An overview on the main features of

KRATOS MULTI-PHYSICS DEMpack

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

CIMNE UPC

- 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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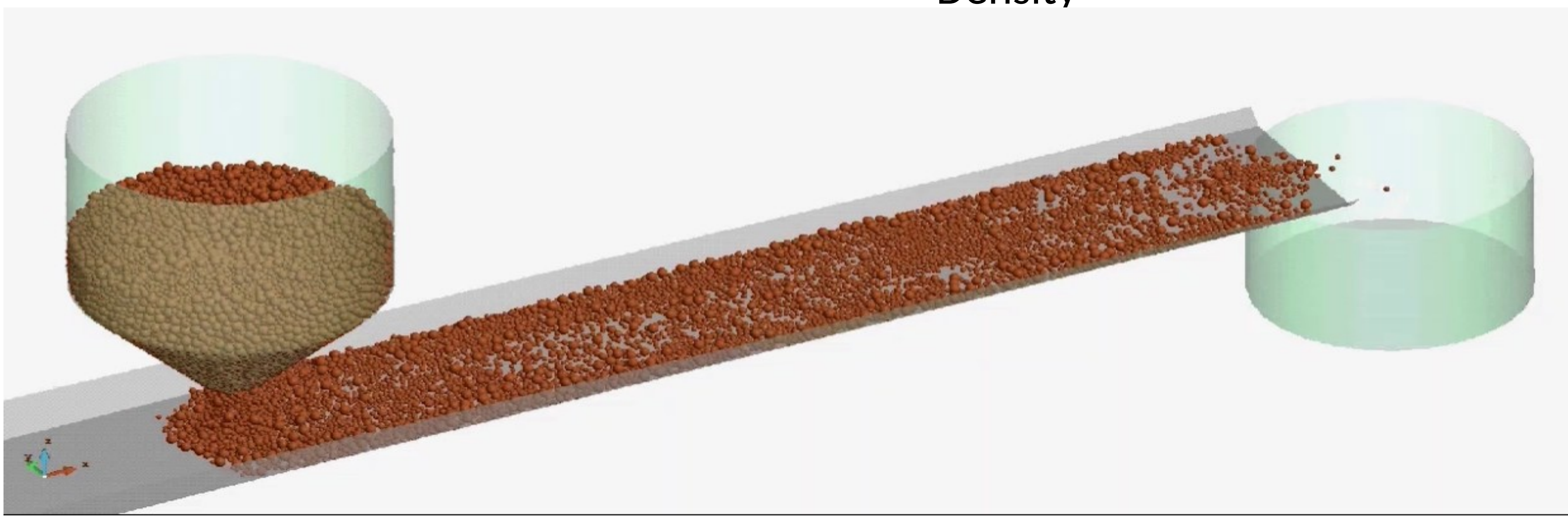
DEM CODE: KRATOS DEMPACK

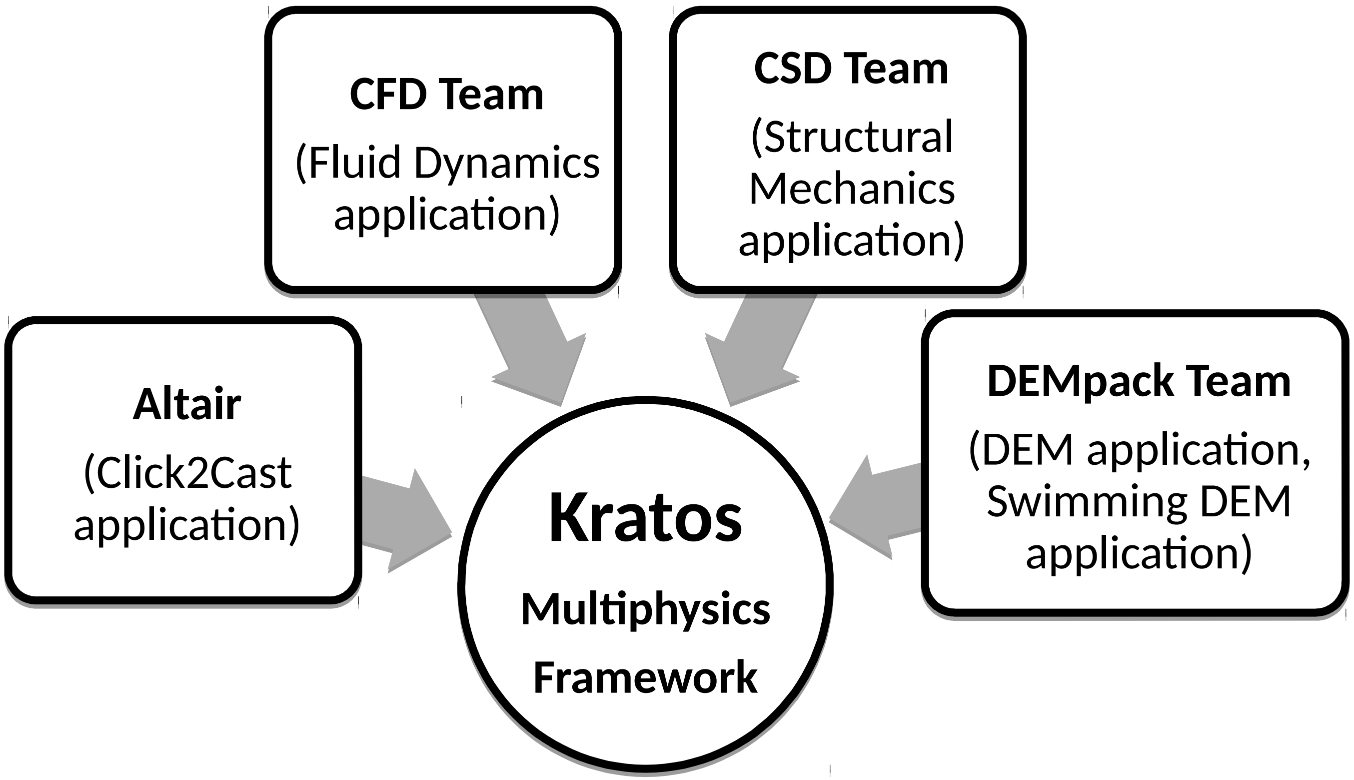
(framework)

