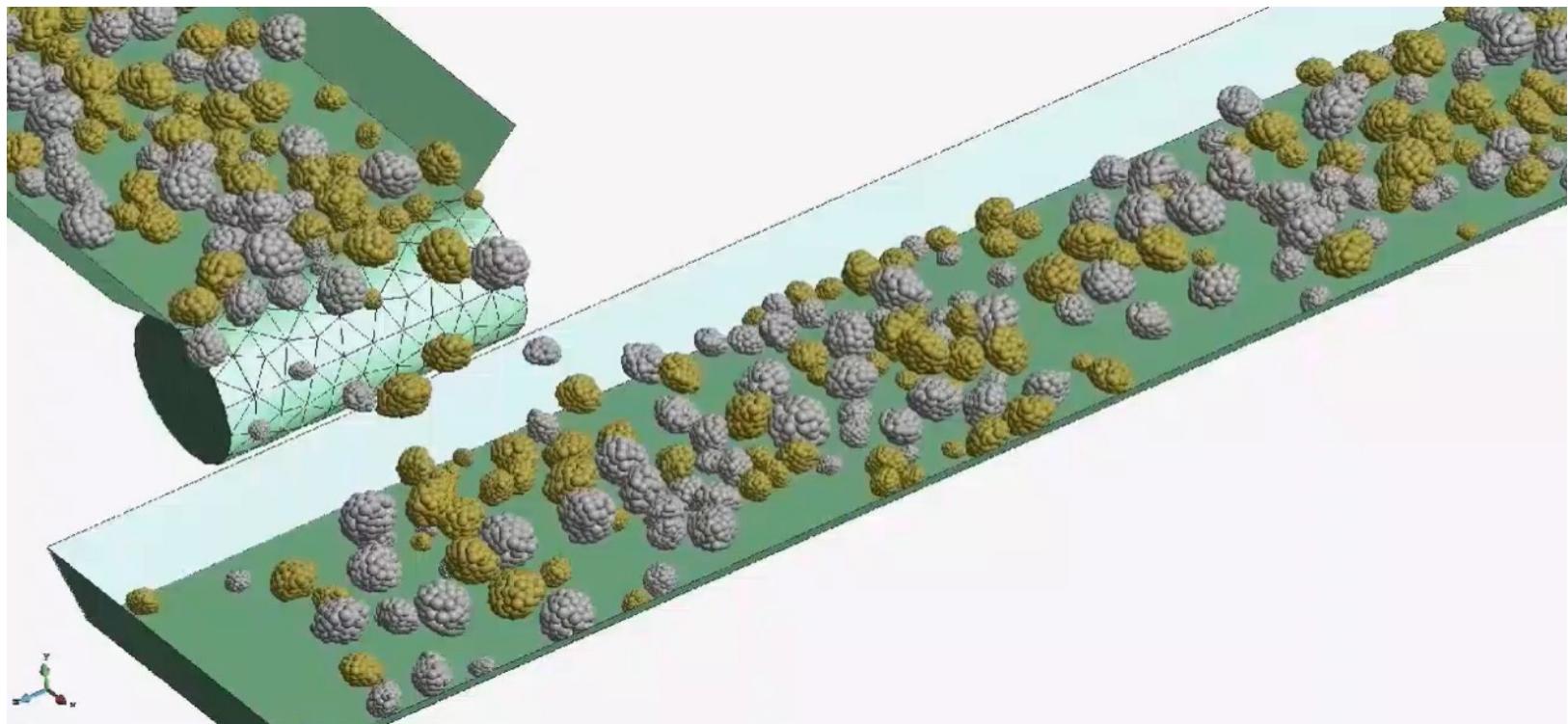
Non spherical particles: Capsules coating



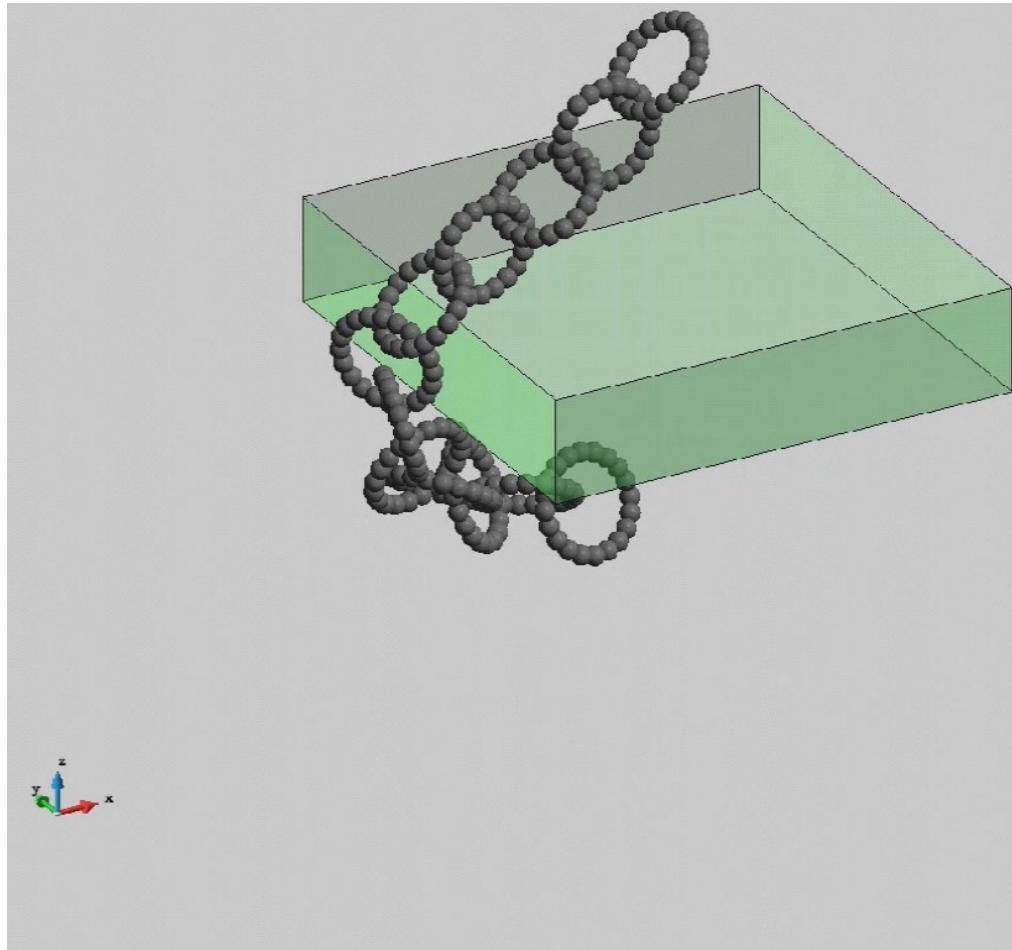
Non spherical particles: Corn seeds



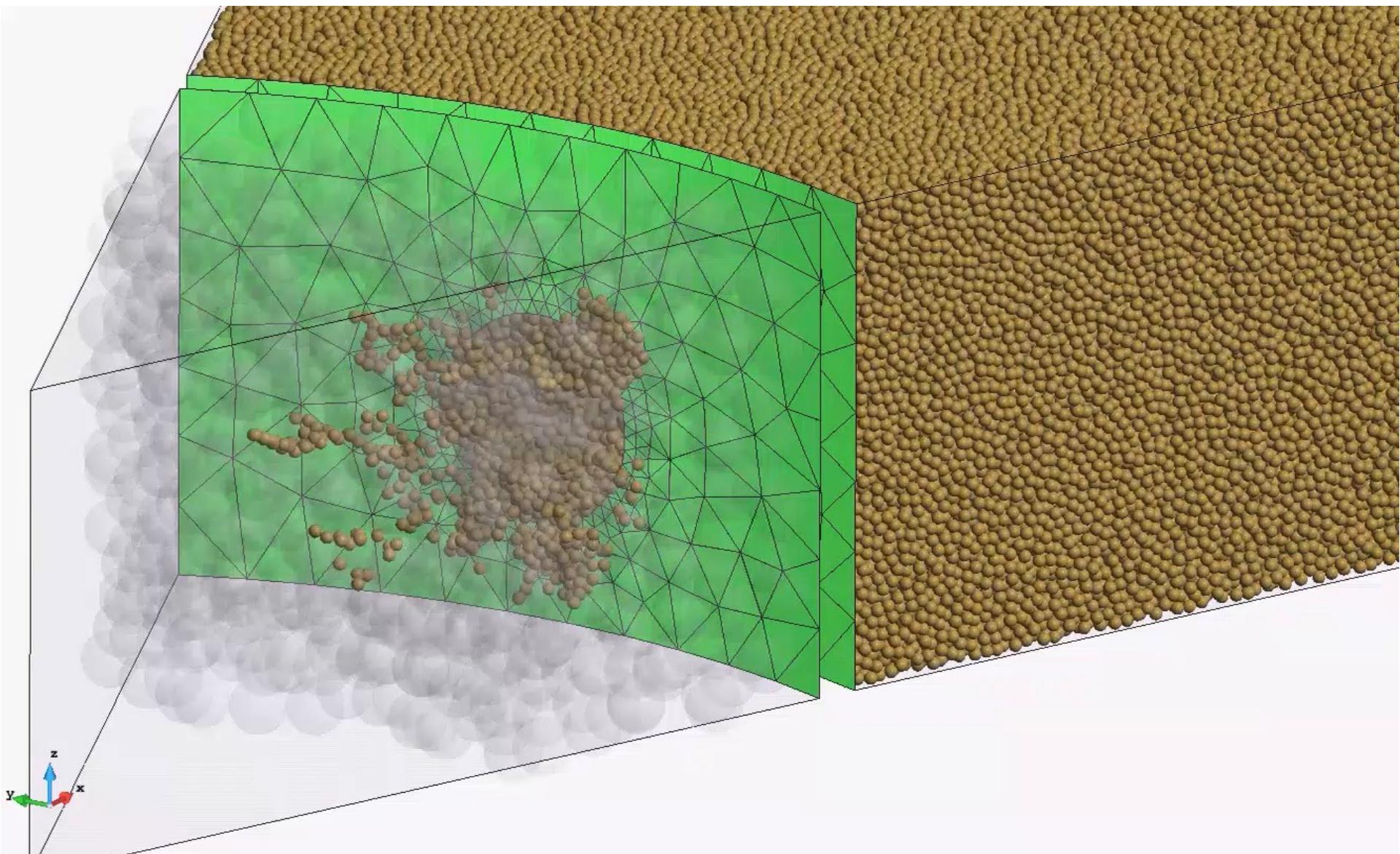
Non spherical particles: Conveyor belt with rocks of different sizes



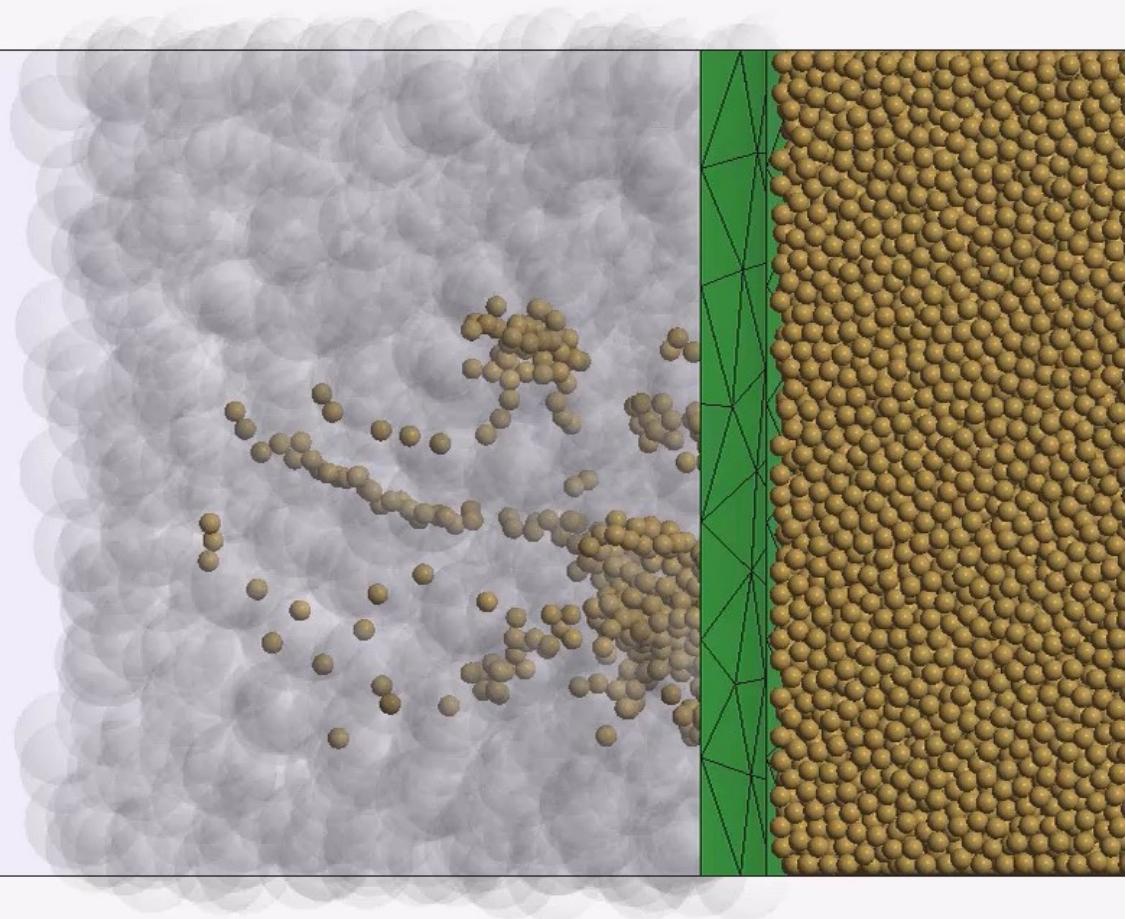
Non spherical particles: Chain made of clusters



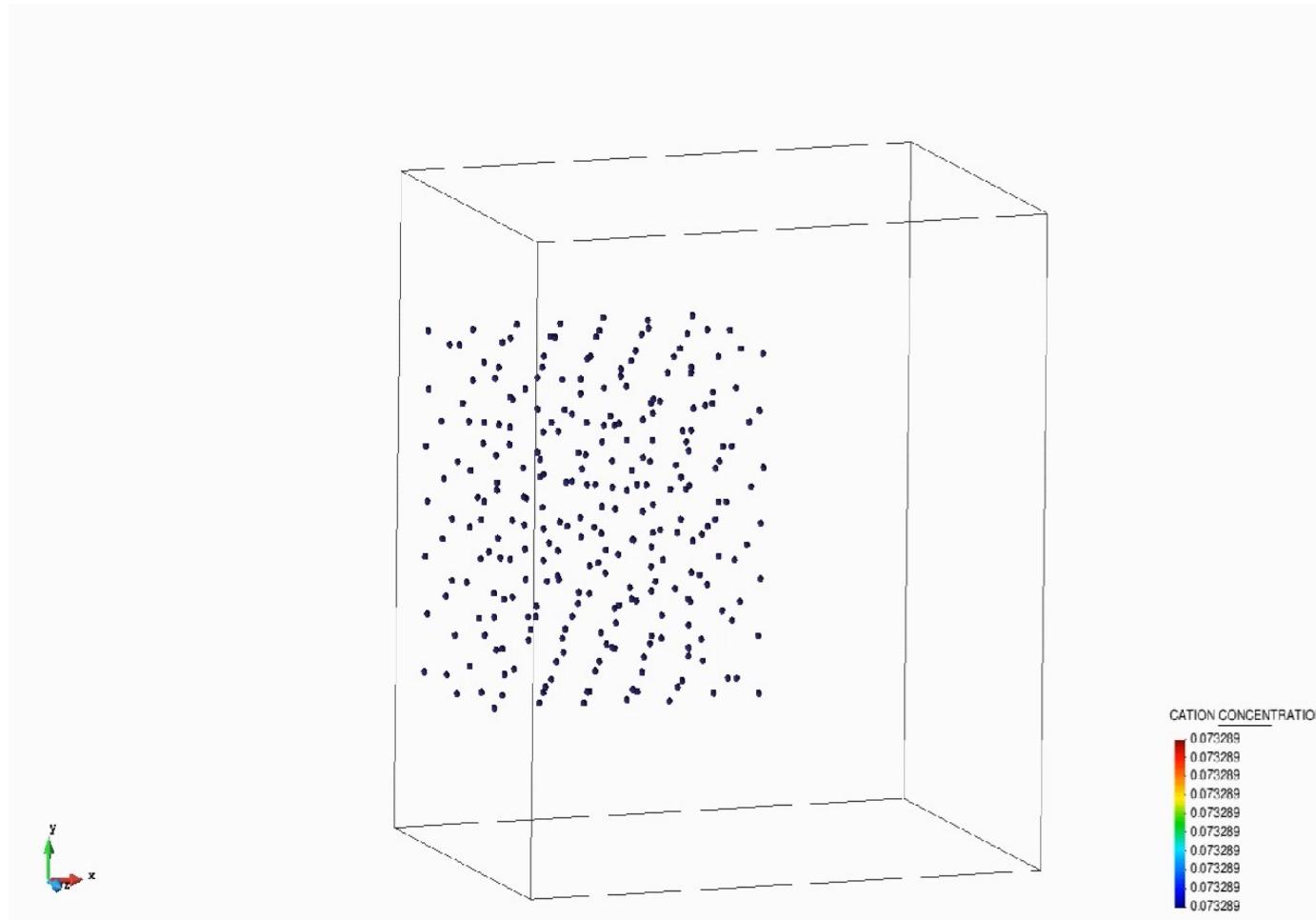
Sand production



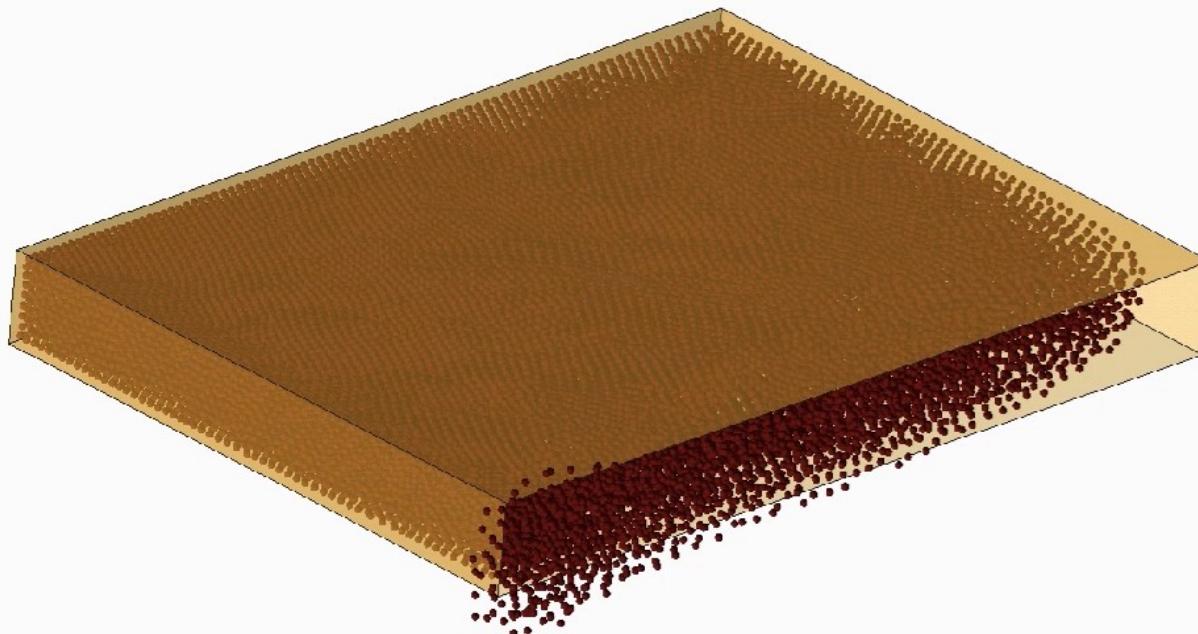
Sand production

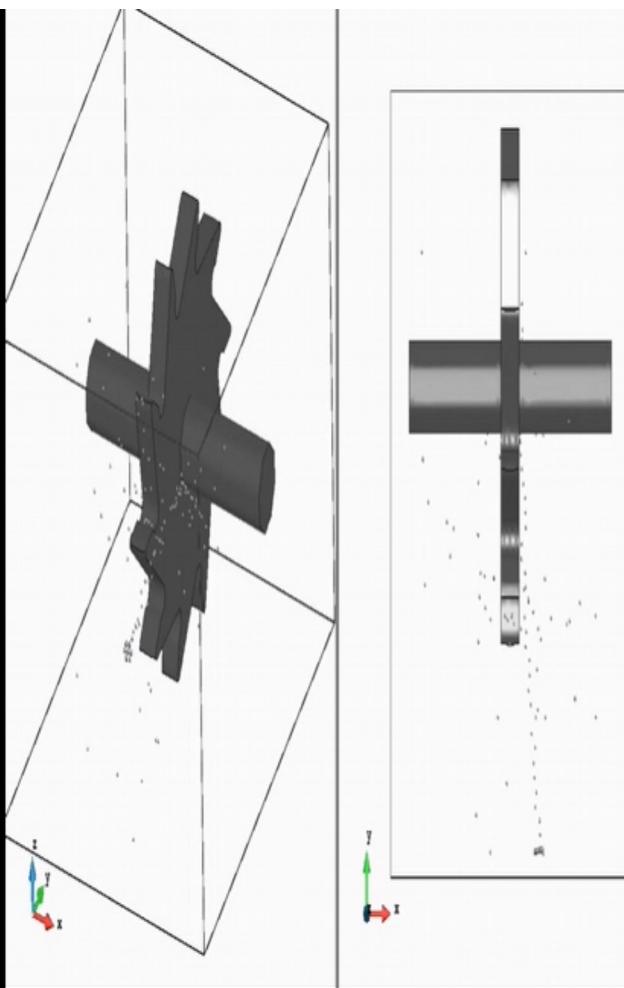


Nano particles ($2\text{e-}7 \text{ m}$). Interaction forces are: diffuse double layer and Van der Waals