(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
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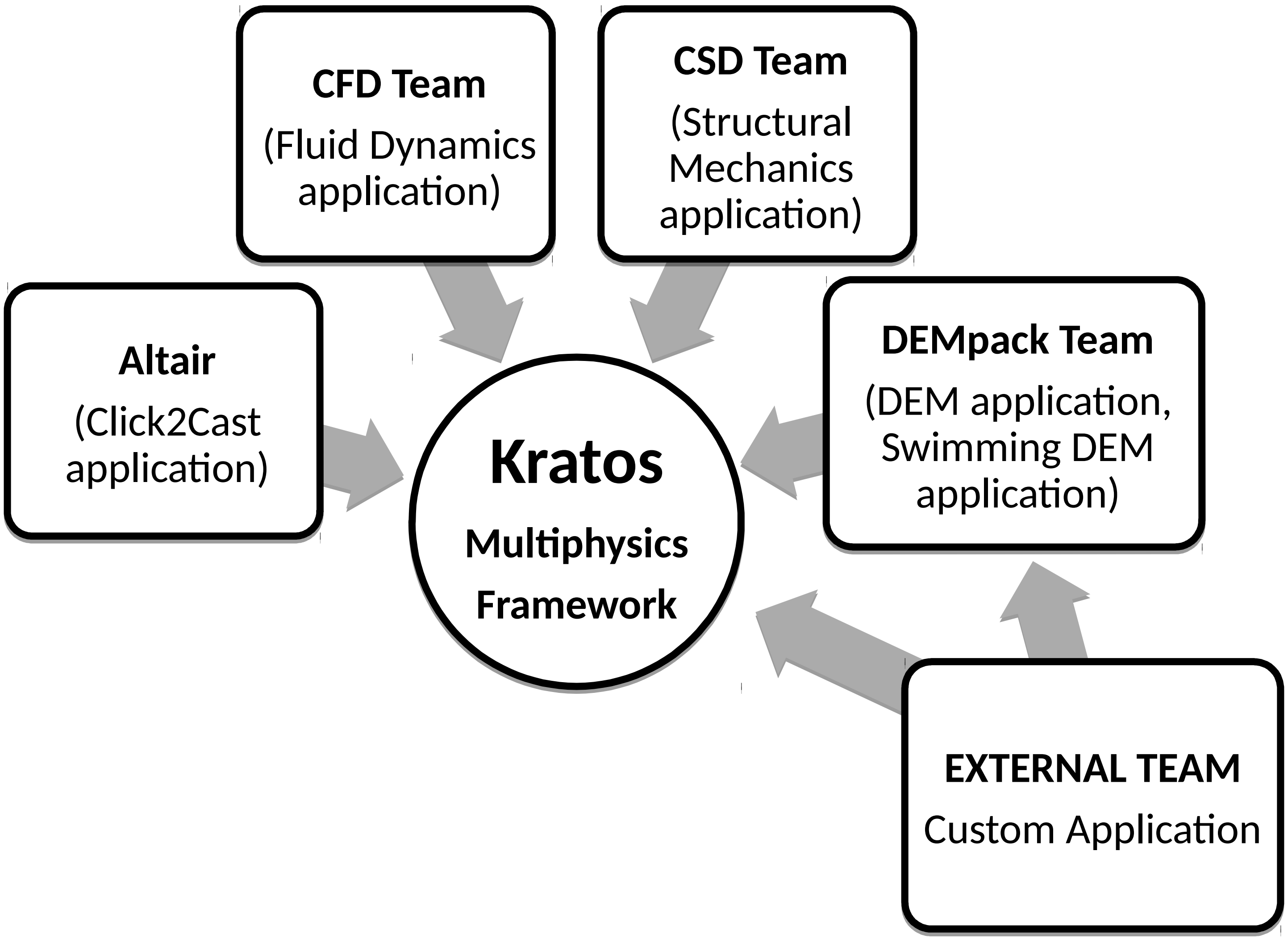

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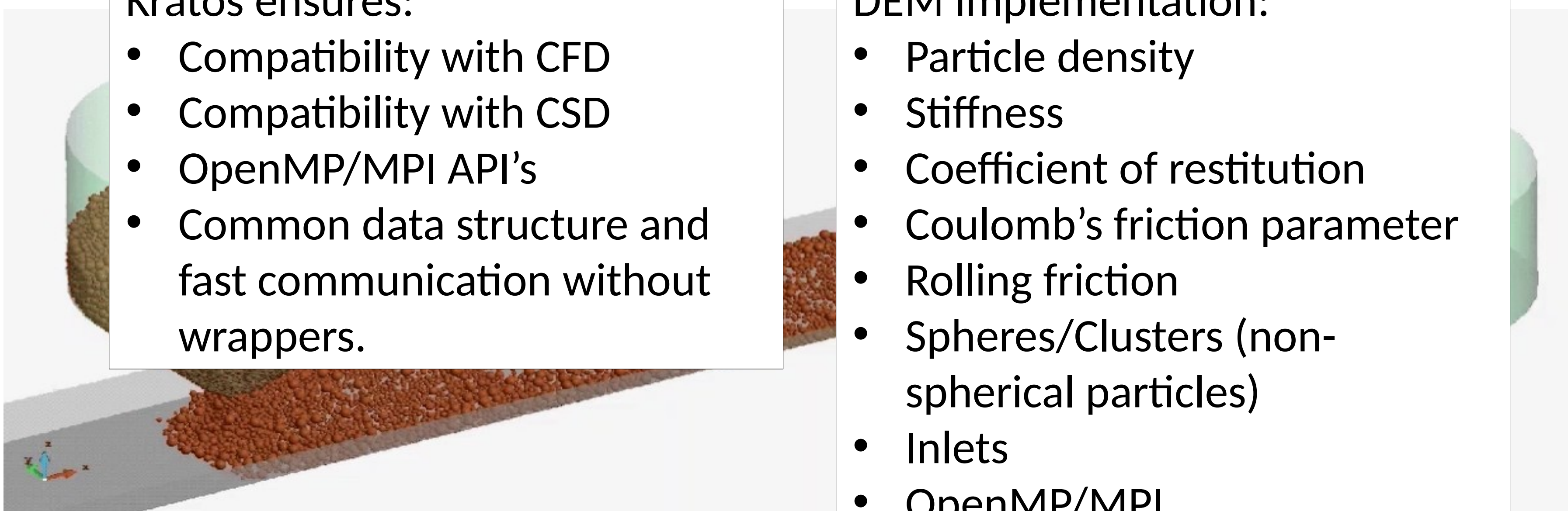
(framework) (application)



Kratos ensures:

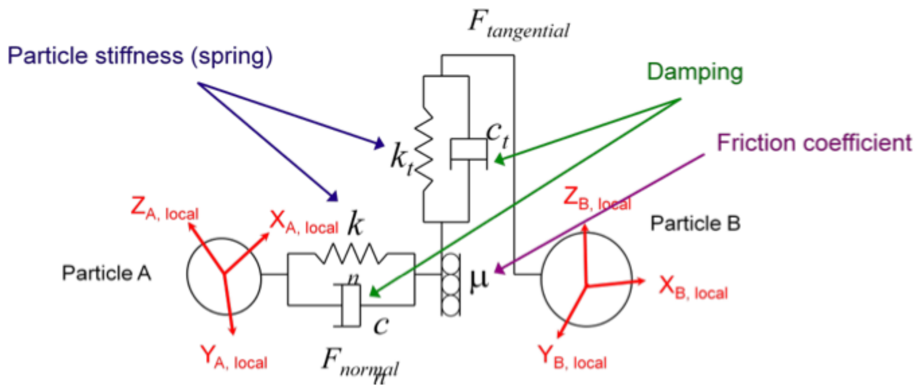
- Compatibility with CFD
- Compatibility with CSD
- OpenMP/MPI API's
- Common data structure and fast communication without wrappers.