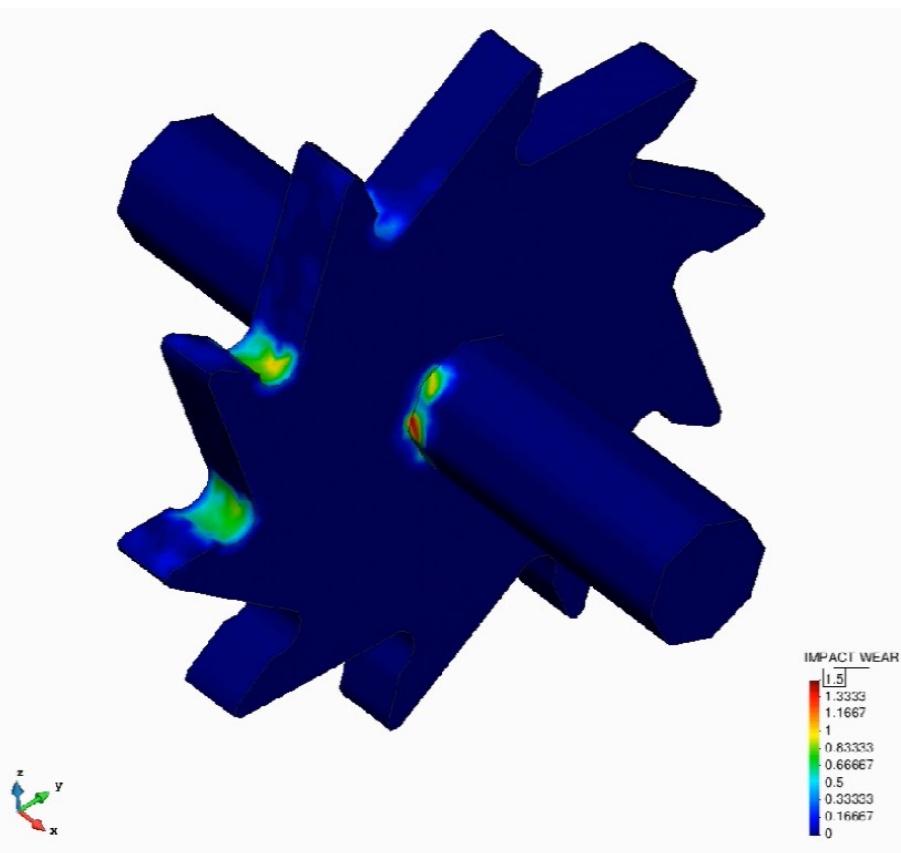
Nano particles ($2\text{e-}7 \text{ m}$). Interaction forces are: diffuse double layer and Van der Waals



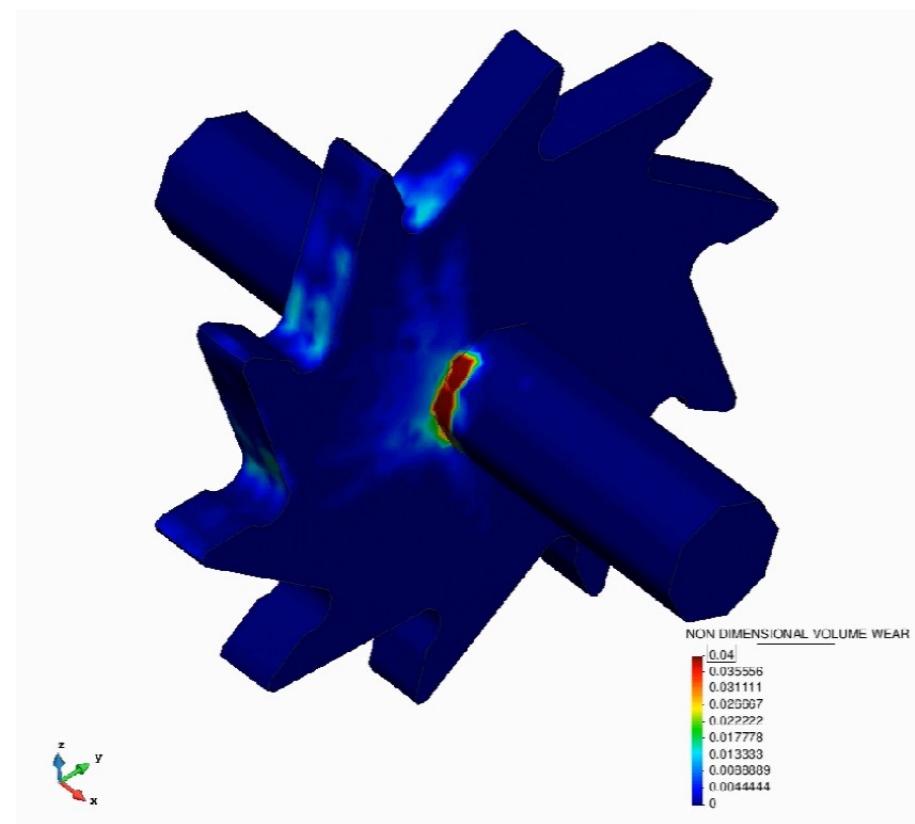


SHOT PEENING

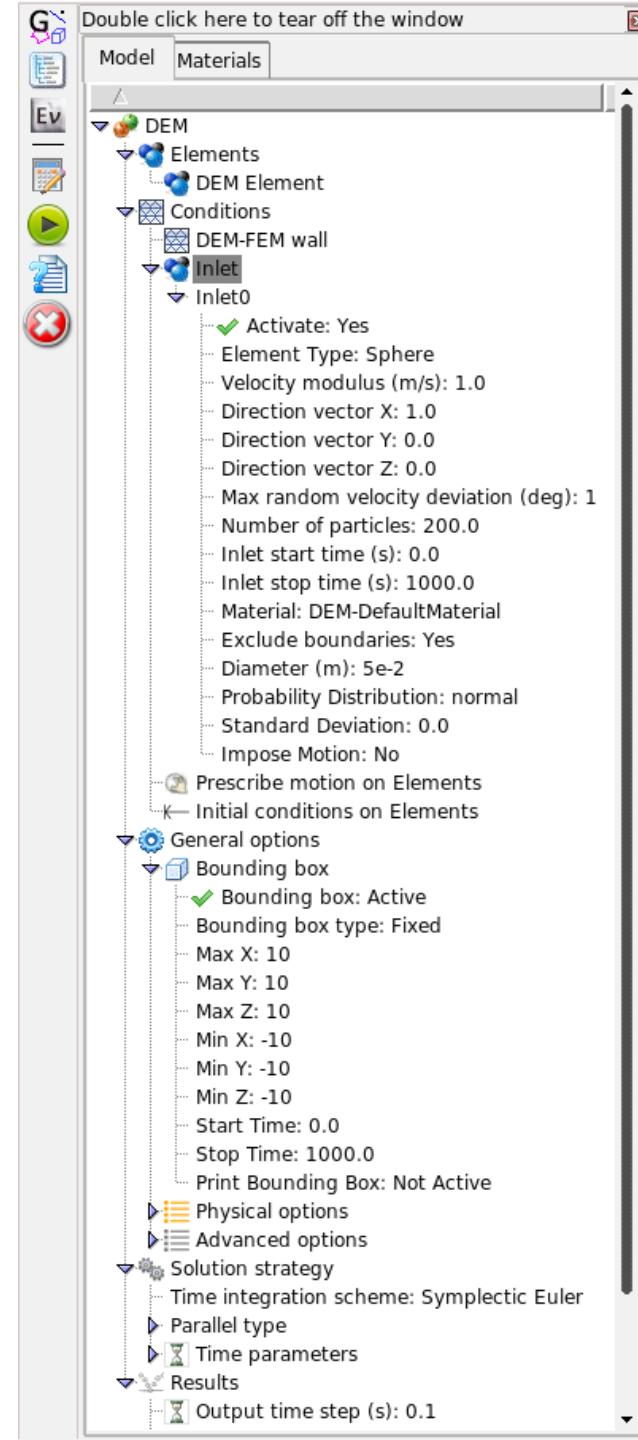
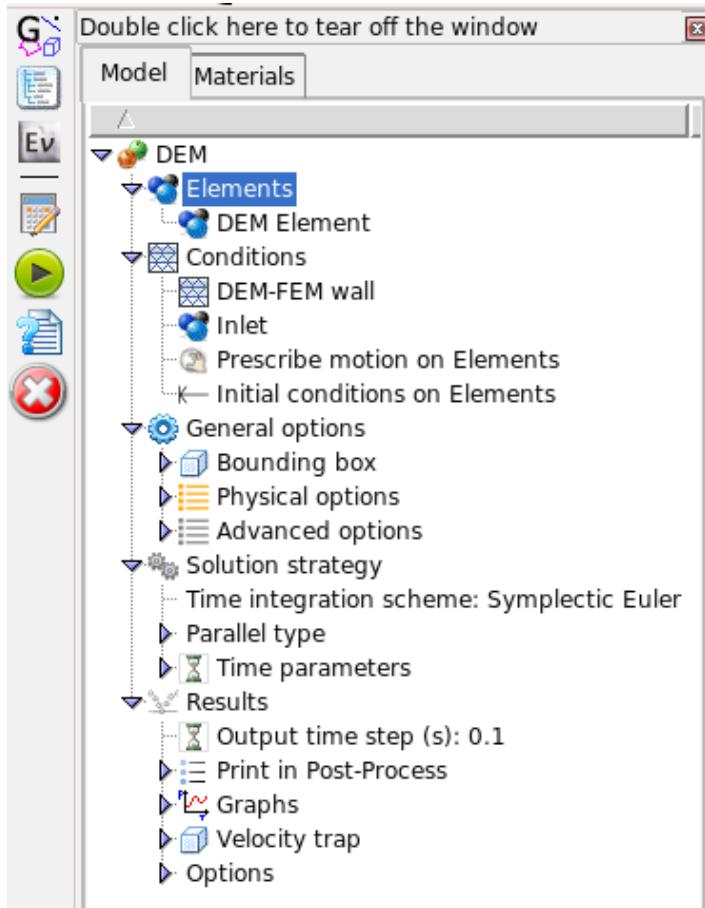
IMPACT EFFECT
(Oka et al (2005)):

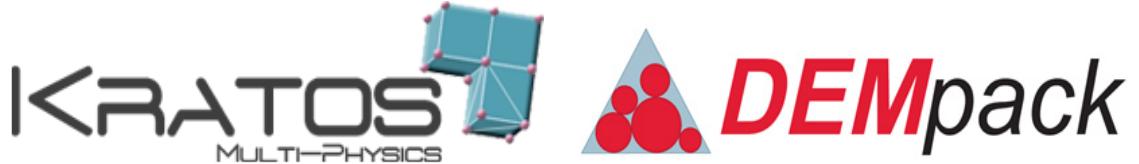


ABRASION BY FRICTION
(Archard):



GUI (for GiD, a pre- and post-processor developed at CIMNE)



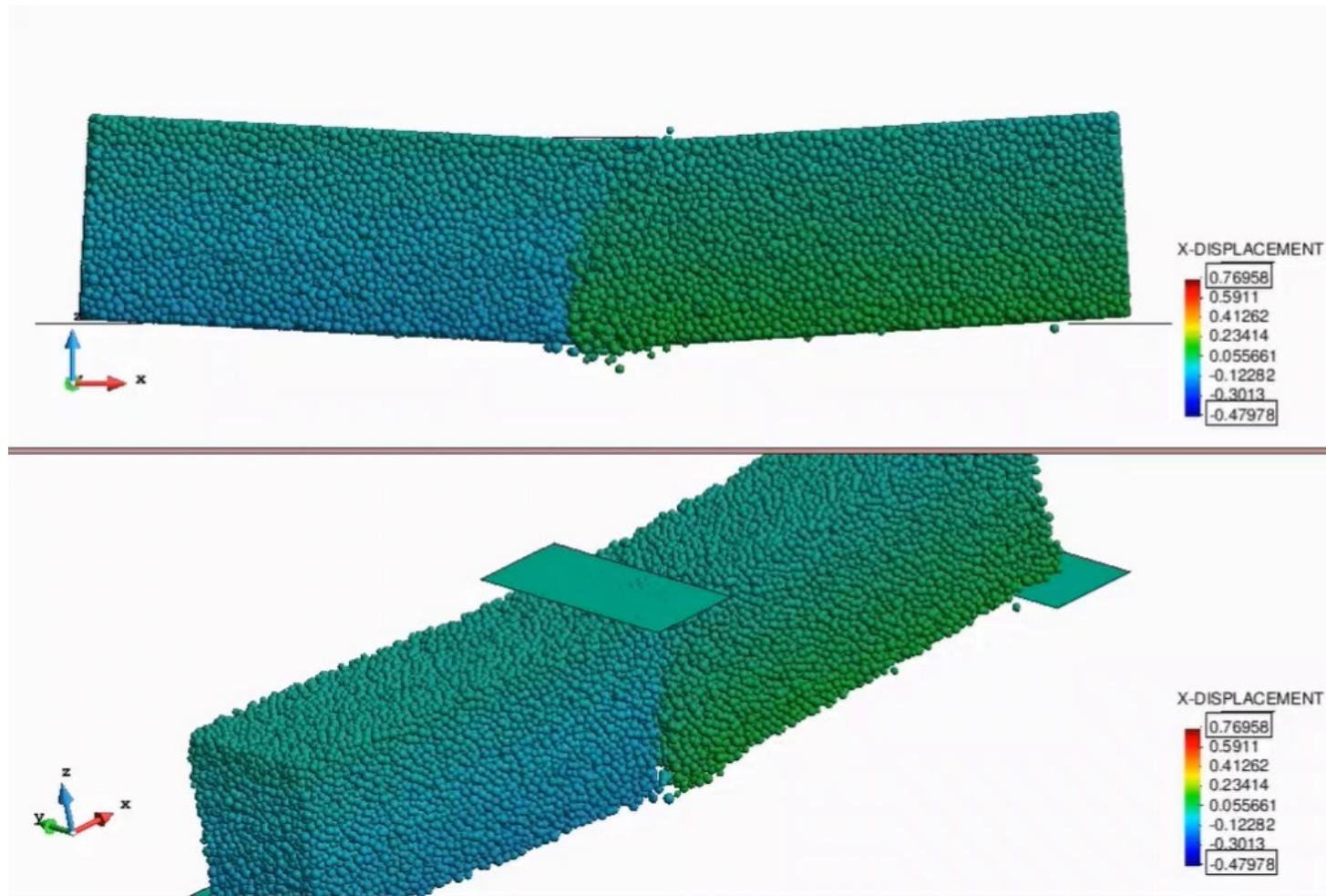


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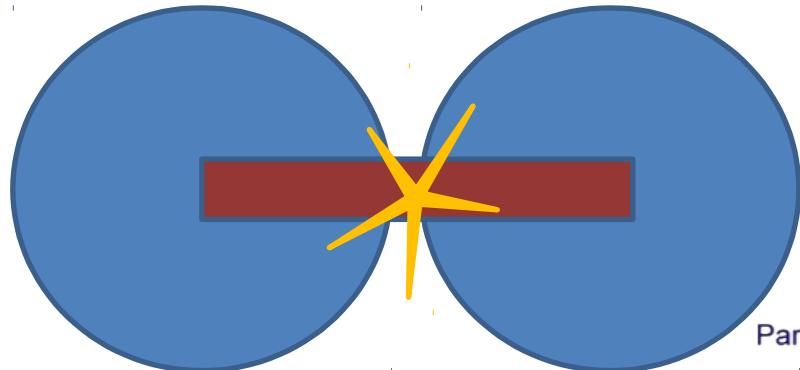
CIMNE^R
International Centre
for Numerical Methods in Engineering

OBJECTIVE: solve relatively large domains (human size), where spheres are not micro, they can measure centimeters or meters.



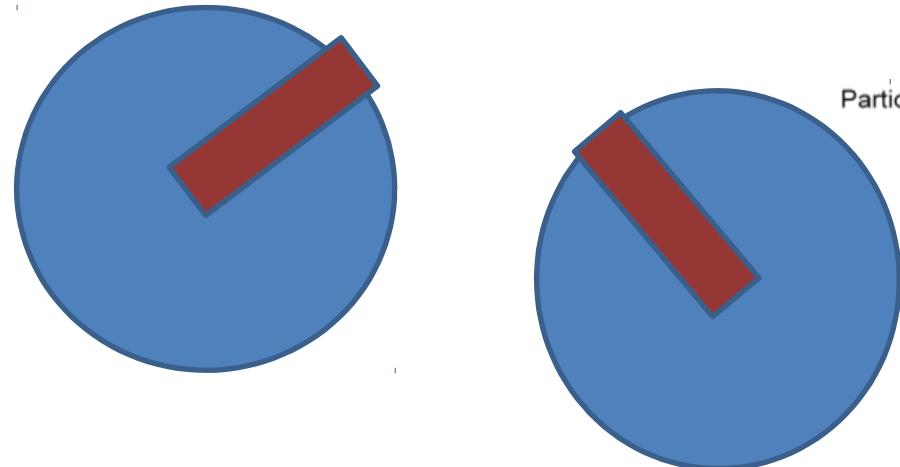
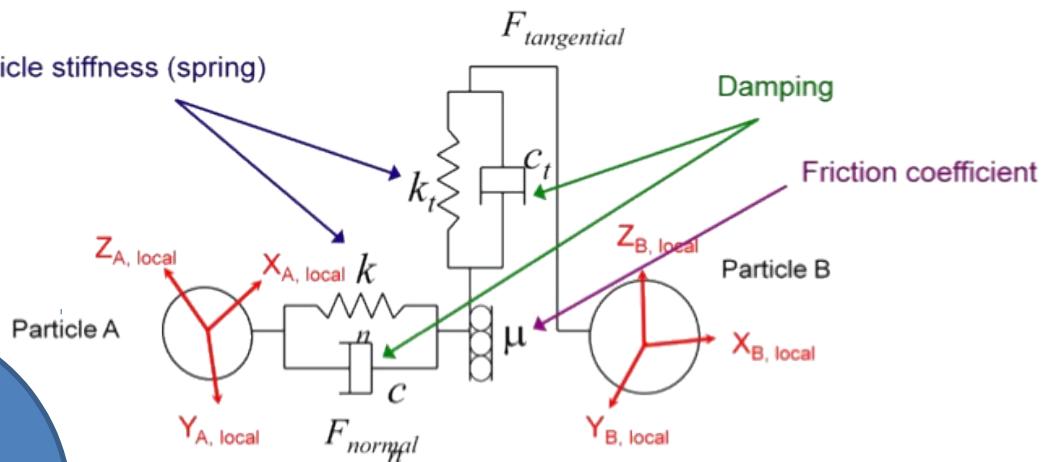
Typically, Young's Modulus and Poisson's Ratio are enough to define the elastic properties of a material. Post-elasticity requires other parameters.

The DEM has been used to model these problems by means of the so called 'Bonded DEM'



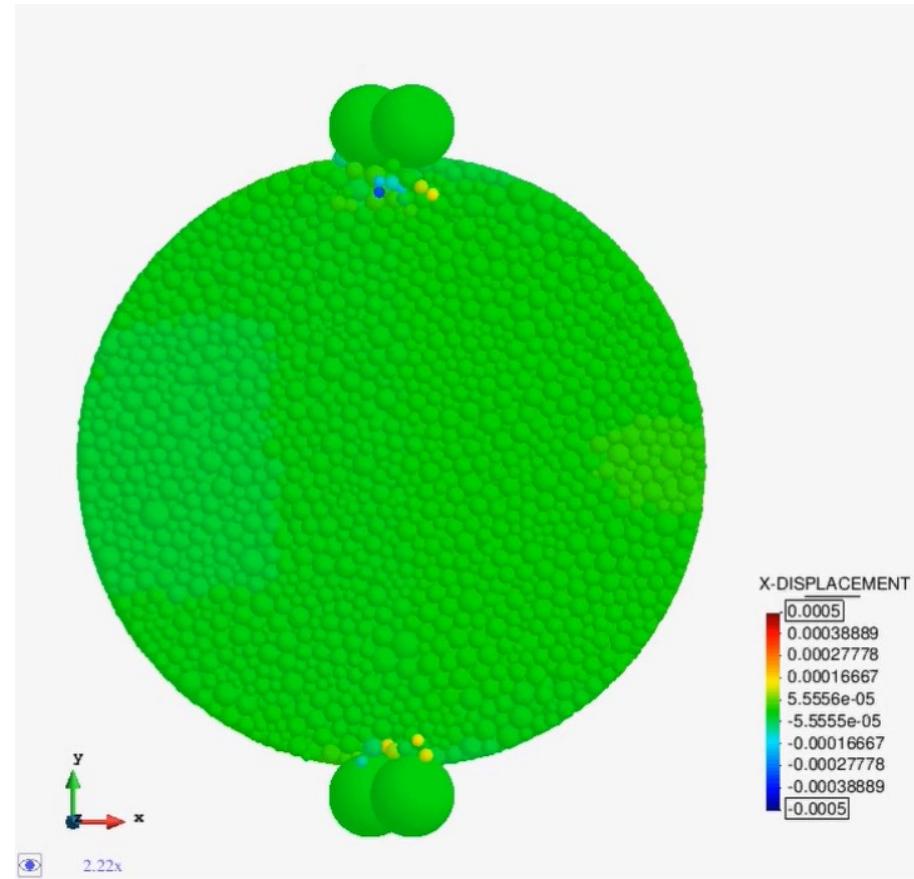
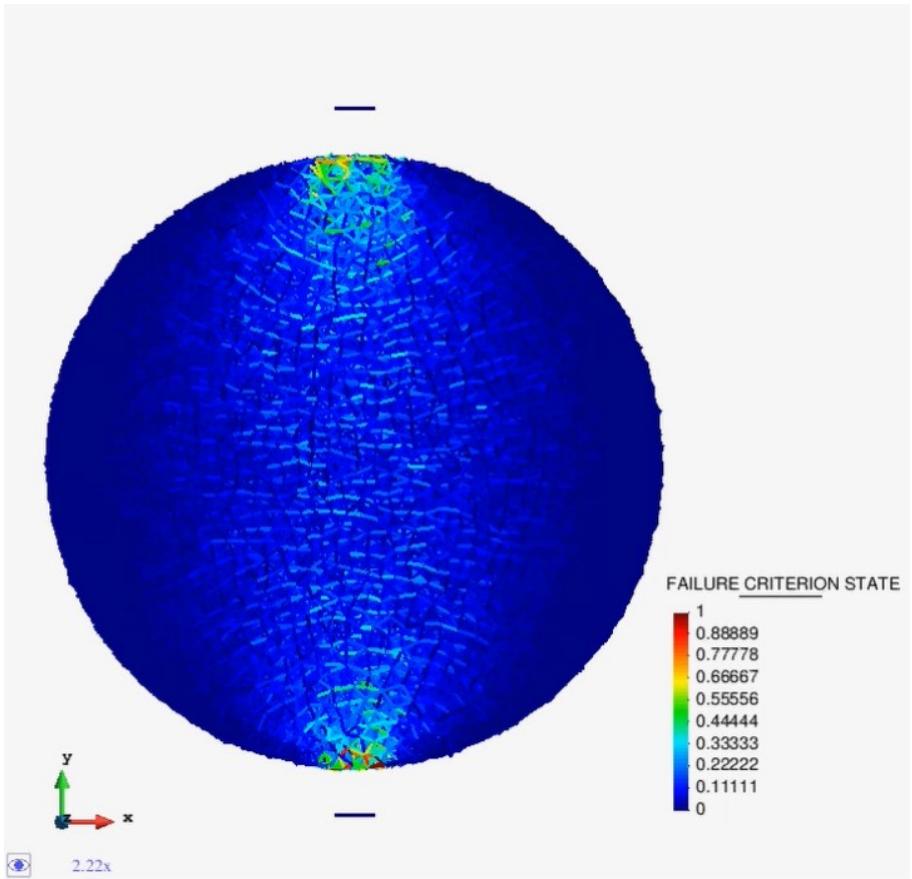
Normal spring actuates in compression and tension

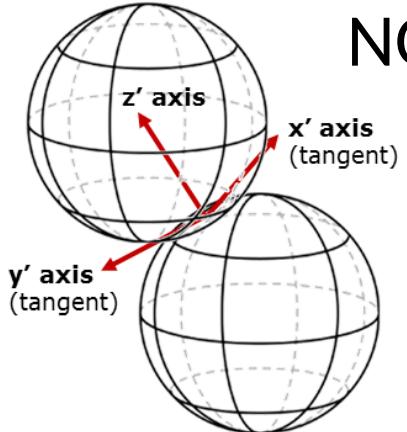
Particle stiffness (spring)



Normal spring actuates in compression only

CONTINUUM SIMULATIONS WITH DEM (CONCRETE). MULTI-FRACTURE Brazilian test





NORMAL FORCE (z' axis)

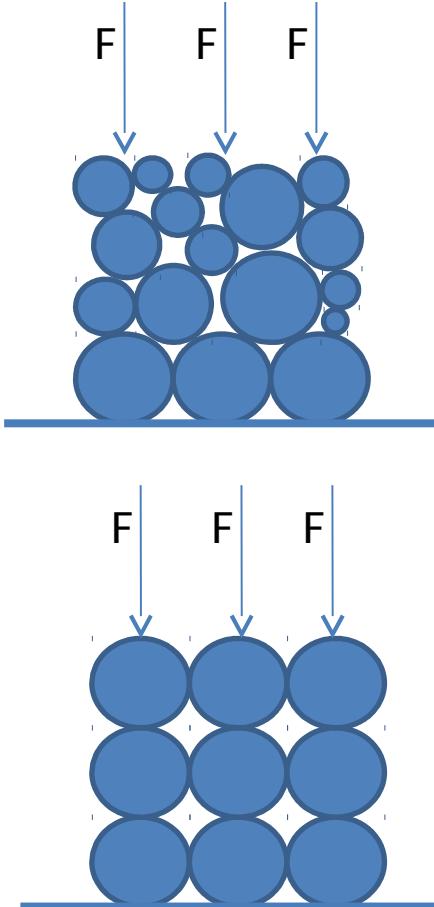
$$\sigma_{z'} = E \varepsilon_{z'}$$

$$\frac{F_{z'}}{A^*} = E \frac{\Delta l}{l} = \frac{E}{R1 + R2} \delta$$

$$F_{z'} = \frac{EA^*}{R1 + R2} \delta$$

$$F_{z'} = K_n \delta$$

+ Weighted Voronoi Diagram...



- Young's Modulus depends on K_t
- Poisson's Ratio depends on K_t
- Perfect Young's Modulus
- Wrong Poisson's Ratio (100% error!)

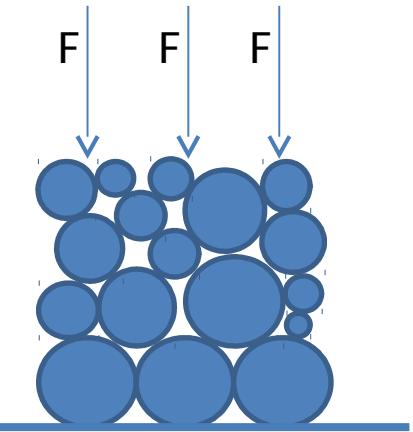
$$F_{z'} = K_n \delta + v A^* (\sigma_{x'} + \sigma_{y'})$$

The stress tensor is used to enrich the force computation

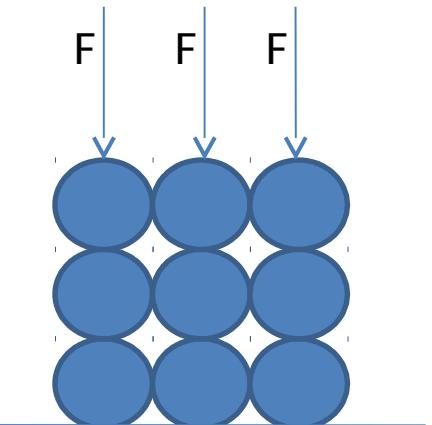
$$F_{x'_i} = k_{ti} \delta_{x'i} + A_i G \left(\frac{\tau_{z'x',i}}{G} - \frac{\delta_{x'i}}{L_i} \right)_{step}$$

$$F_{y'_i} = k_{ti} \delta_{y'i} + A_i G \left(\frac{\tau_{z'y',i}}{G} - \frac{\delta_{y'i}}{L_i} \right)_{step}$$

- Good Young's Modulus
- Good Poisson's Ratio

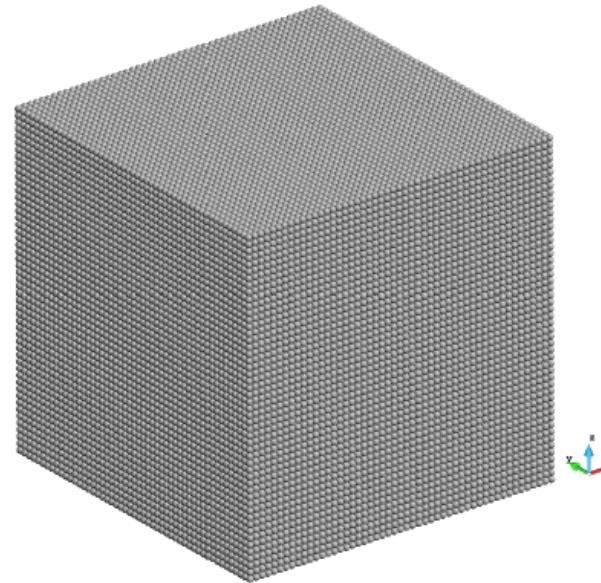


- Good Young's Modulus
- Good Poisson's Ratio

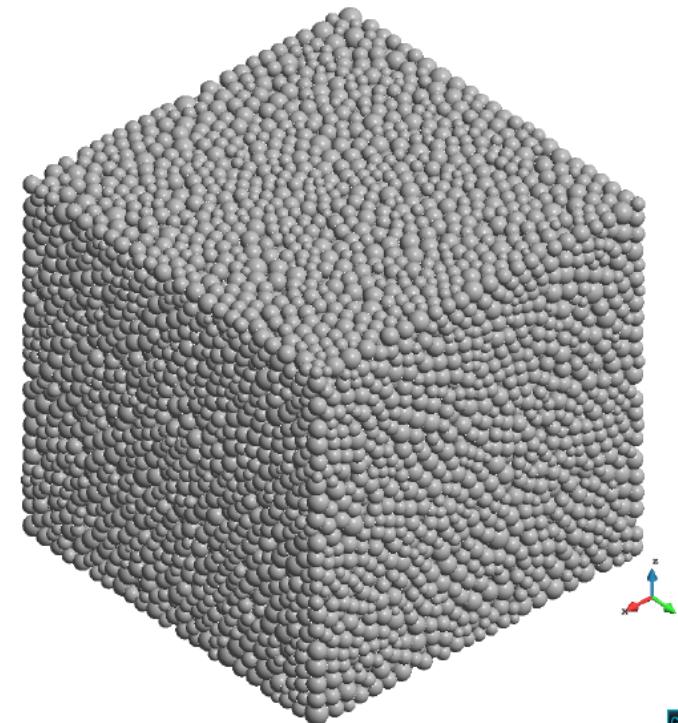


VALIDATION

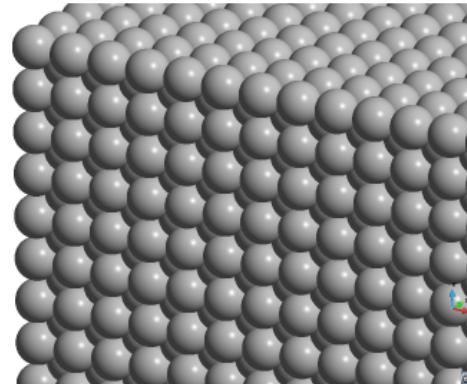
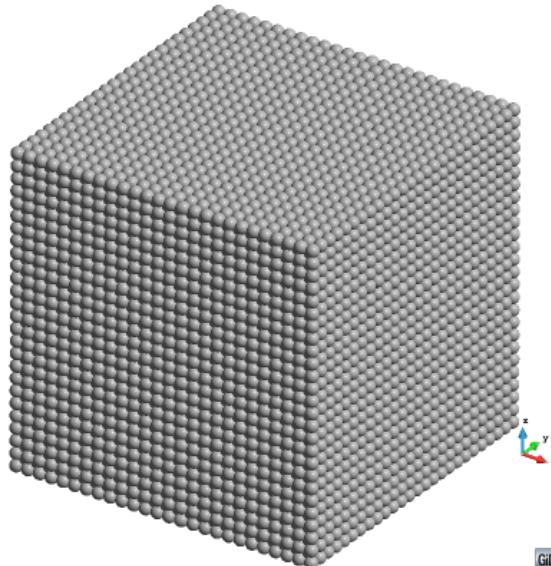
Cartesian packing



Random packing

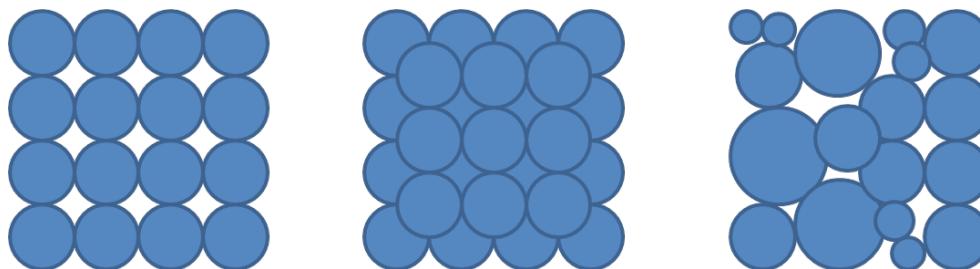


Staggered packing



VALIDATION TESTS: EFFECT OF ADDING THE NEW TERMS BASED ON THE STRESS TENSOR. NO CALIBRATION NEEDED.

3D packings:



Input parameters: $E = 1.0e9, \nu = 0.2$

Error in computed values	Cartesian fine packing		Staggered fine packing		Random fine packing	
	Standard DEM	Improved DEM	Standard DEM	Improved DEM	Standard DEM	Improved DEM
Young's modulus E	-0.6 %	-0.6 %	-20.8 %	+0.7 %	-22.0 %	-0.2 %
Poisson's ratio ν	-100.0 %	+1.45 %	-43.0 %	+0.4 %	-29.0 %	-3.0 %

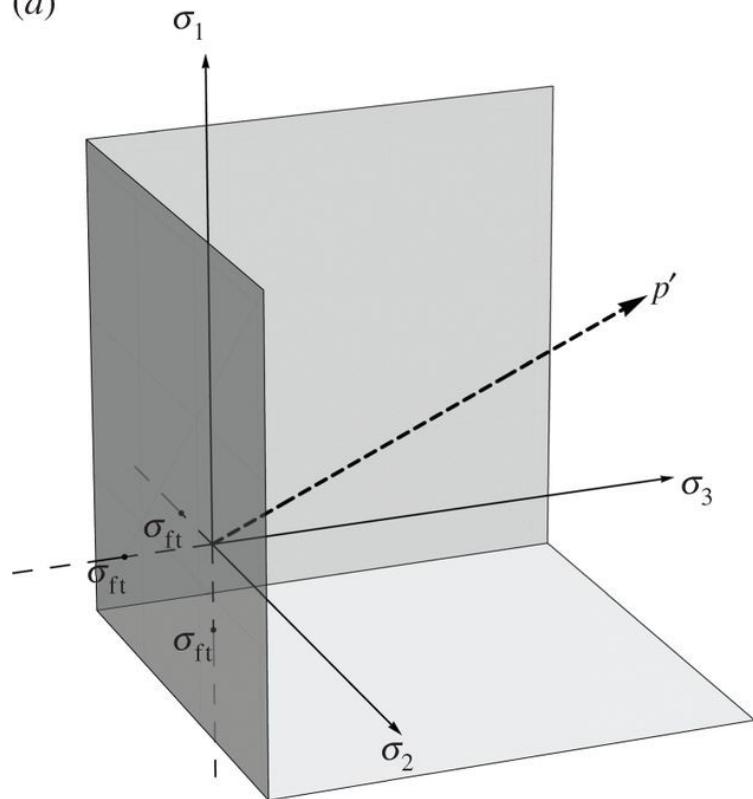
Input parameters: $E = 1.0e9, \nu = 0.35$

Error in computed values	Cartesian fine packing		Staggered fine packing		Random fine packing	
	Standard DEM	Improved DEM	Standard DEM	Improved DEM	Standard DEM	Improved DEM
Young's modulus E	-0.6 %	-0.6 %	-23.0 %	+0.7 %	-28.0 %	-0.2 %
Poisson's ratio ν	-100.0 %	+0.22 %	-64.0 %	-2.9 %	-62.0 %	-3.5 %

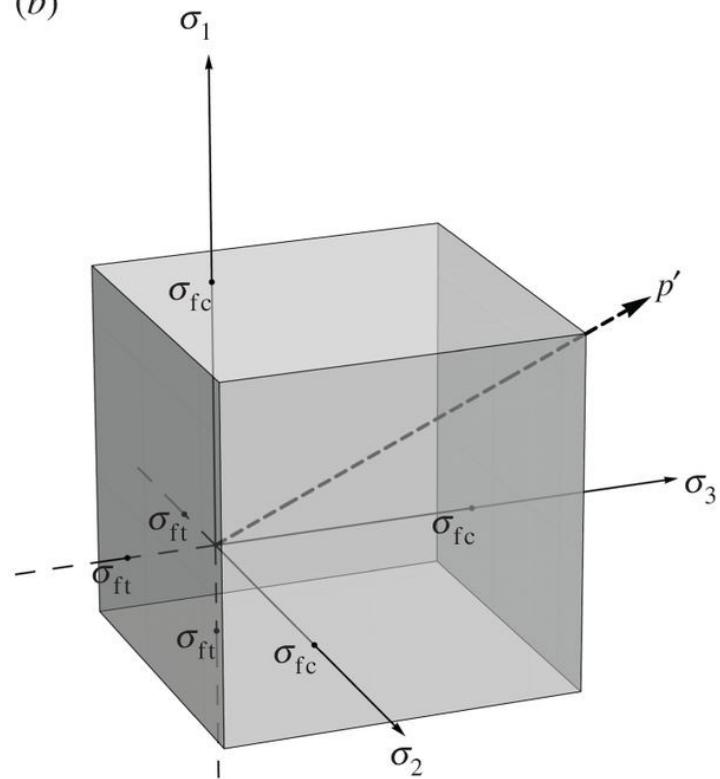
Celigueta, M. A., Latorre, S., Arrufat, F., & Oñate, E. (2017). Accurate modelling of the elastic behavior of a continuum with the Discrete Element Method. *Computational Mechanics*, 1-14.