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.



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

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

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

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

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

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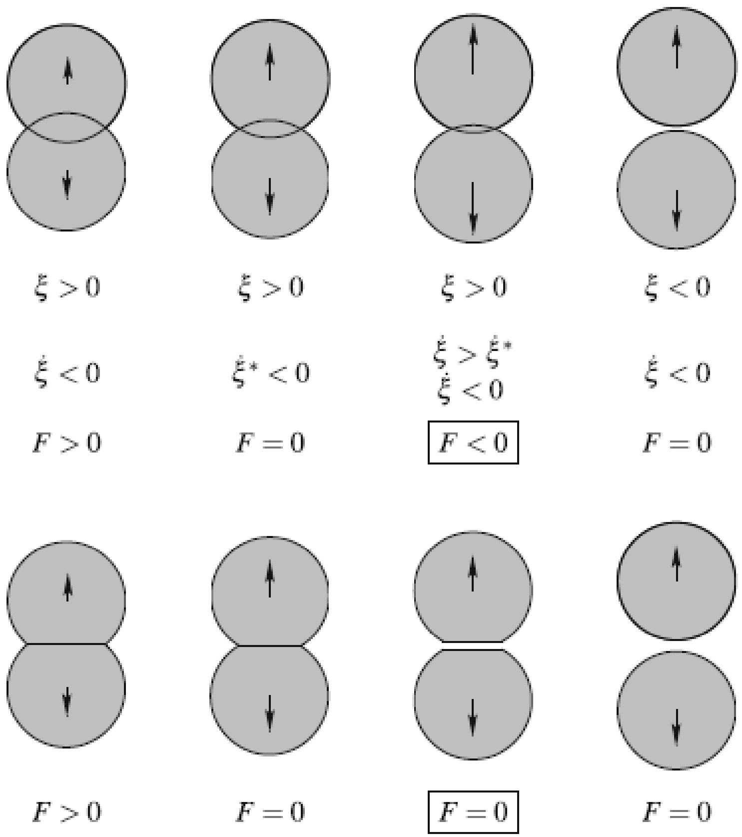


shorter contact time, so
stronger damping to ensure fullfilment of the Coefficient of Restitution.

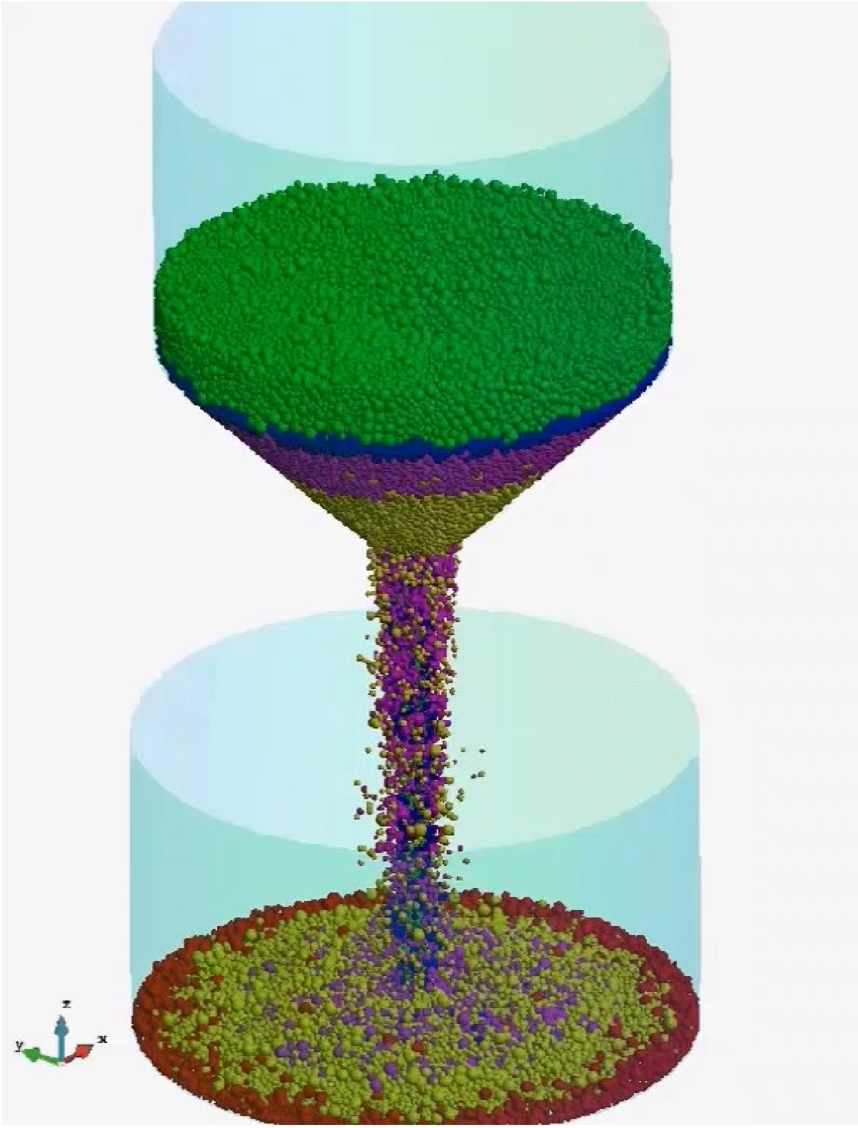
Other features:

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

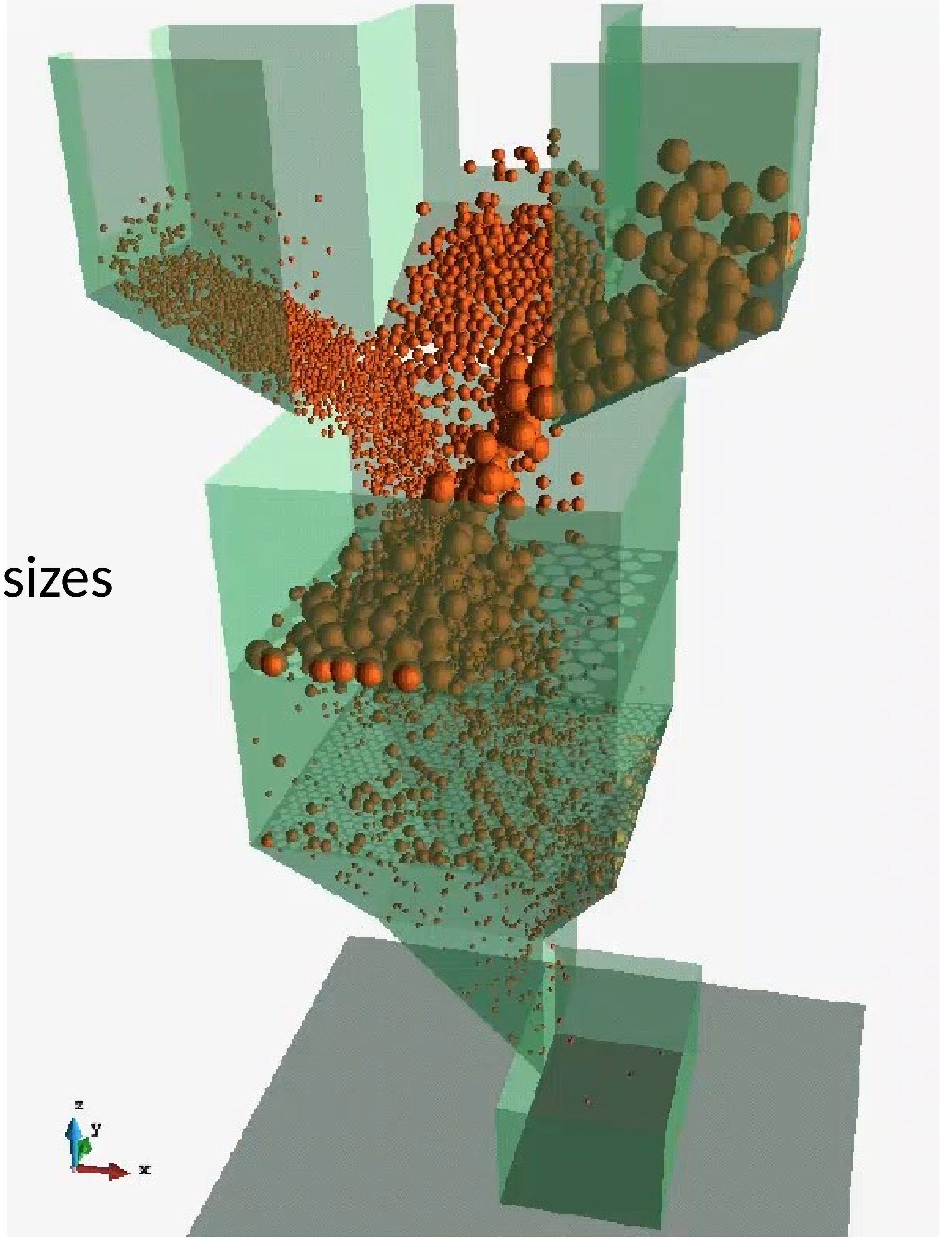
No tractions allowed!

T. Schwager, T. Pöschel, *Coefficient of restitution and linear-dashpot model revisited*, Granular Matter 9 (2007) 465–469.

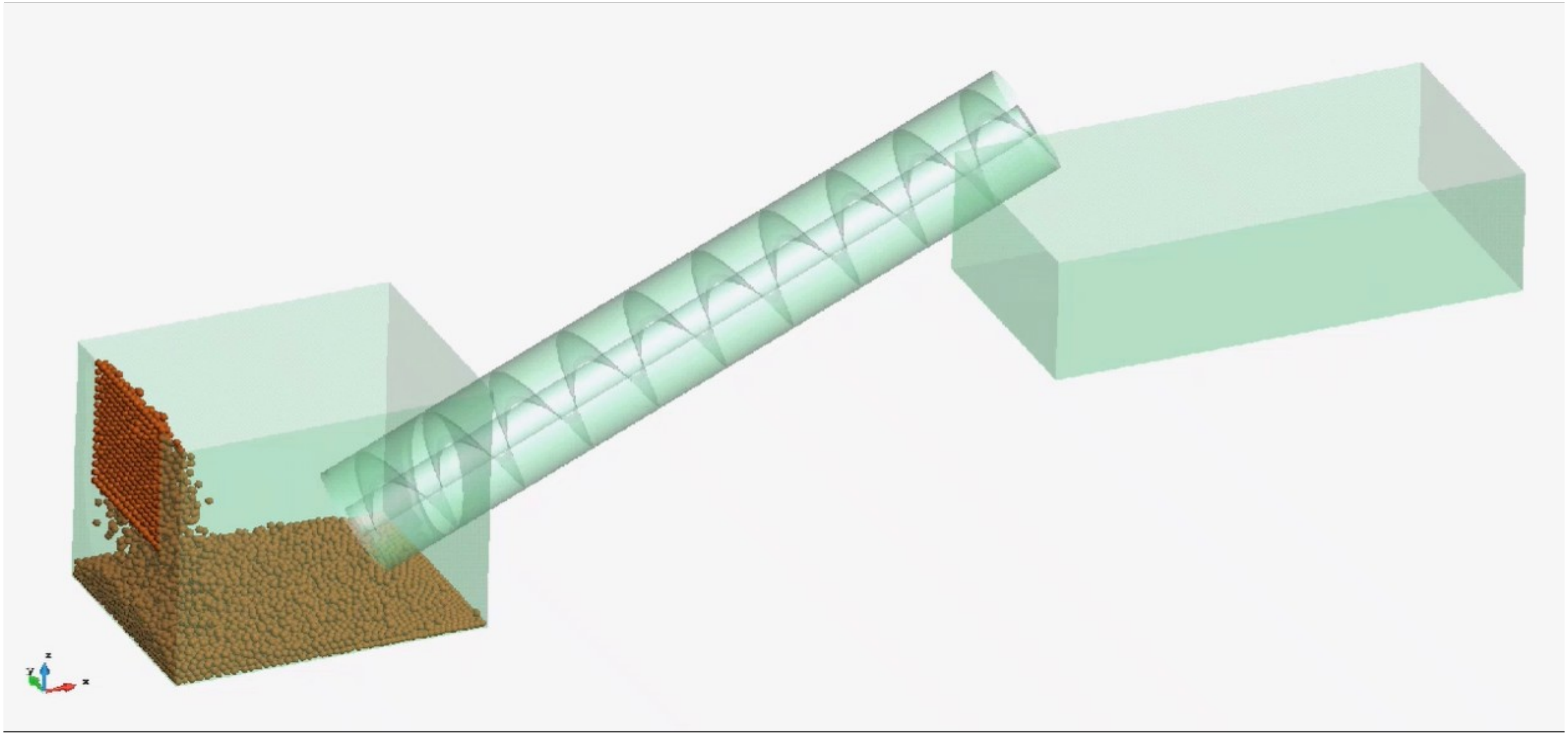
DISCONTINUUM METHODS (PARTICLES) FOR GRANULAR FLOWS



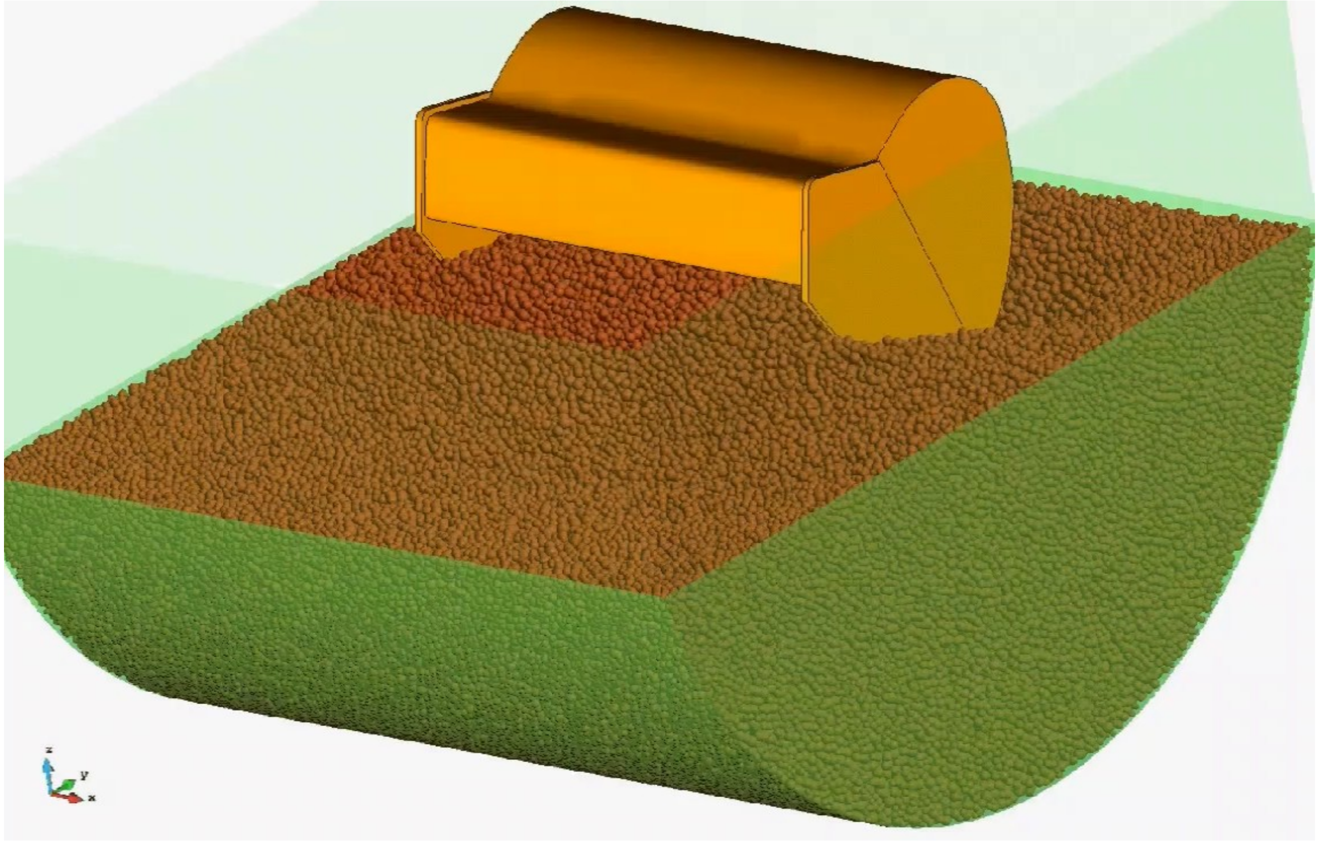