RANKINE YIELD CRITERION (FOR EXAMPLE)

(a)



(b)



Stress tensor

$$\boldsymbol{\sigma}$$

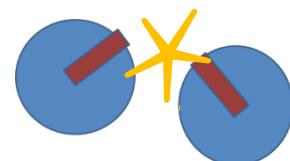


Principal Stresses

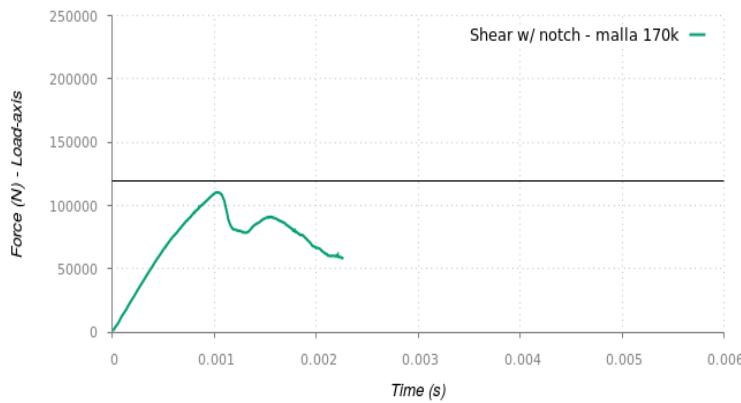
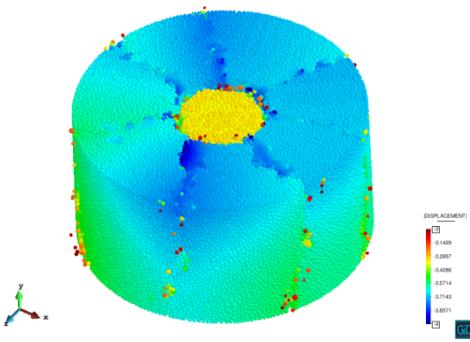
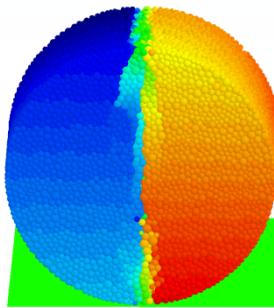
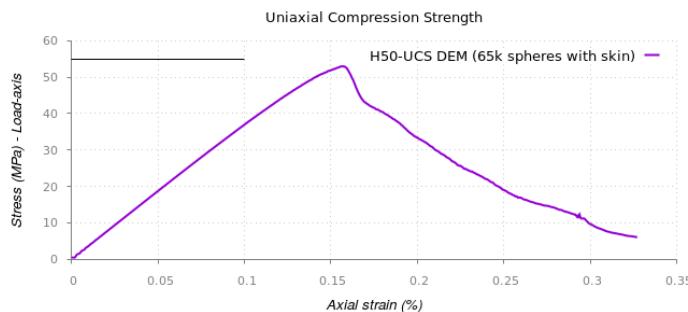
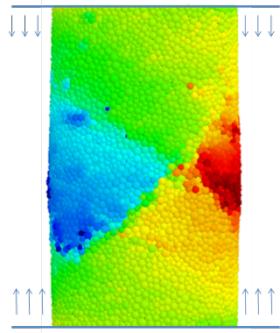
$$\sigma_1, \sigma_2, \sigma_3$$



Bond breakage



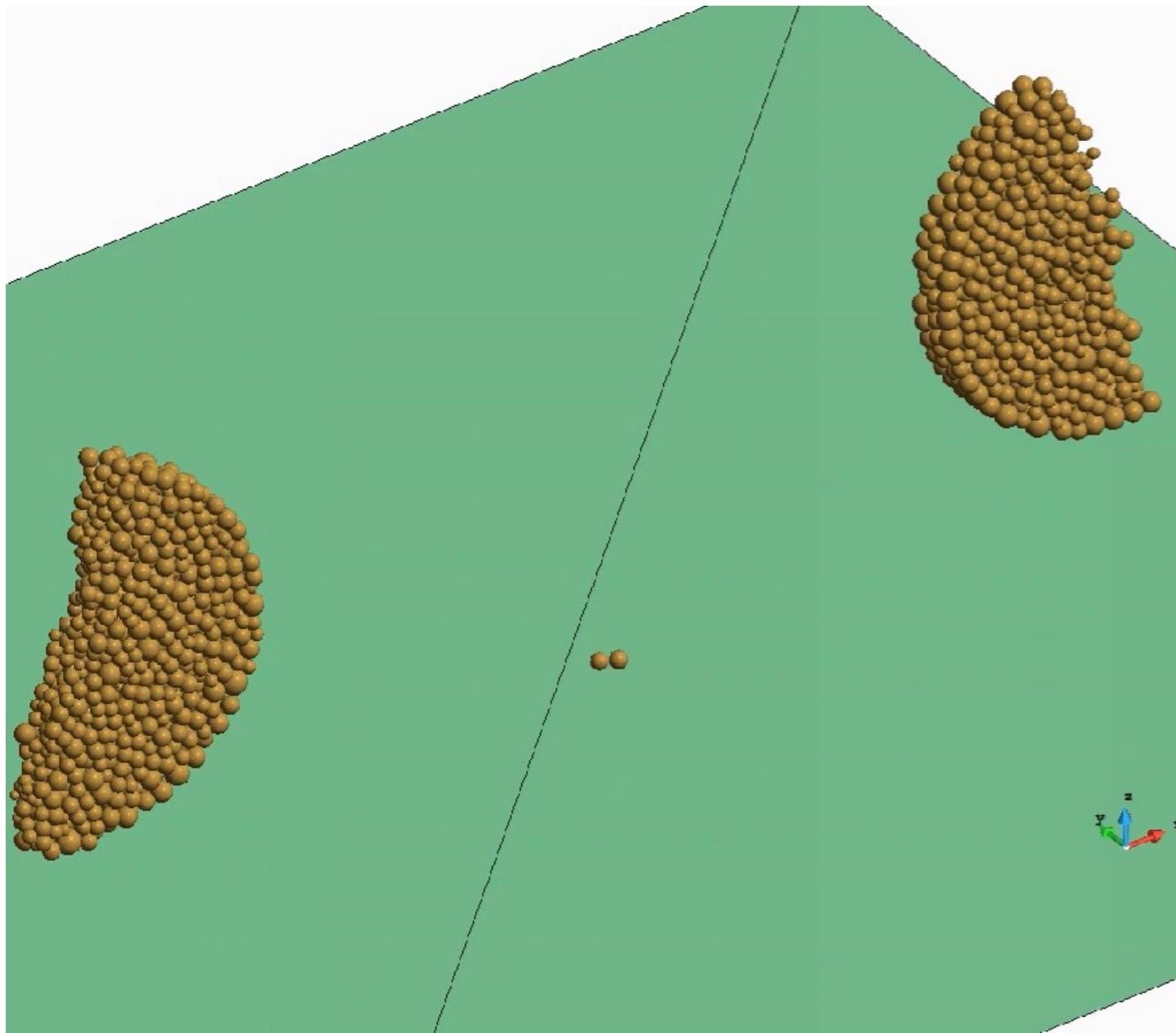
50 MPa Concrete



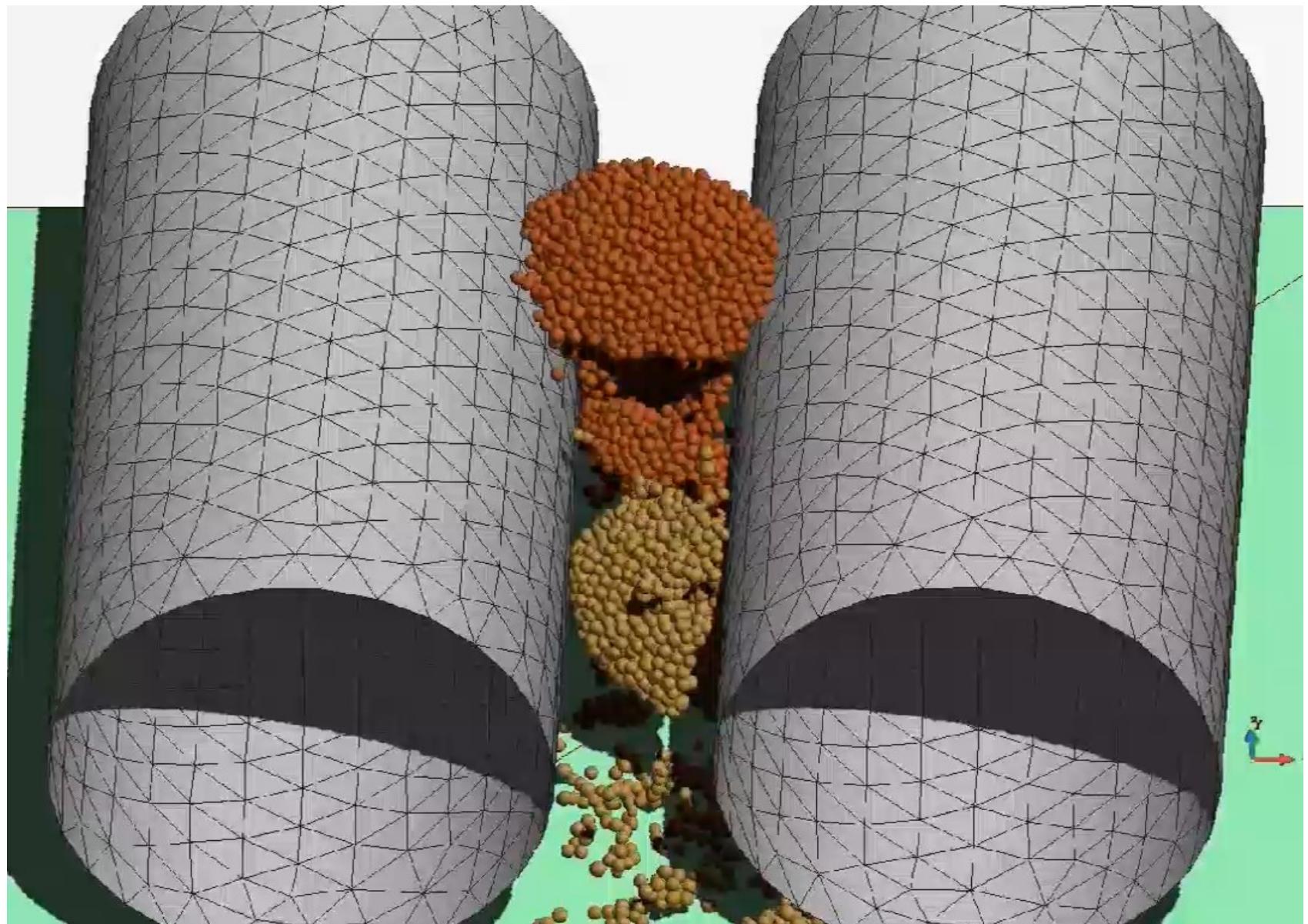
Just one micro parameter was calibrated (σ_{ft})

Just two micro parameters were calibrated (plus) (same σ_{ft} plus μ)

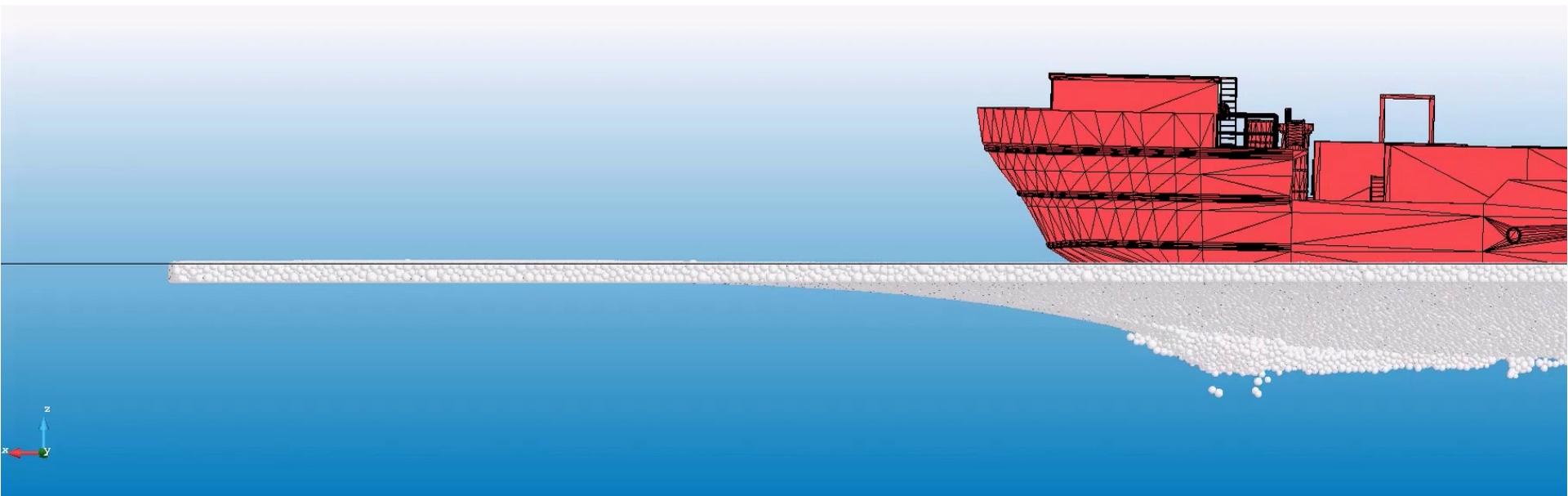
Large displacements and rotations are allowed



Fragments can break again



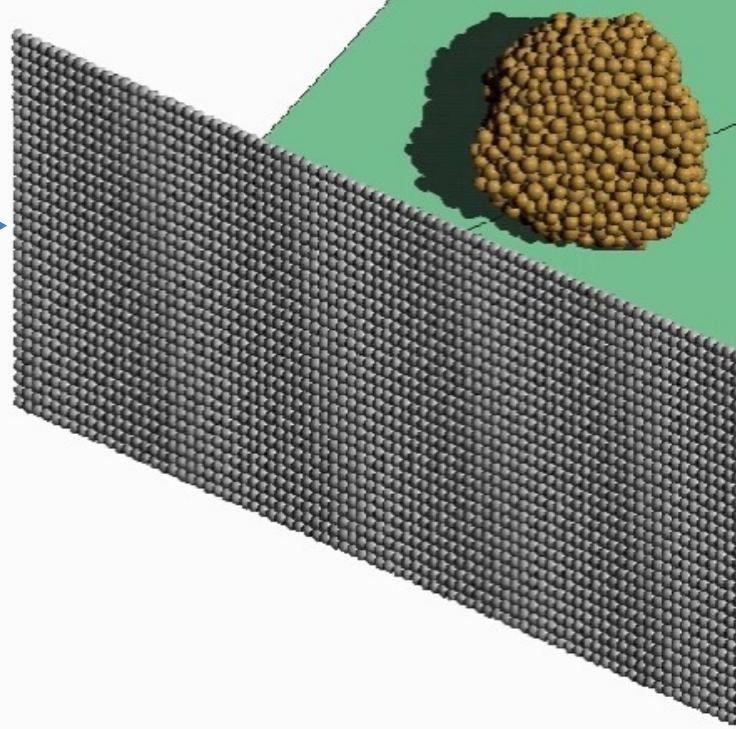
Icebreakers (understanding ice-ship interactions)



Water is not modeled as a fluid. A ‘virtual sea level’ is used for buoyancy and damping.

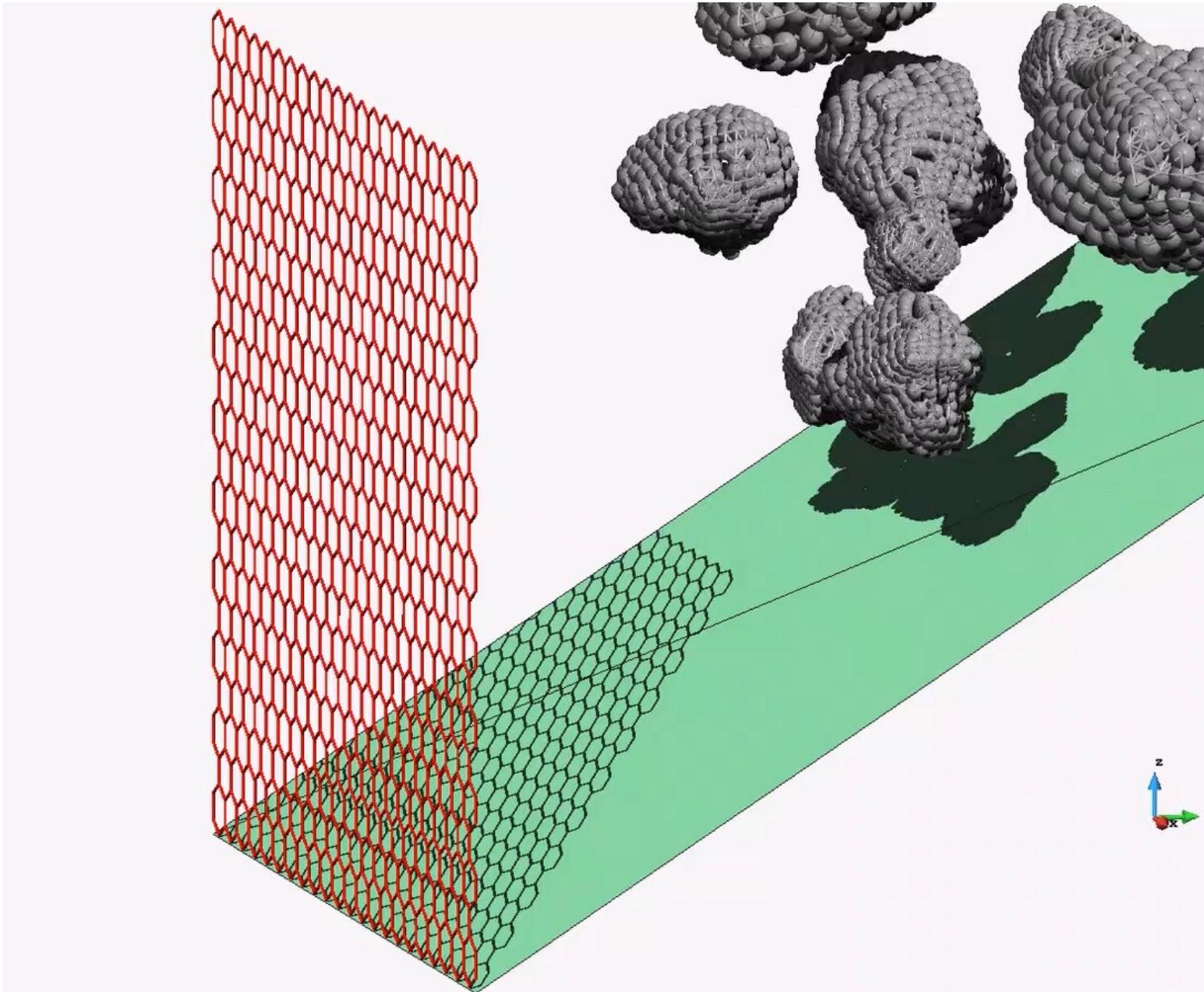
1 rock discretized with
cohesive DEM (rolling)

1 single layer of
bonded DEM

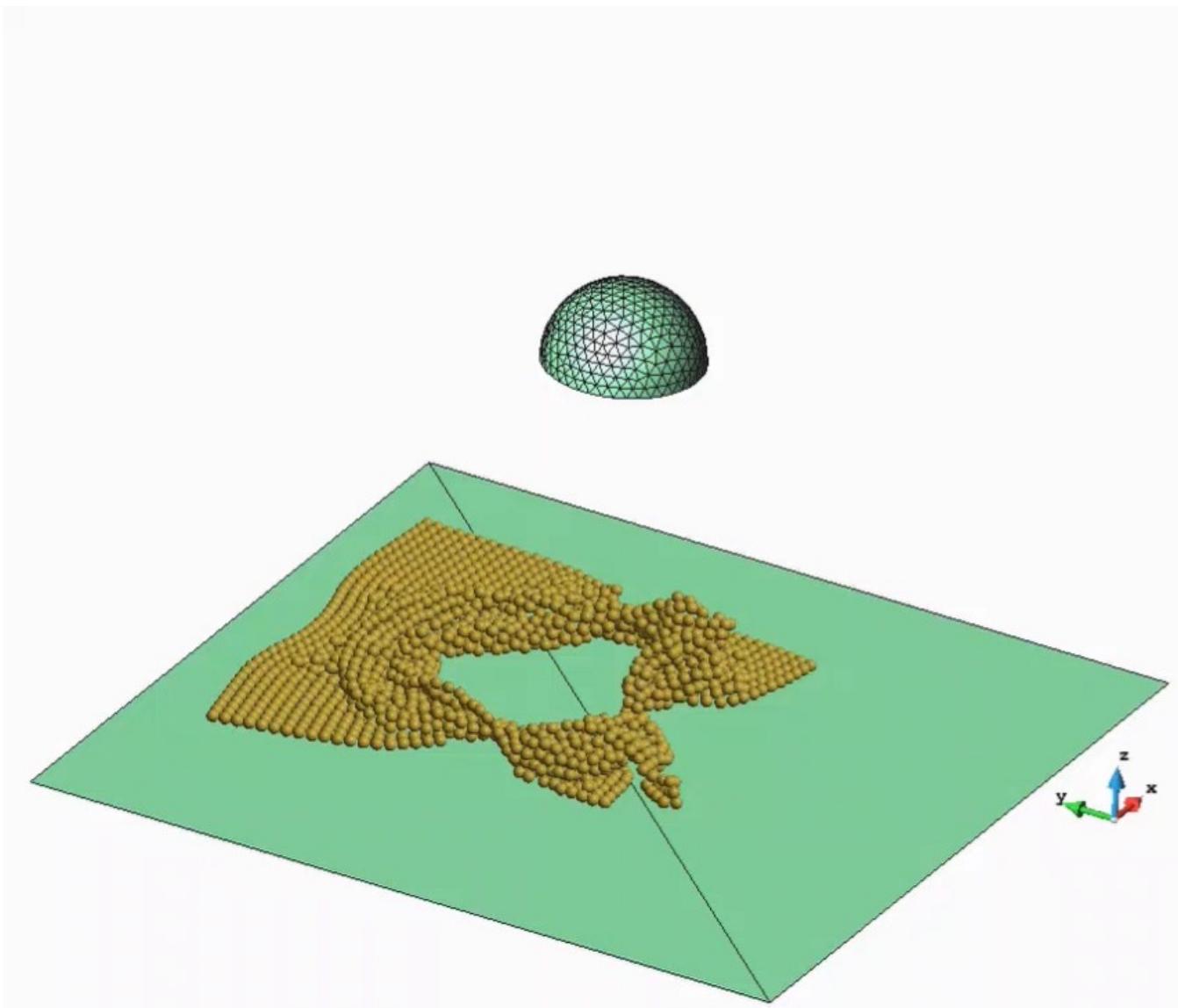


Rockfall protection nets (roads safety)