Sieve, 3 diferent sizes



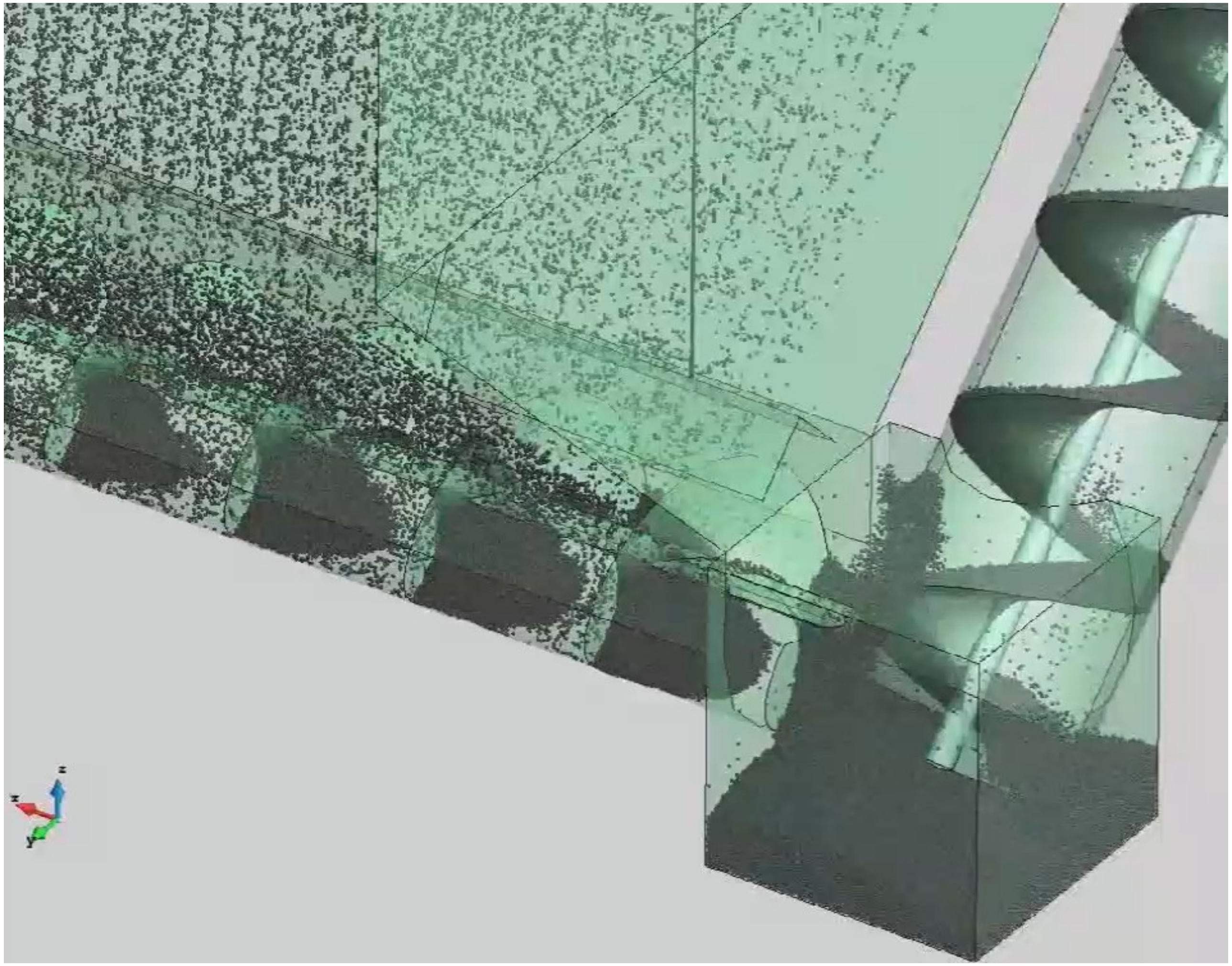
Archimedes screw for granular matter



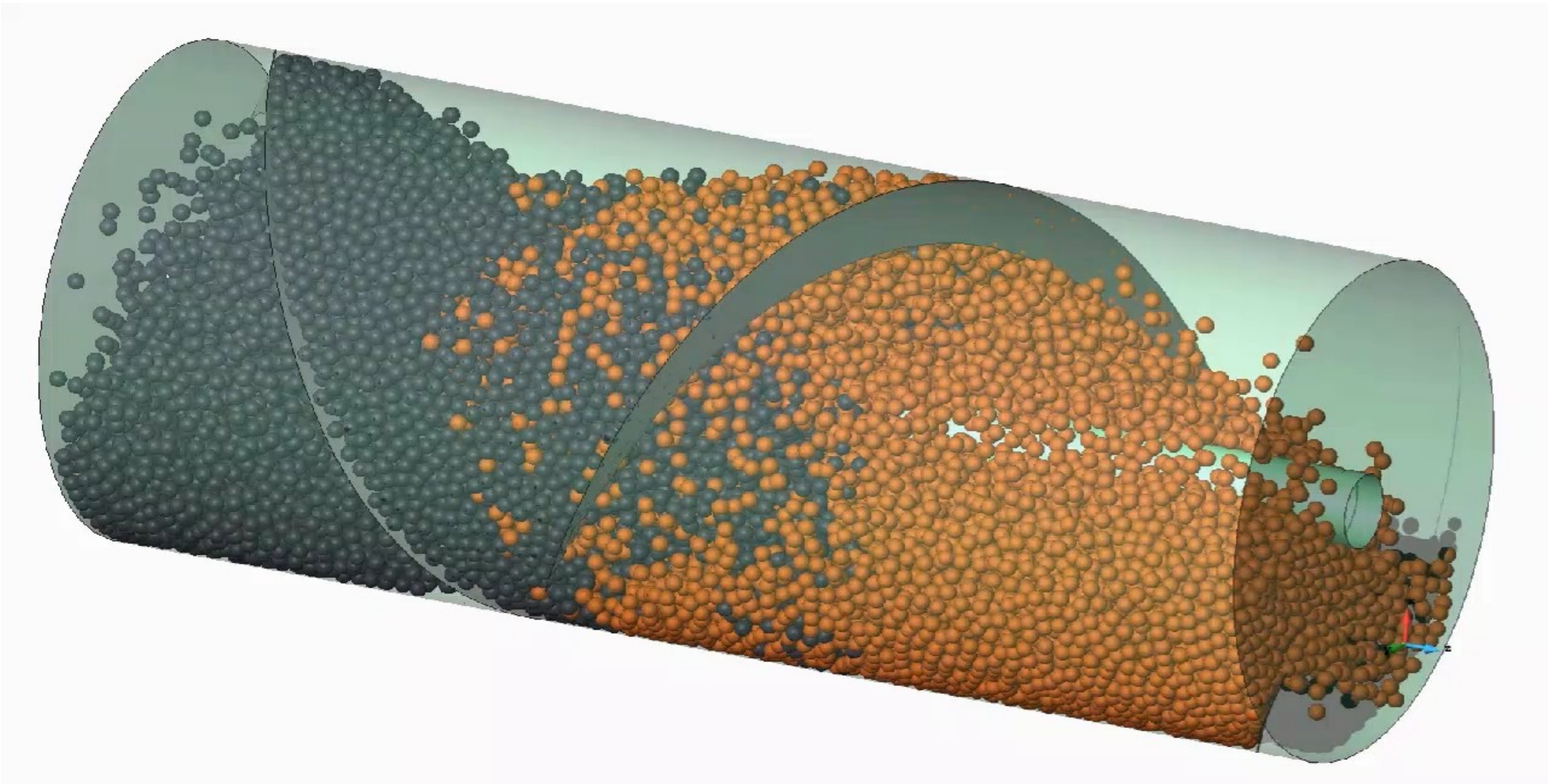
Mining bucket