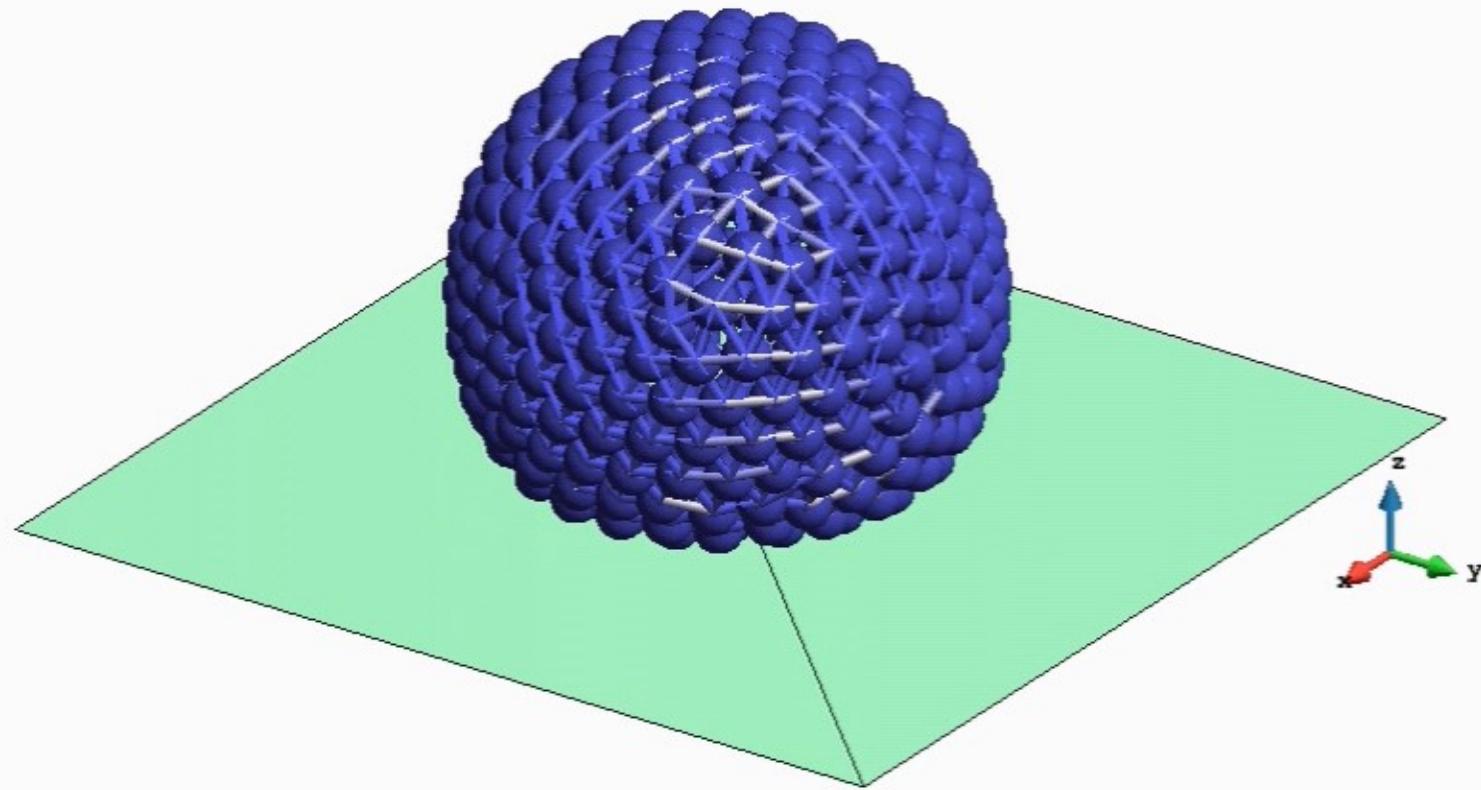
(hidden spheres)



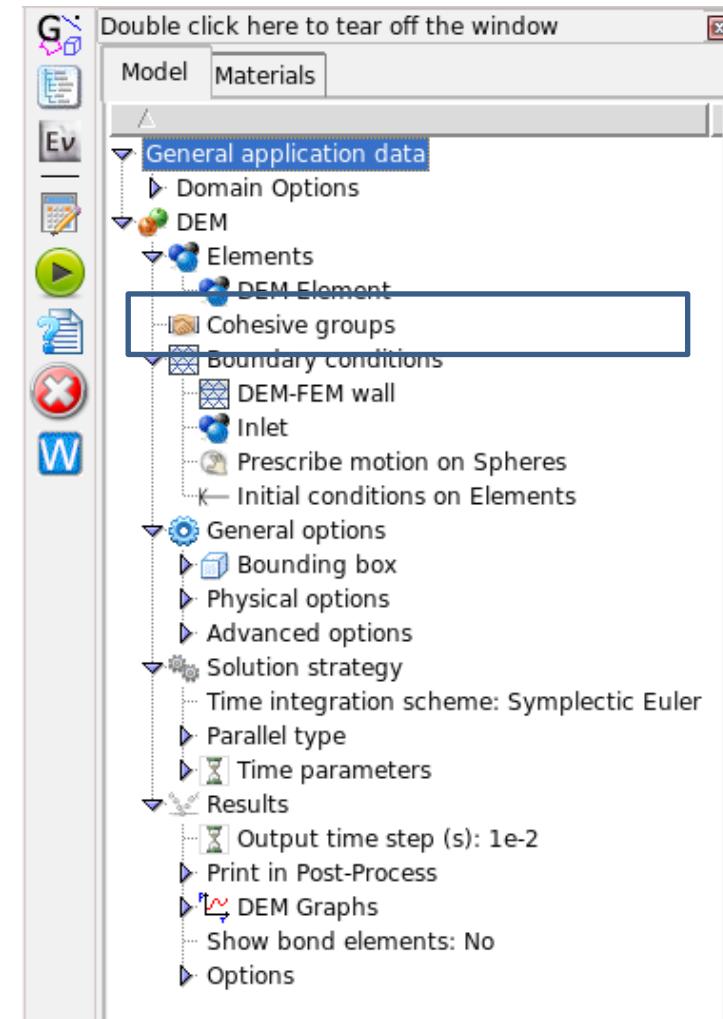
Fabrics breakage.



Bending stiffness in fabrics

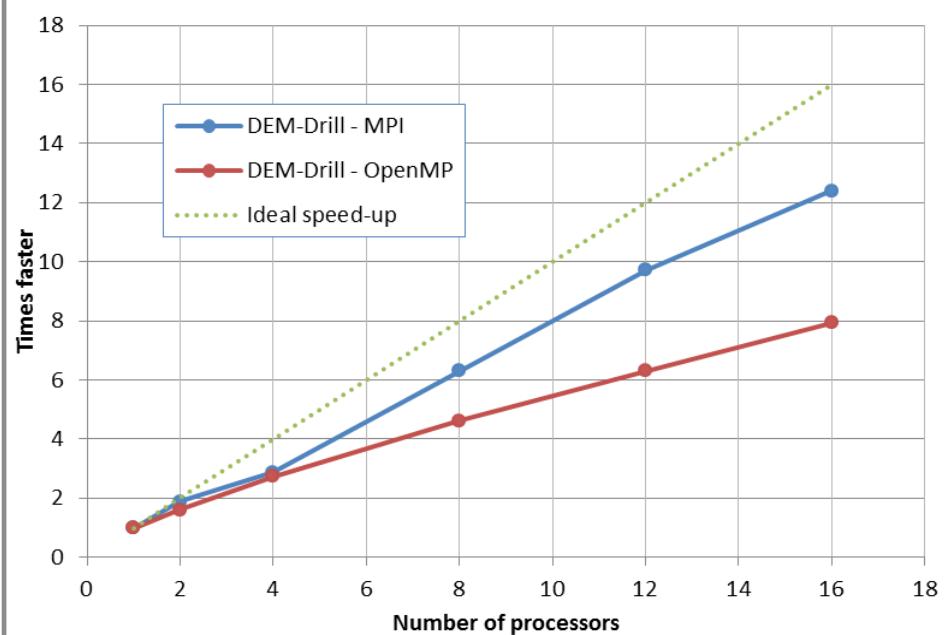
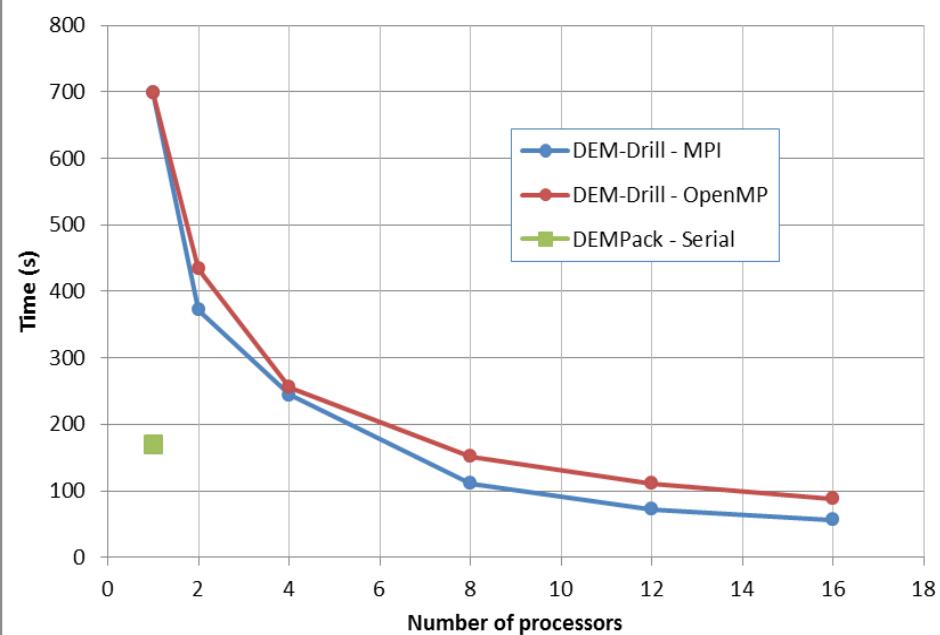


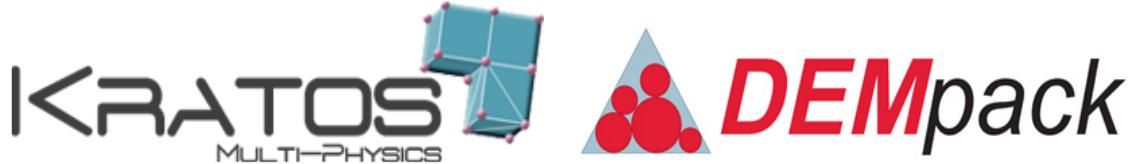
GUI (for GiD, a pre- and post- processor developed at CIMNE)



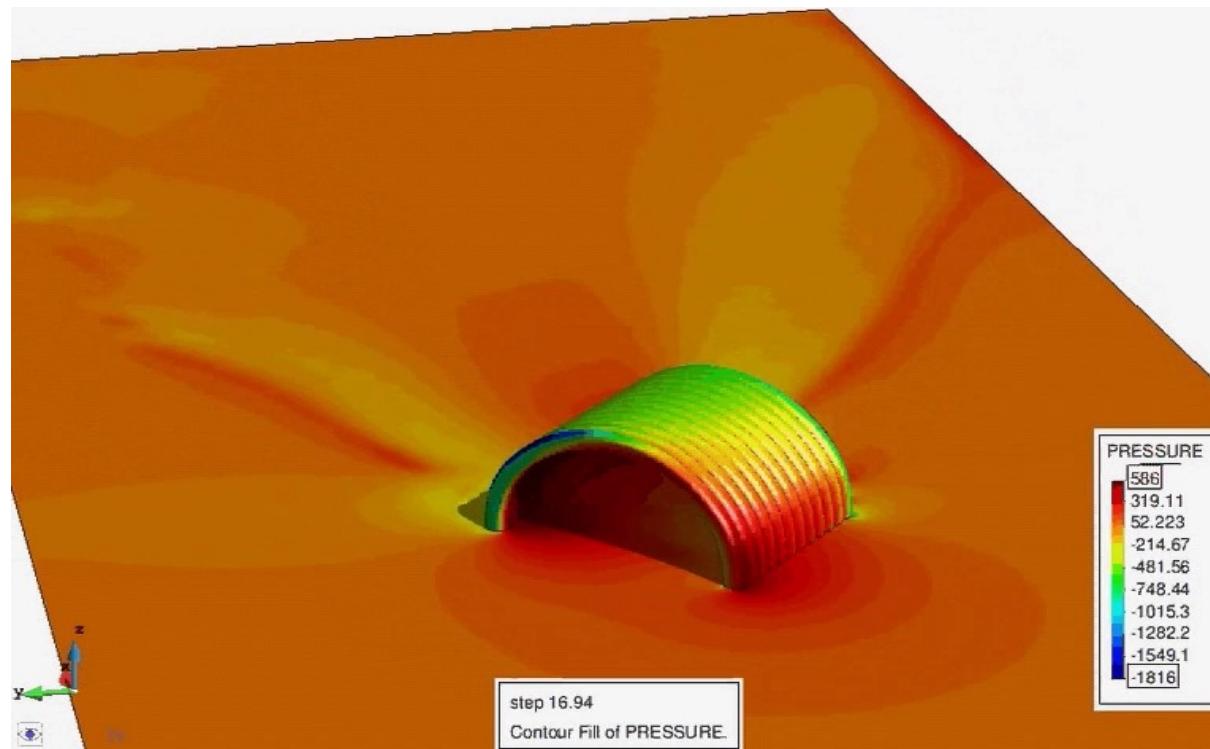
CONTINUUM SIMULATIONS WITH DEM (CONCRETE). MULTI-FRACTURE SPEED-UP

Number of processors	DEMPack-serial	DEM-Drill	DEM-Drill	DEM-Drill	DEM-Drill
	Time (s)	Time (s) OpenMP	Speed-up OpenMP	Time (s) MPI	Speed-up MPI
1	170.55	699.25	1	699.25	1
2		434.03	1.735908803	372.29	1.878
4		255.35	3.083239595	243.92	2.867
8		151.23	5.301740812	111.01	6.299
12		111.05	7.17539267	71.9	9.725
16		88.04	8.562949078	56.35	12.41





- What is Kratos - DEMpack?
- DEMpack – non-cohesive (granular materials, slightly cohesive soils)
- DEMpack – cohesive (rocks, concrete, fabrics)
- **DEMpact – CFD (strong 2-way coupling)**
- DEMpack – CSD (plasticity, damage)
- Wizards



KRATOS CFD
MULTI-PHYSICS

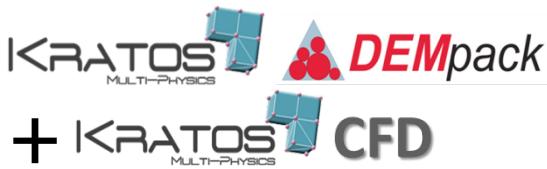
+

KRATOS
MULTI-PHYSICS

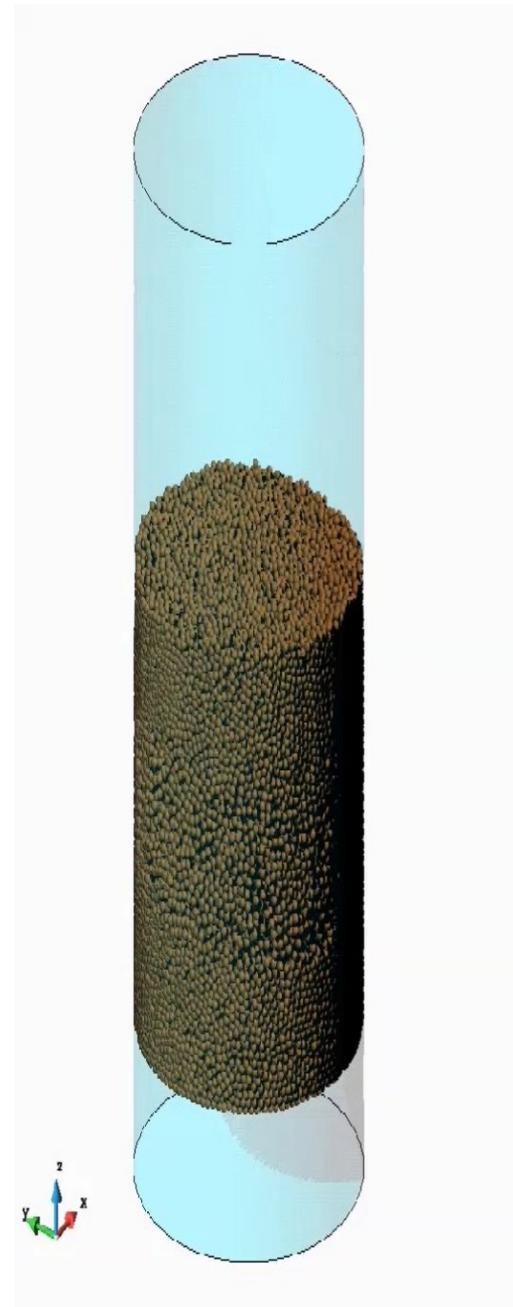
DEMpack

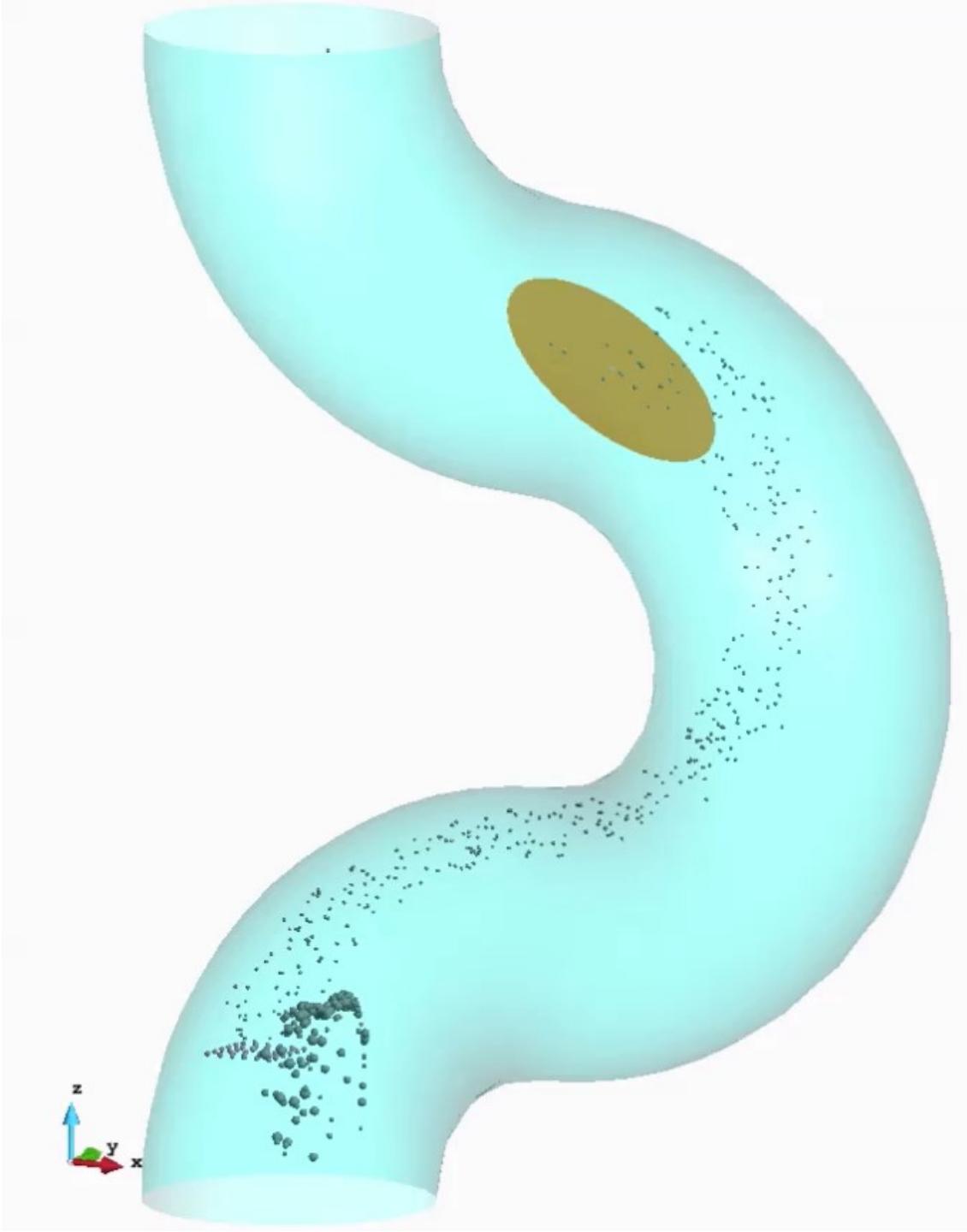


Fluidized bed

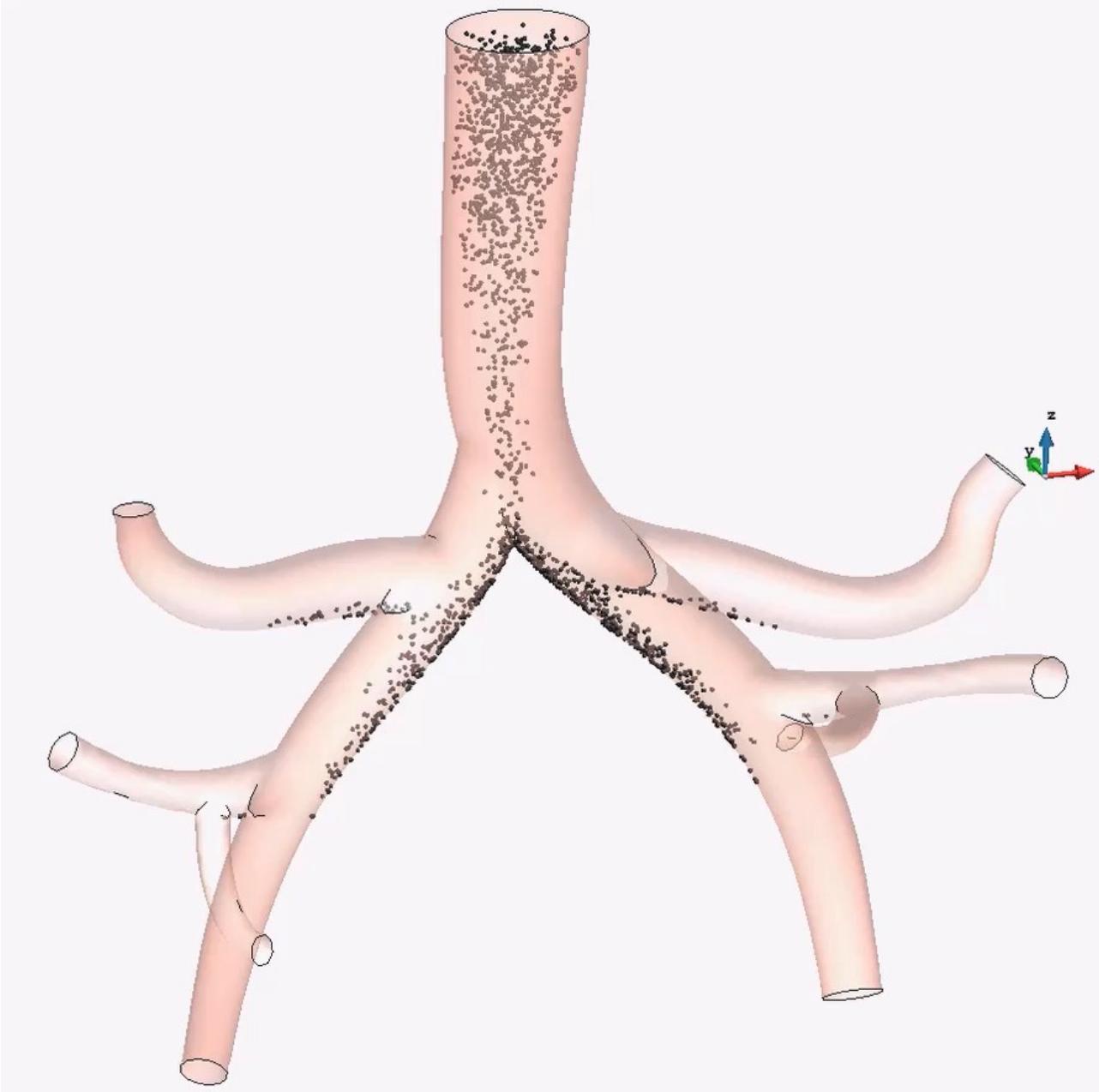


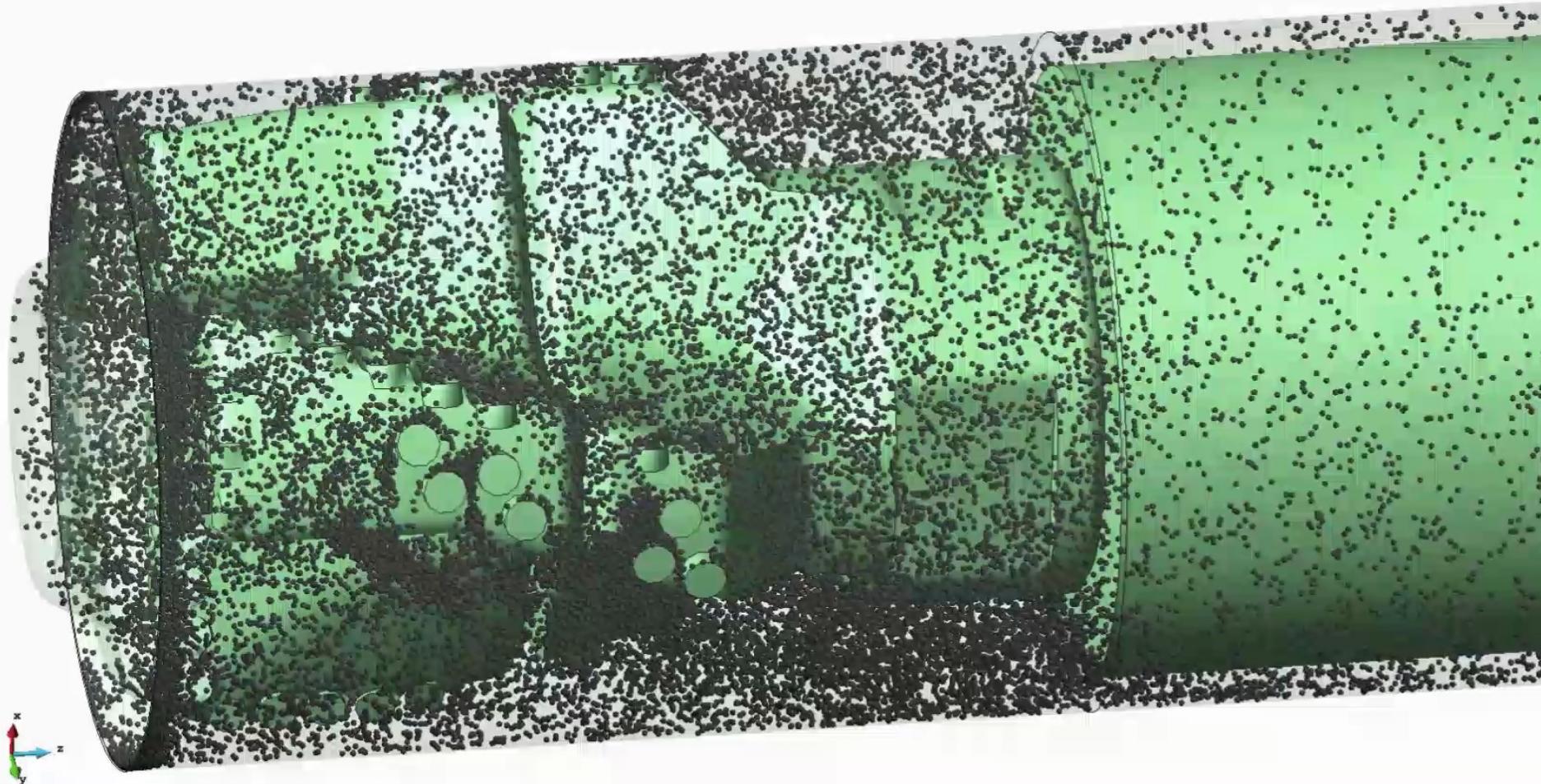
Ascending fluid



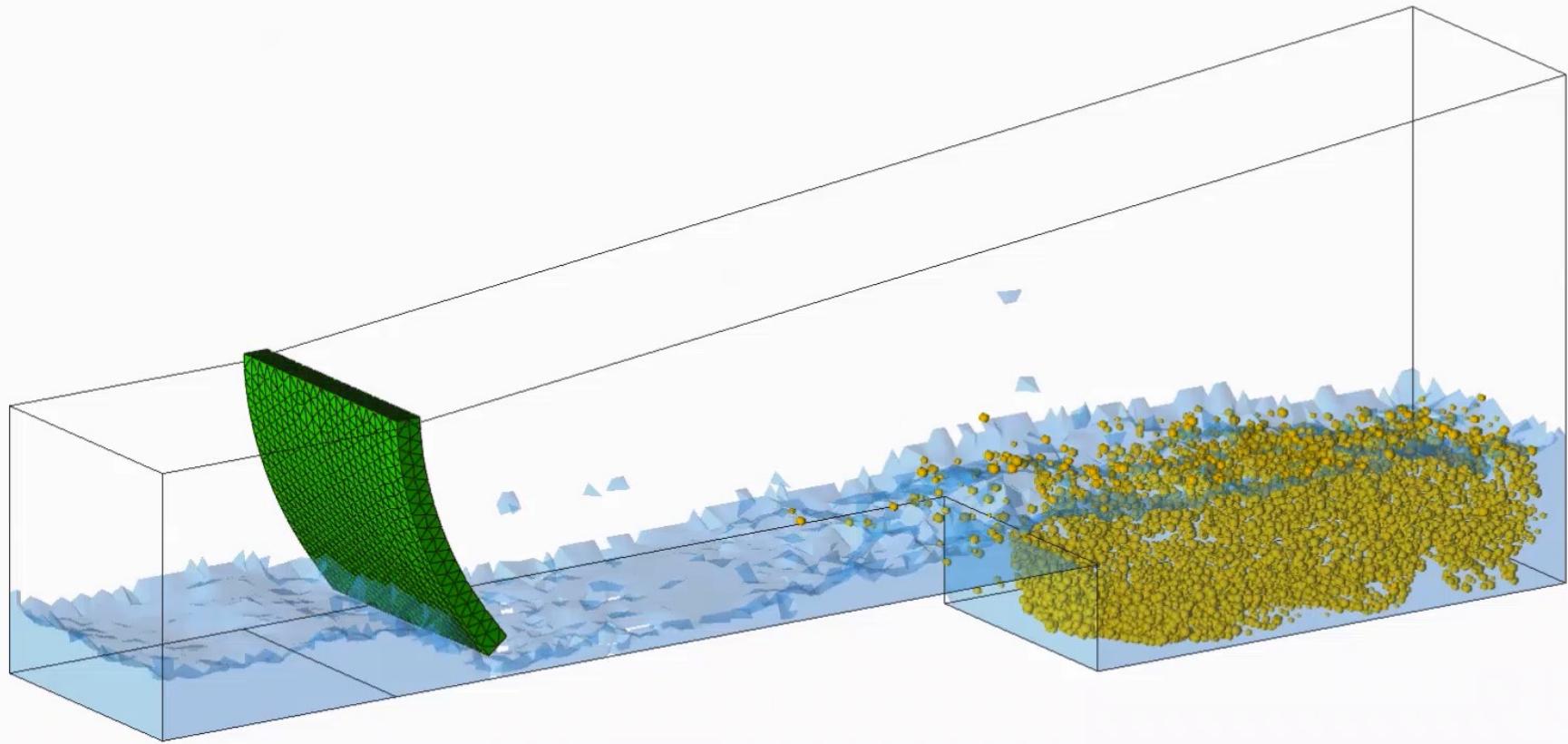


Biomedical studies (lung soiling)

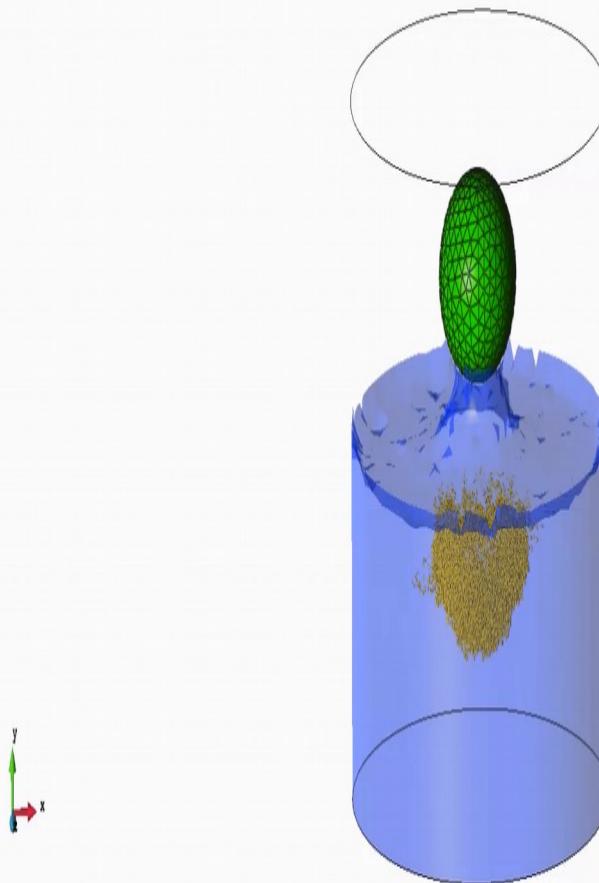




Free surface flows (PFEM + DEM)



Free surface flows (PFEM + DEM)



GUI (for GiD, a pre- and post-processor developed at CIMNE)

Double click here to tear off the window

Model Materials

General application data

- Project information
- Toggle debug/release: Release
- Simulation Options

Physical options

- Gravity modulus: 9.81
- Direction X: 0.0
- Direction Y: 0.0
- Direction Z: -1.0

Coupling parameters

- Coupling level: Full two-way
- Time averaging mode: Take newest values

Hydrodynamic Force Model

- Pick each individual force: Yes
- Drag Force type: Stokes
- Virtual mass force type: Zuber
- Saffman lift Force type: Saffman
- Magnus lift force type: Oesterle
- Hydrodynamic torque type: Dennis
- Drag Modifier type: Hayder
- Viscosity modification type: Einstein
- Include Faxen Terms: No

Post-Processing variables

- Gradient Calculation Mode: Superconvergent Recovery
- Velocity Laplacian Calculation Mode: Finite Element Projection

Results

Options

- Result format: Binary
- Result file: Multiple files

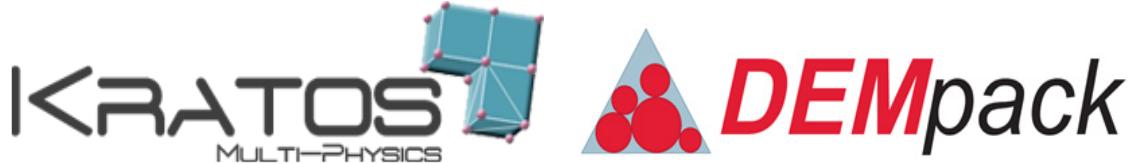
Nodal values to be printed for post-process

- Particle's results
- Fluid phase nodal values
 - Body Force: Yes
 - Fluid Fraction: Yes
 - Fluid Fraction Gradient: Yes
 - Hydrodynamic Reaction on Fluid: Yes
 - Pressure: Yes
 - Pressure gradient: Yes
 - Solid Fraction: Yes
 - Time-Averaged Hydrodynamic Reaction on Fluid: Yes
 - Velocity: Yes
 - Velocity Laplacian: Yes
 - Velocity Laplacian Rate: Yes

Fluid

Analysis data

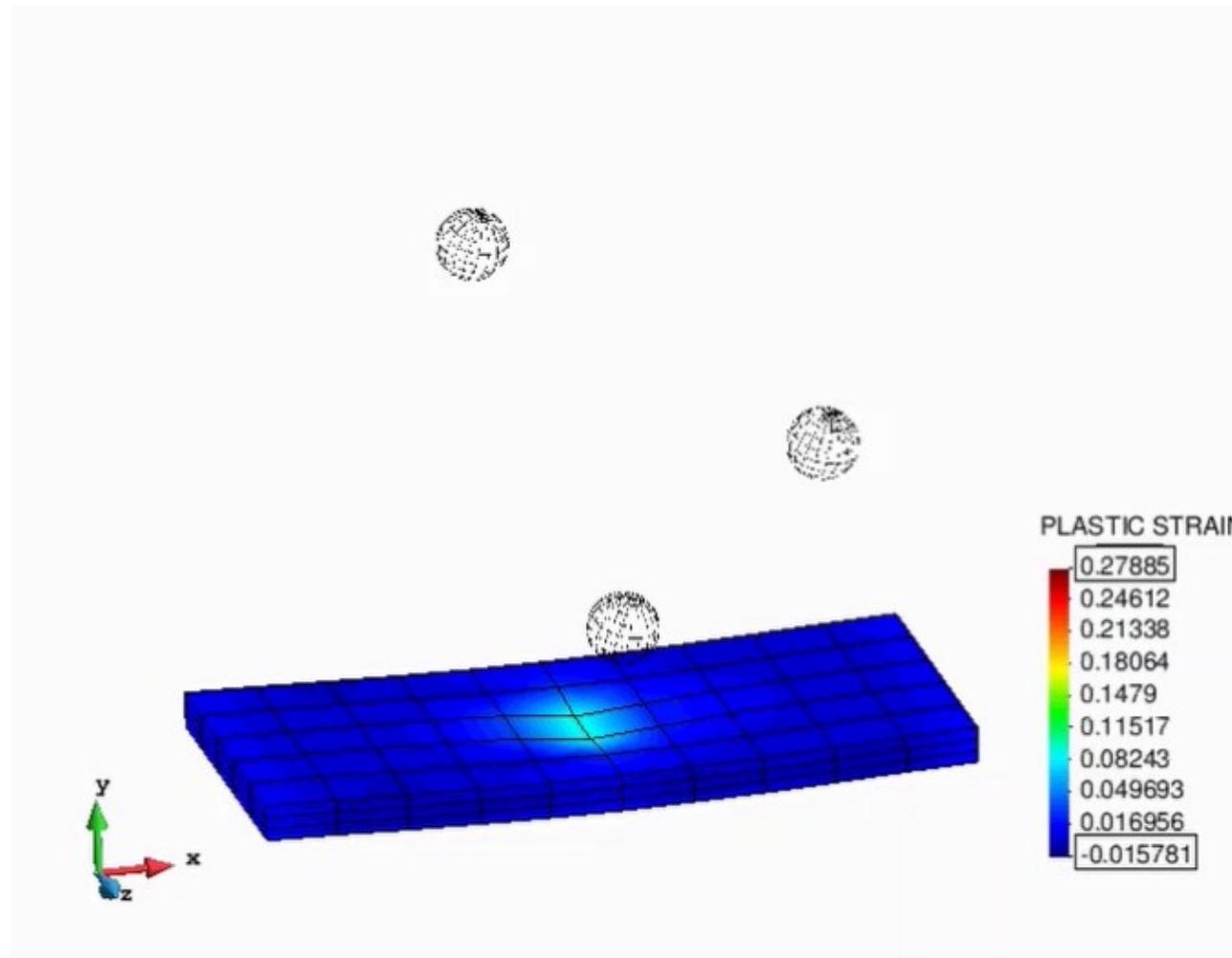
- Solver type: Monolithic



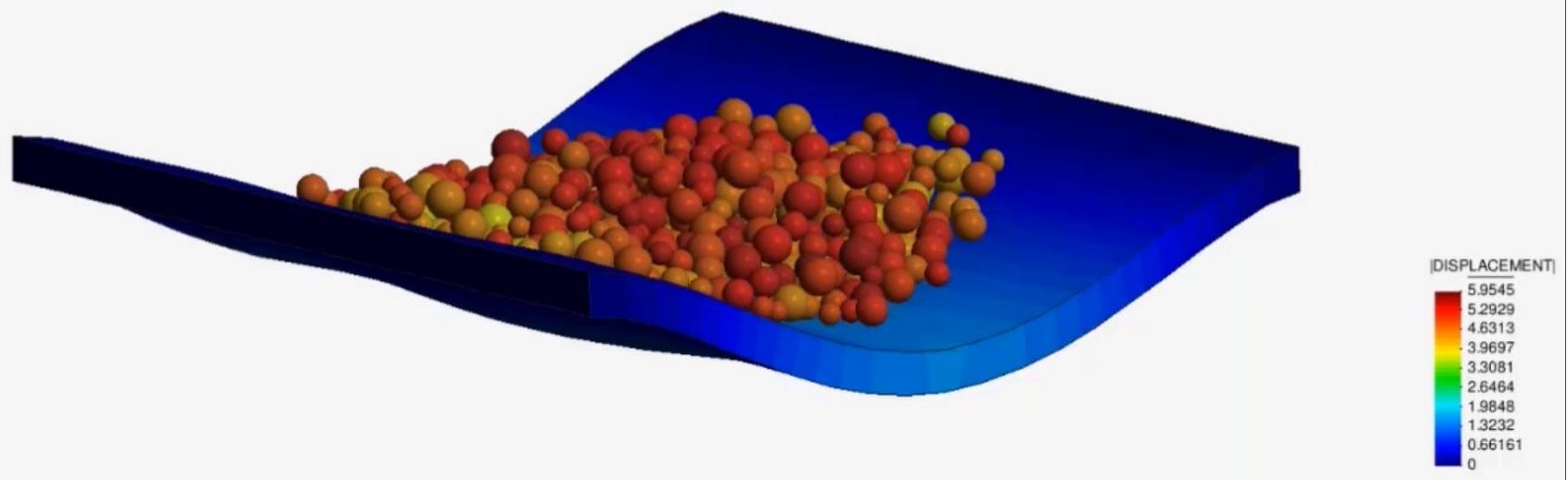
- What is Kratos - DEMpack?
- DEMpack – non-cohesive (granular materials, slightly cohesive soils)
- DEMpack – cohesive (rocks, concrete, fabrics)
- DEMpack – CFD (strong 2-way coupling)
- DEMpack – CSD (plasticity, damage)
- Wizards

DEM impacts on elasto-plastic solid

Impact duration and evolution of forces is crucial to calculate the actual plastic strain in the solid. This means that the time step is the same for both the DEM and the solid. CSD uses an explicit scheme.