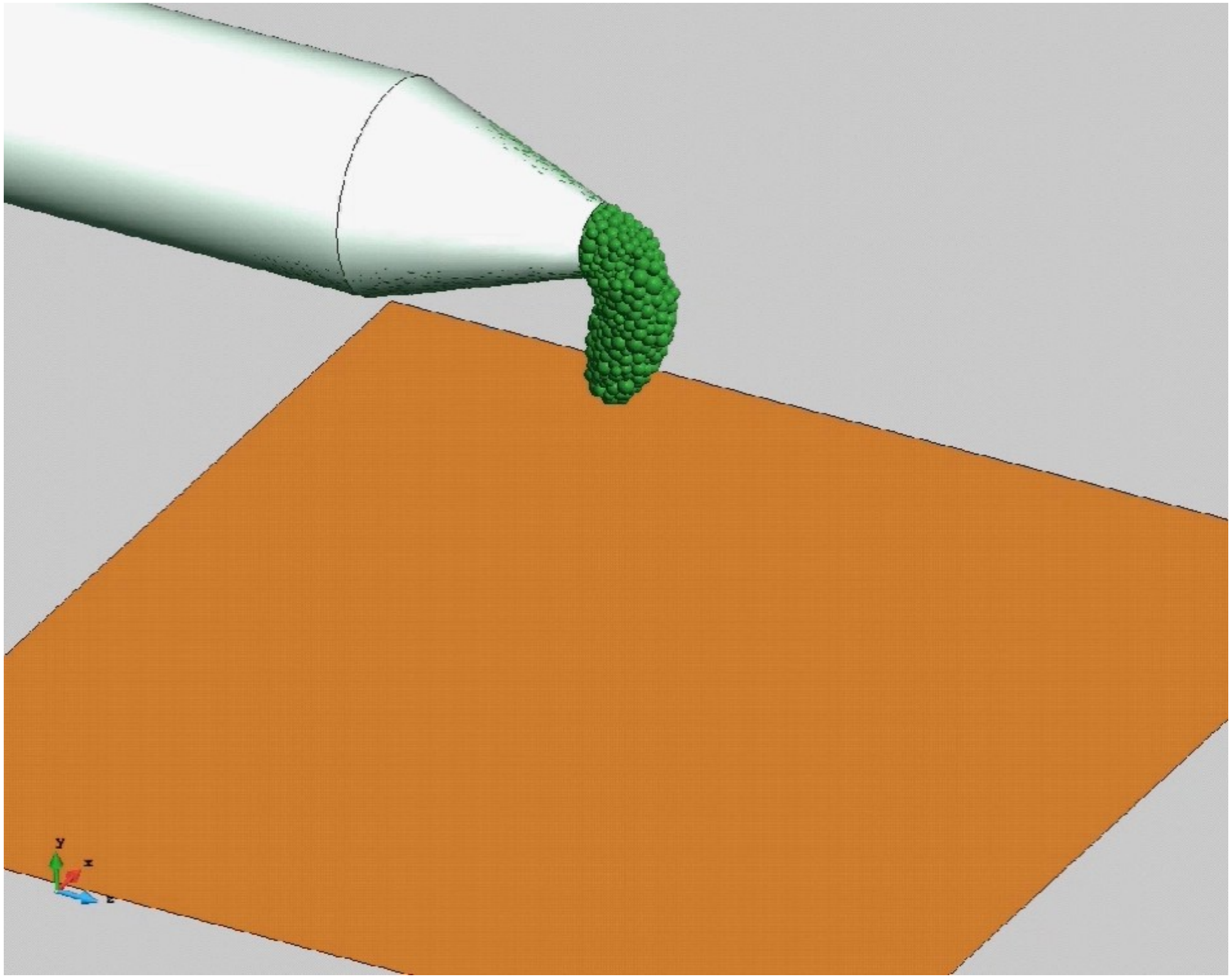
Feeding and conveying



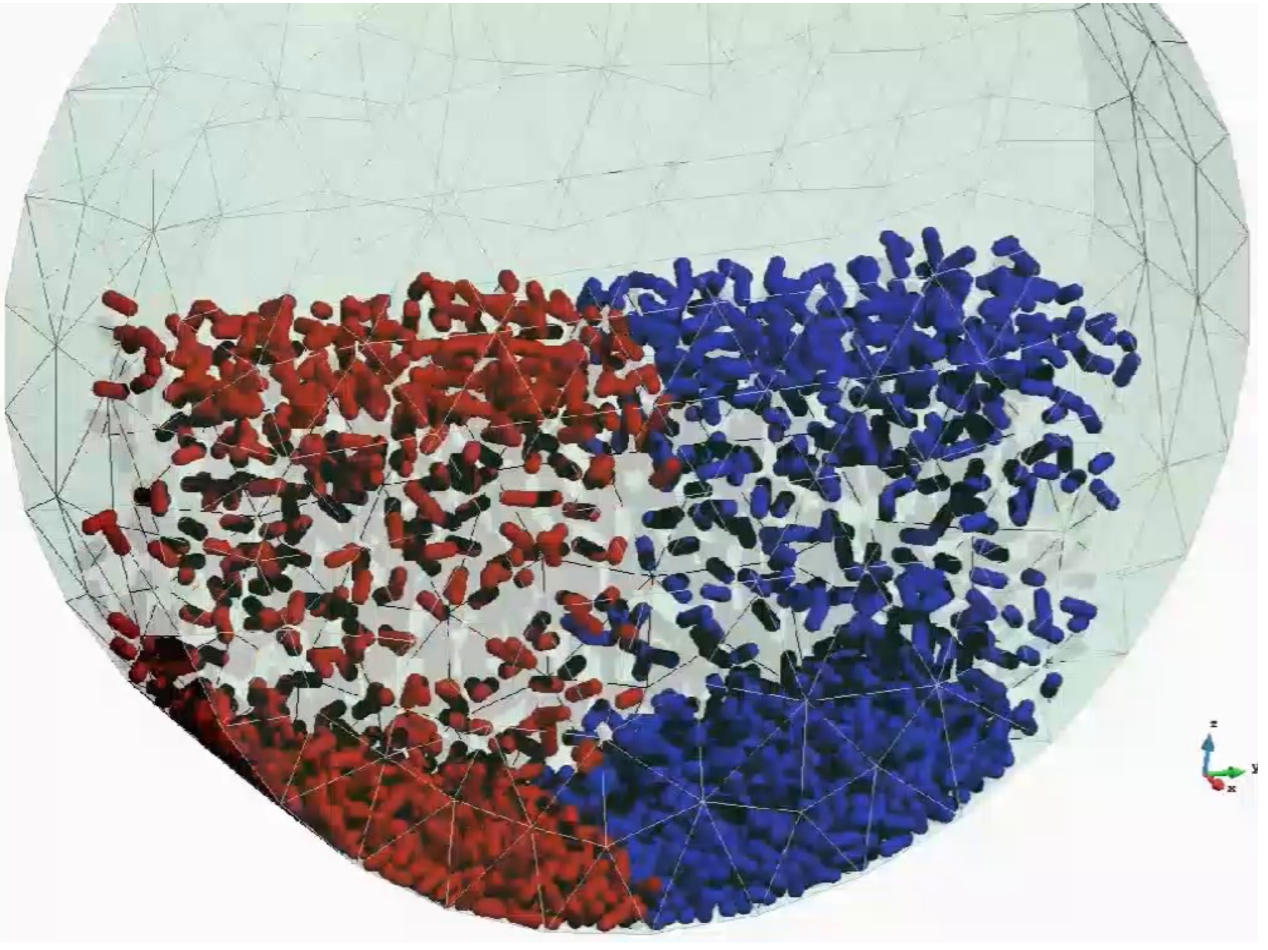
Mixing processes