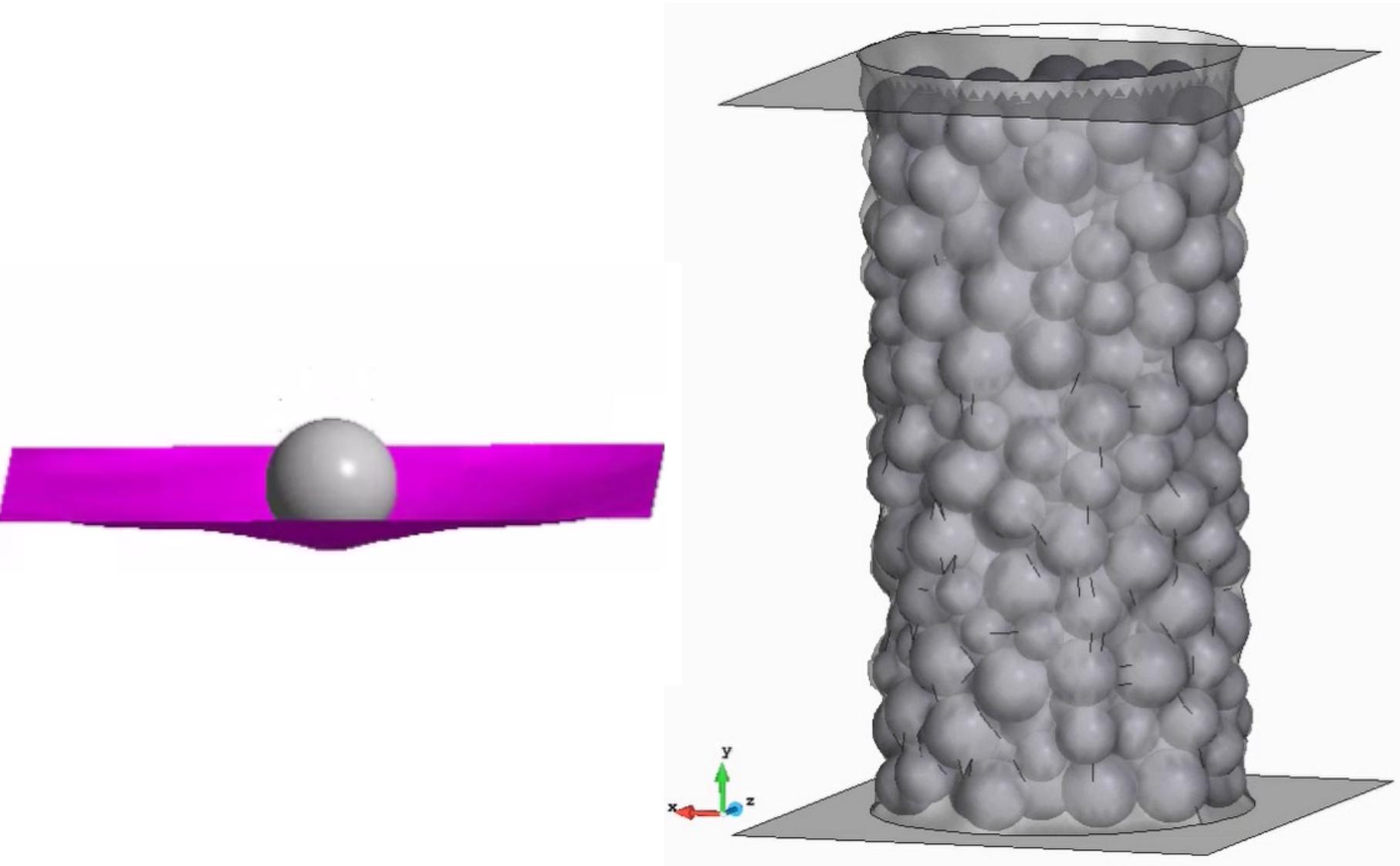


Interaction between particles and elastic plate

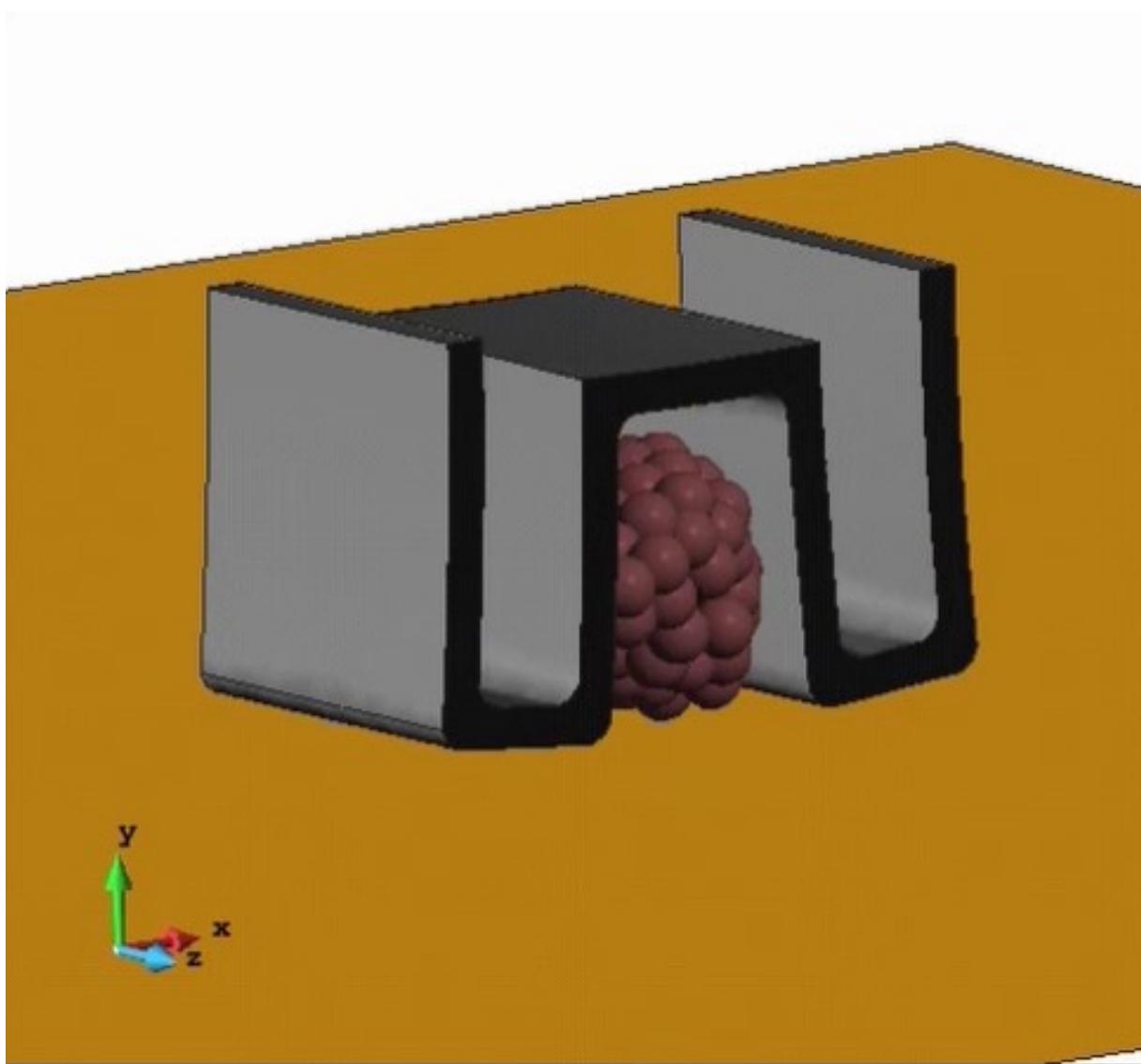


Santosusana, M., Irazábal, J., Oñate, E., Carbonell, J.M. *The Double Hierarchy Method. A parallel 3D contact method for the interaction of spherical particles with rigid FE boundaries using the DEM.*
DOI:10.1007/s40571-016-0109-4

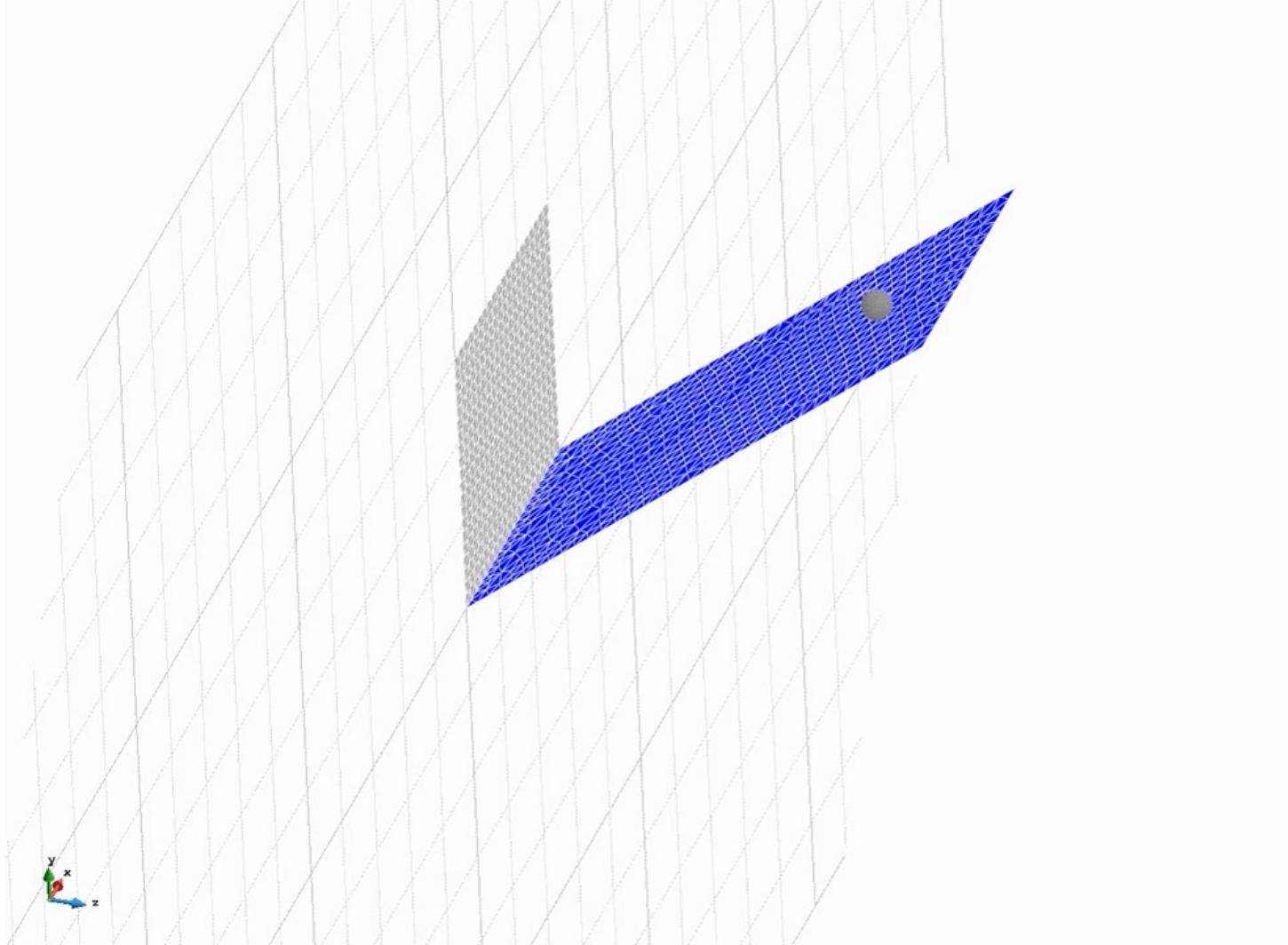
Triaxial test (wrapper structural membrane):

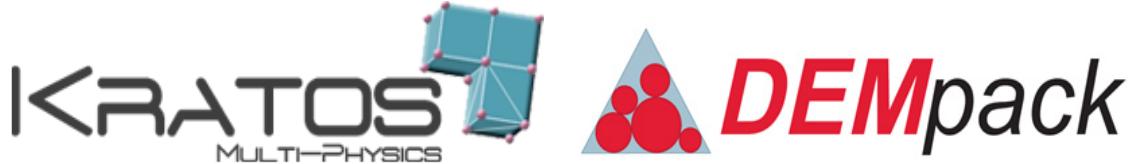


Truck tyre and stone



Coupling DEM-Structure (beams) – WIP in TUM





- What is Kratos - DEMpack?
- DEMpack – non-cohesive (granular materials, slightly cohesive soils)
- DEMpack – cohesive (rocks, concrete, fabrics)
- DEMpack – CFD (strong 2-way coupling)
- DEMpack – CSD (plasticity, damage)
- Wizards

Features of a ‘Wizard’:

- A Graphical User Interface which allows to launch a computation in a very short time (computation might take hours or more, though)
- Little or no effort in creating geometries or meshes
- Limited and very specific capabilities and output
- Optimized for a specific task

SpreadDEM v1.0

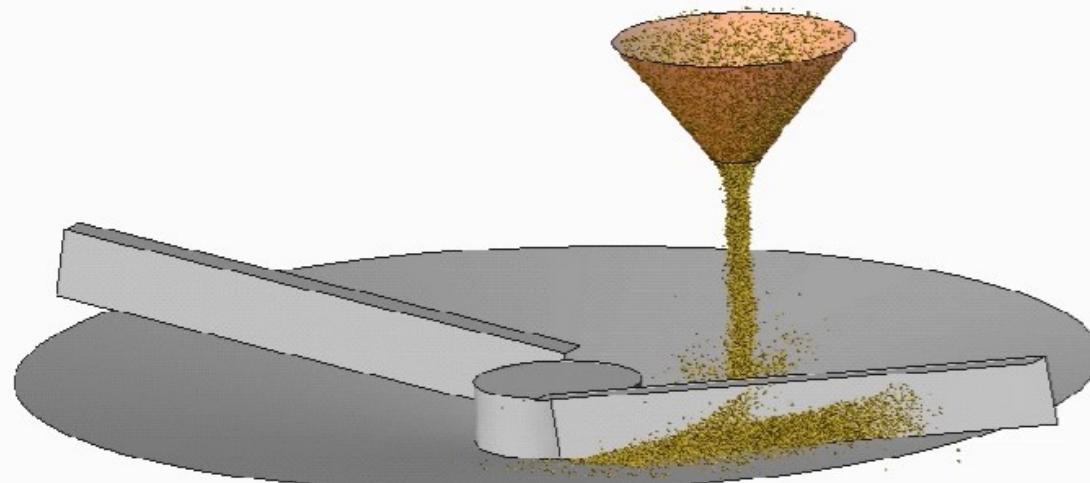


(presented in Gid Workshop 2018)

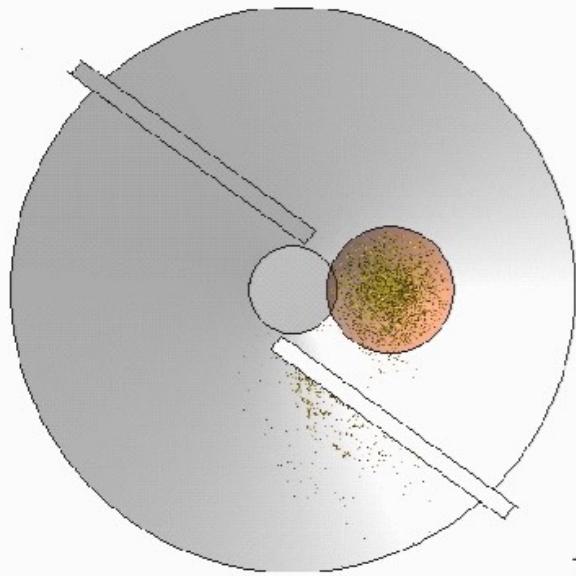


Fertilizer (or seeds) spreader

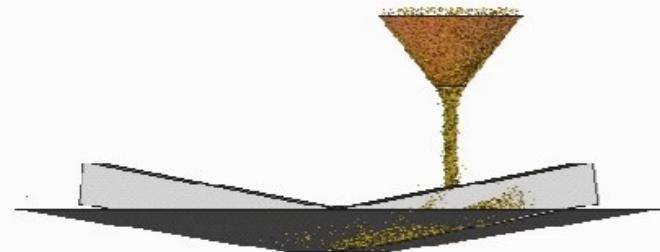




Time = 0.32 s



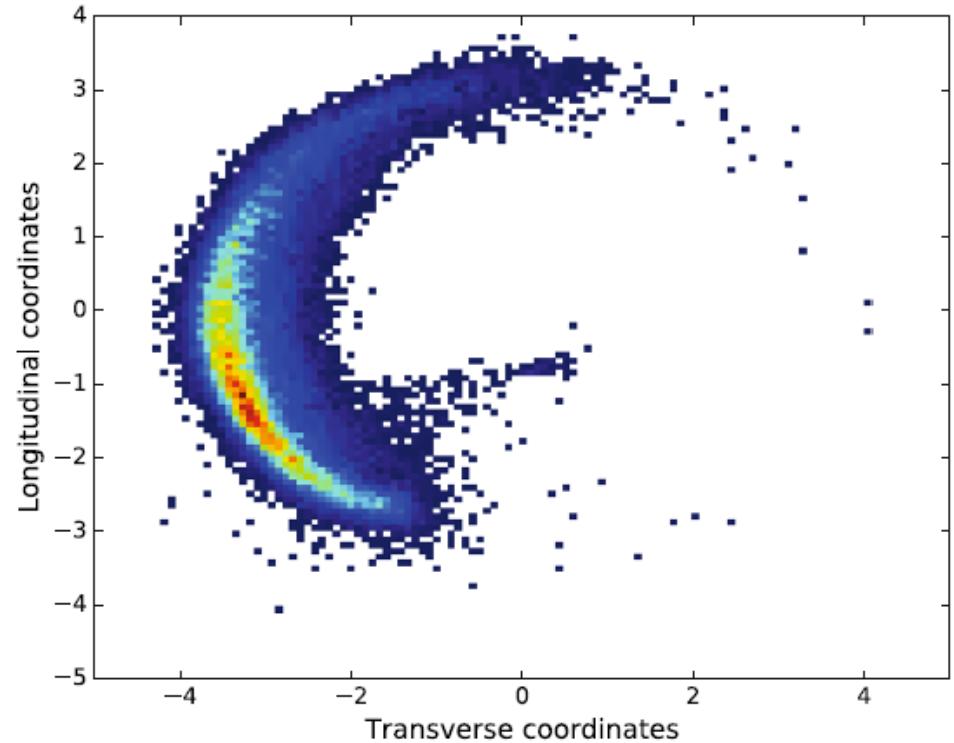
Time = 0.32 s



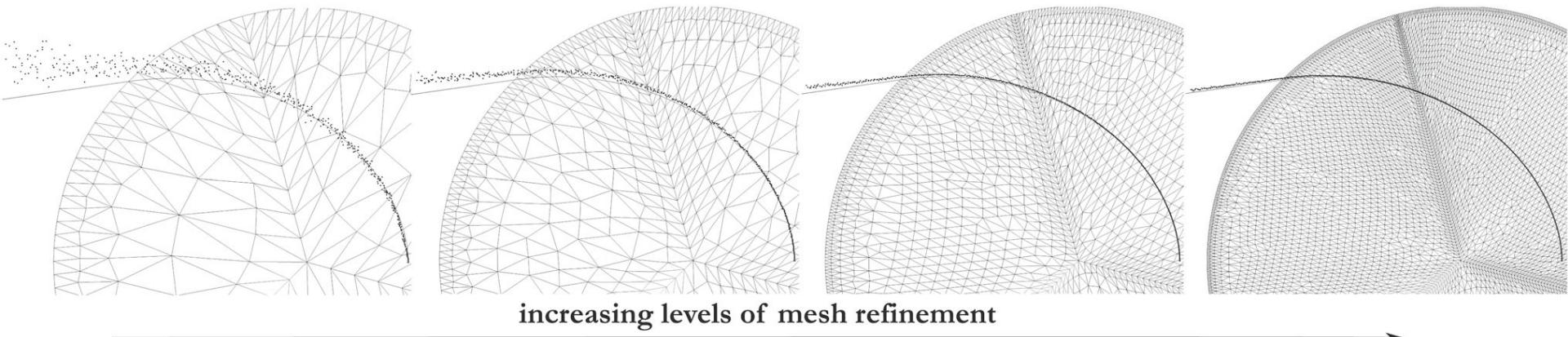
70

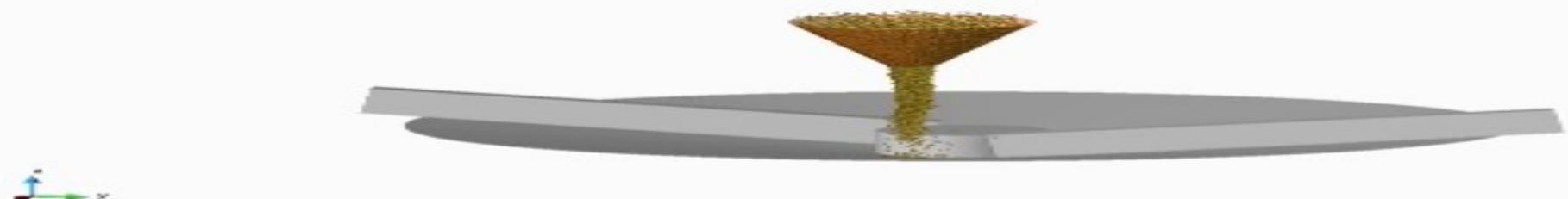
Time = 0.32 s

Dispersion patterns:



Accuracy assessment:







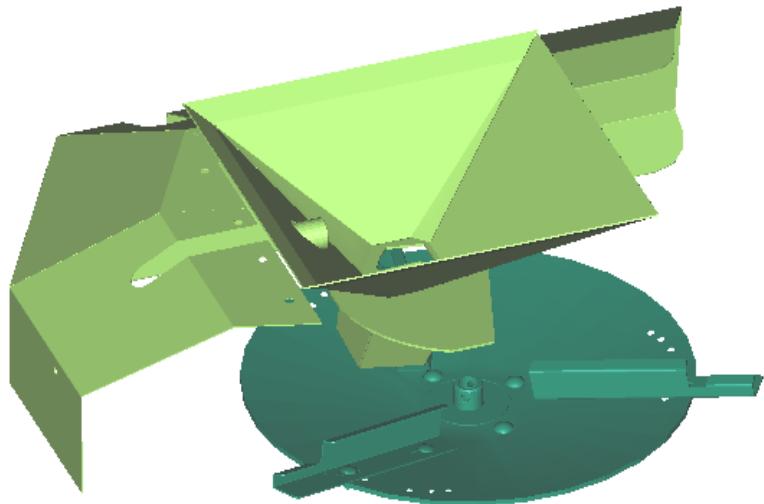
STEP 1. Model

Rotative parts imported

Angular velocity of the discs

Rotation axis

Fixed parts imported



SpreadDEM

SpreadDEM ① Model ② Fertilizer ③ Inlet ④ Conditions ⑤ Settings ⑥ Results

Model units: m

Discs / rotating bodies:

Disc1	<input type="button" value="Move"/>	<input type="button" value="Duplicate"/>	
<input type="checkbox"/> Move			
Kinematics Disc 1			
Angular velocity: 800 rpm			
Rotation axis:			
Initial node:	Pick	Final node:	Pick
X 0.00 m	0.00 m	Z 0.00 m	1.00 m
Y 0.00 m	0.00 m		
<input type="checkbox"/> Display vector			

Duplicate disc: Yes

Duplicate to the side: Left Right

Distance between axis: 0.9 m

Show duplicated disc

Fixed / rigid bodies:

Rigid1	<input type="button" value="Move"/>	<input type="button" value="Duplicate"/>
Rigid2		
Rigid3		
<input type="checkbox"/> Move		

< Back Next > Exit



STEP 2. Fertilizer

Fertilizer properties

Density

Friction angle

Granulometry

SpreadDEM

SpreadDEM 1 Model 2 Fertilizer 3 Inlet 4 Conditions 5 Settings 6 Results

Material properties

Material:	Customized-fertiliser	<input checked="" type="checkbox"/> Advanced properties
Density:	1035 kg/m ³	Coef. of restitution: 0.2
Friction angle:	20 deg	Sphericity: 1

Particle Size Distribution

Granulometry Probability distribution

Sieve aperture [mm]	Percentage passing [%]
2	0
3.3	37
4.75	95
5.5	100

Granulometry curve

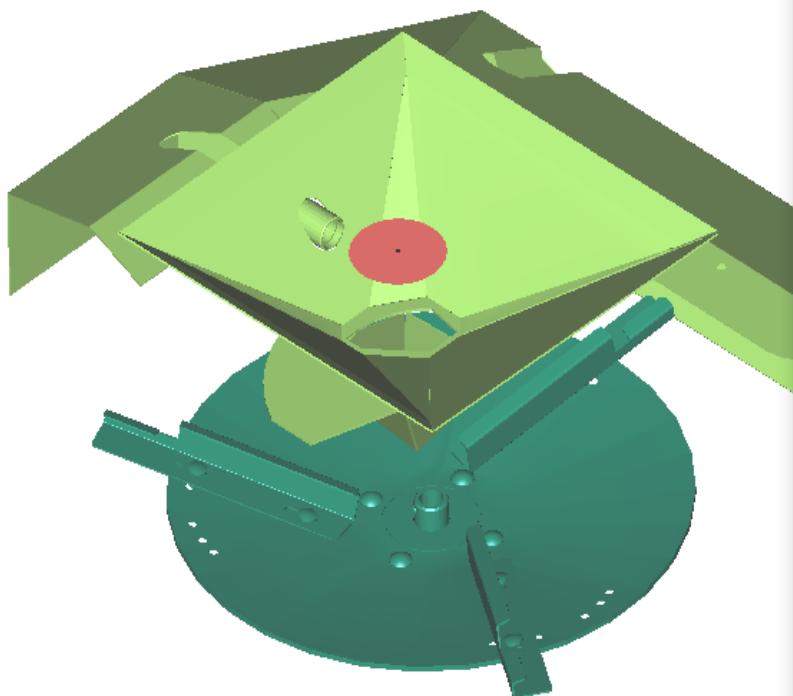
Refresh graph

< Back Next > Exit



STEP 3. Inlet

Inlet of fertilizer particles
Mass flow
Inlet geometry and position



SpreadDEM

SpreadDEM

1 Model 2 Fertilizer 3 Inlet 4 Conditions 5 Settings 6 Results

Inlet of fertilizer particles

Inlet1

+ -

Inlet 1

Mass flow: 100 kg/mir

Inlet radius: 0.05 m

Inlet center: X -0.08 m, Y 0.04 m, Z 0.26 m

Orientation:

Initial node: Final node:

Pick Pick

X 0.00 m Y 0.00 m Z 0.00 m

X 0.00 m Y 0.00 m Z -1.00 m

< Back Next > Exit





STEP 4. Conditions

Gravity

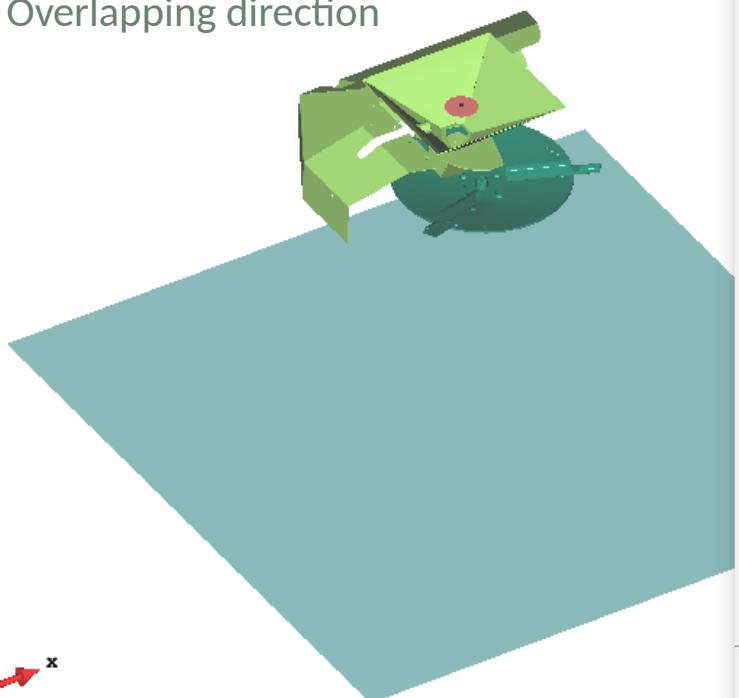
Wind conditions

Ground plane

Distance to floor

Slope of the ground

Overlapping direction



SpreadDEM

① Model ② Fertilizer ③ Inlet ④ Conditions ⑤ Settings ⑥ Results

Gravity

Gravity module: 9.81 m/s²

Gravity direction: X 0.0
Y 0.0
Z -1.0

Wind conditions

Wind module: 0 [m/s]

Wind direction: X 1.0
Y 0.0
Z 0.0

Ground plane

Ground point:

Pick

X 0 m
Y 0 m
Z -0.75 m

Slope of the ground:

X direction 0 deg
Y direction 0 deg

Show ground plane

Ground point Point on the ground plane

X direction Y direction Direction of travel

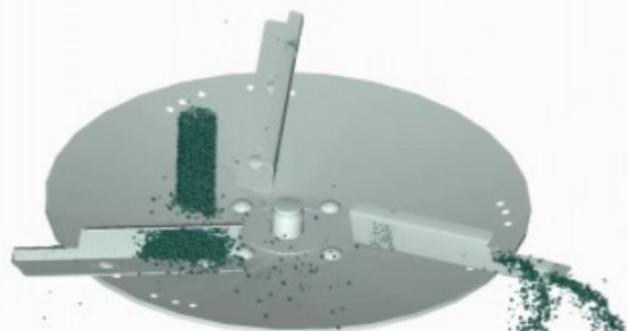
Overlapping direction

The overlapping configuration can be changed after the simulation if no wind effect is computed.

< Back Next > Exit



SpreadDEM v1.0

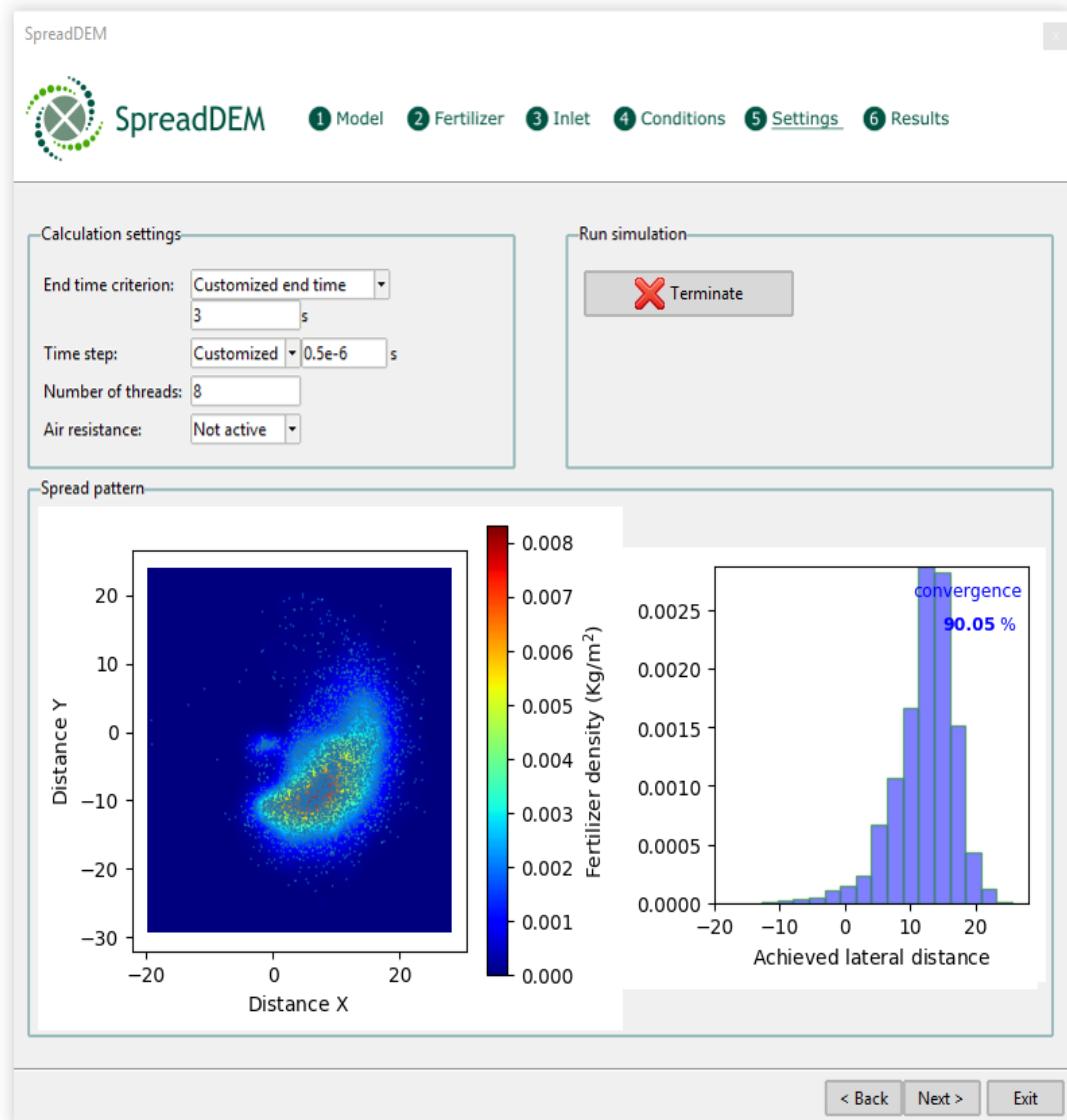




STEP 5. Settings

Calculation settings

Spread pattern during simulation





STEP 6. Results

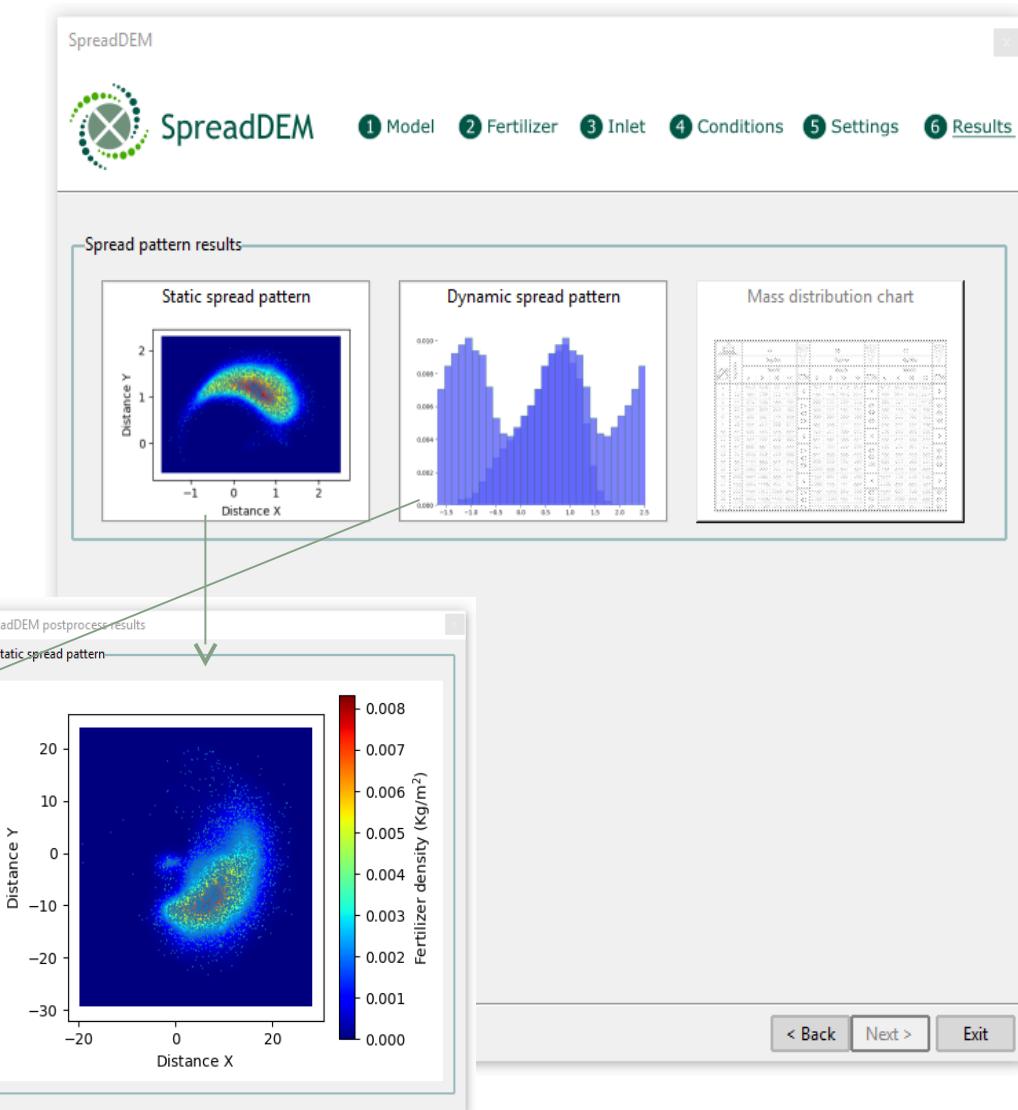
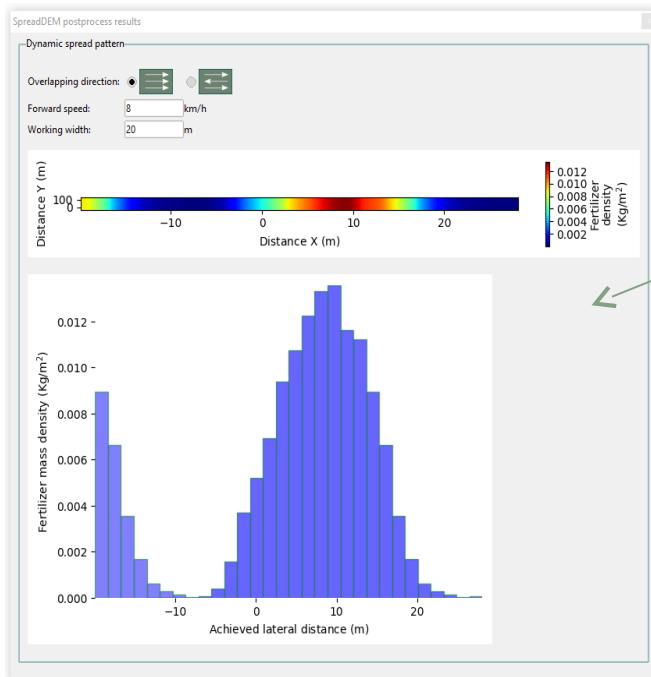
Static spread pattern

Dynamic spread graph according to:

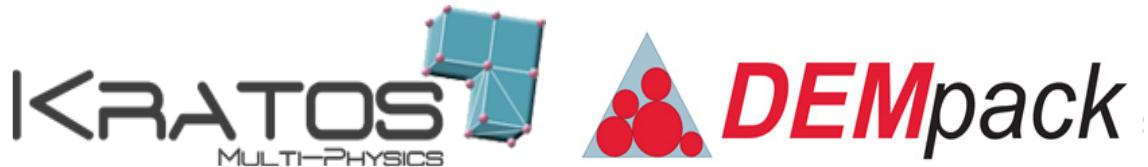
Overlapping direction

Forward speed

Working width



An overview on the main features of



<http://www.cimne.com/dem/>

gcasas@cimne.upc.edu

maceli@cimne.upc.edu

spreaddem@cimne.upc.edu