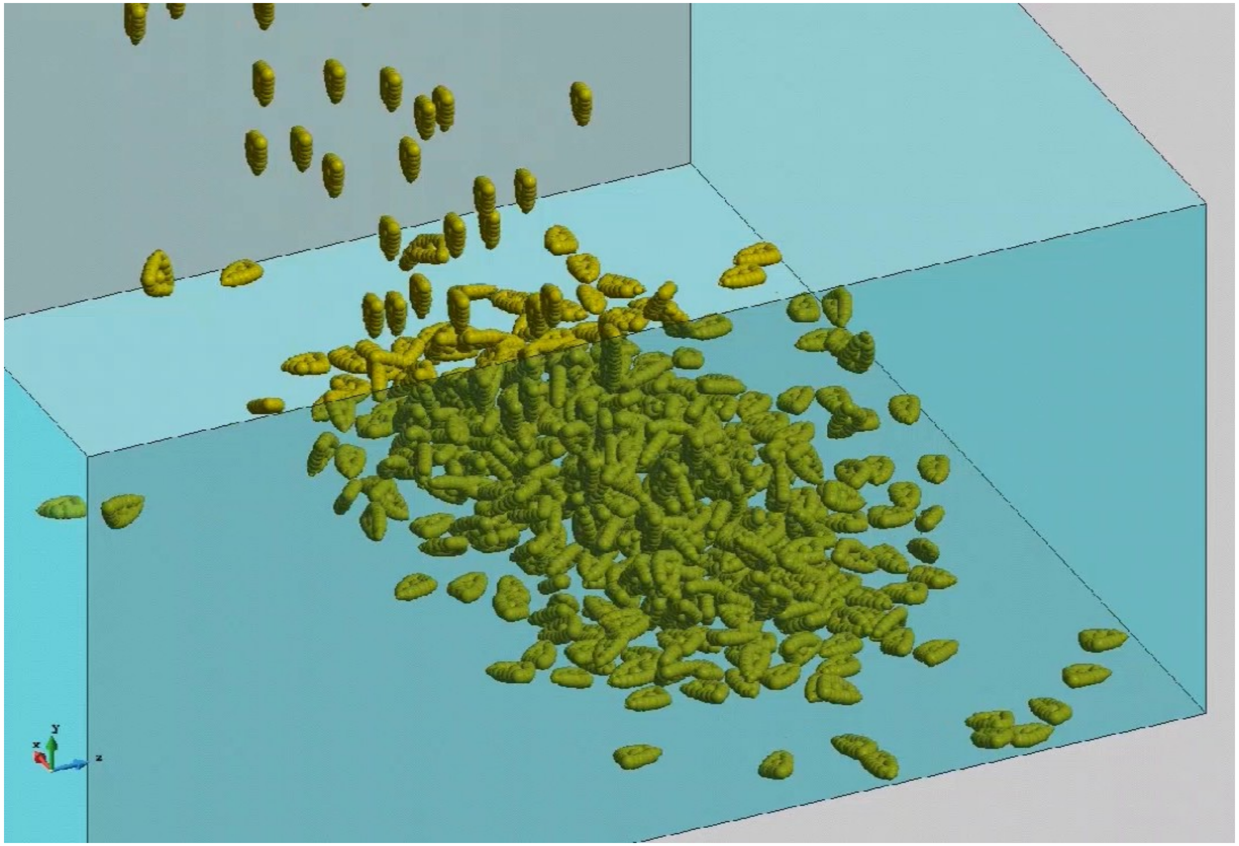
Cohesive materials (JKR, MDT models)



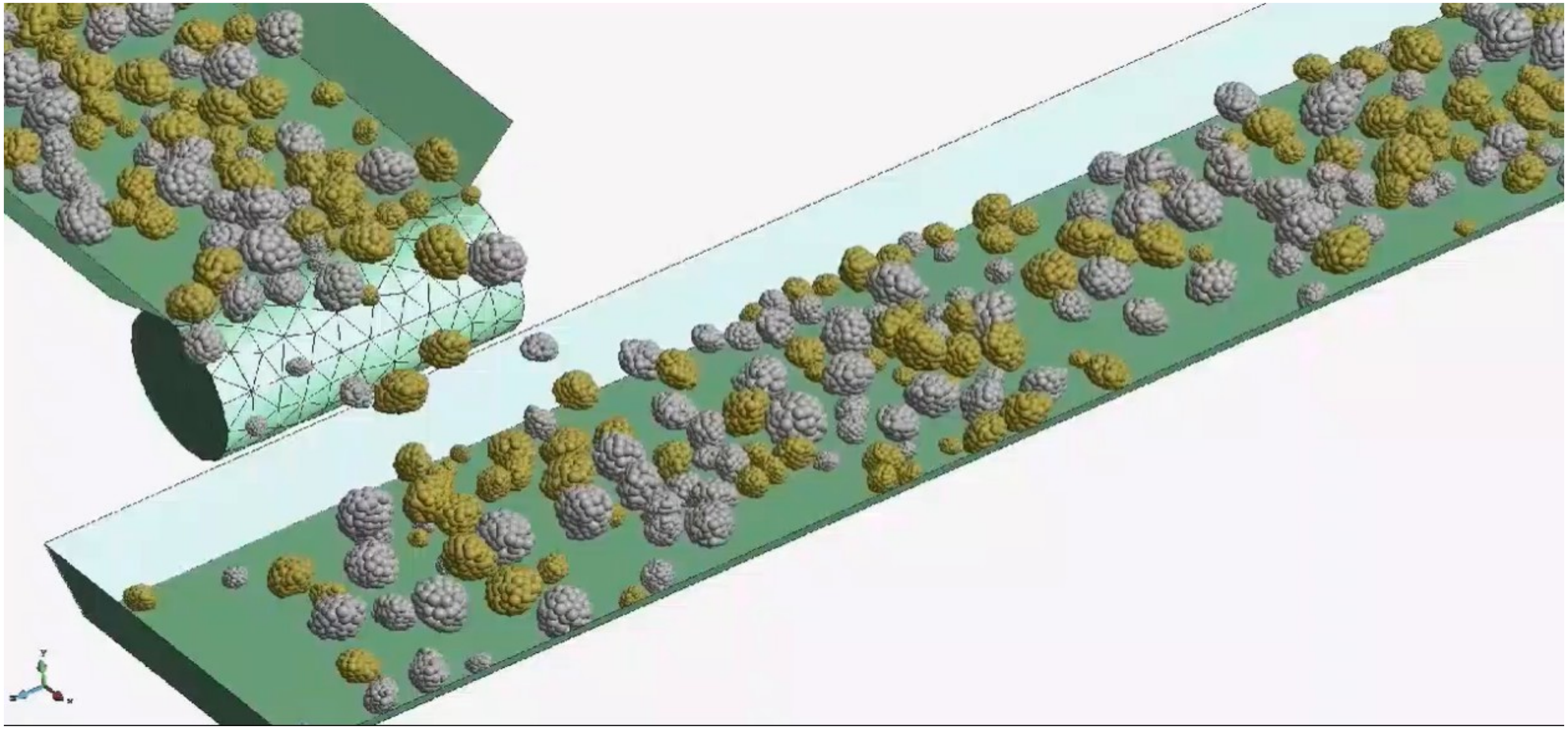
Non spherical particles: Capsules coating



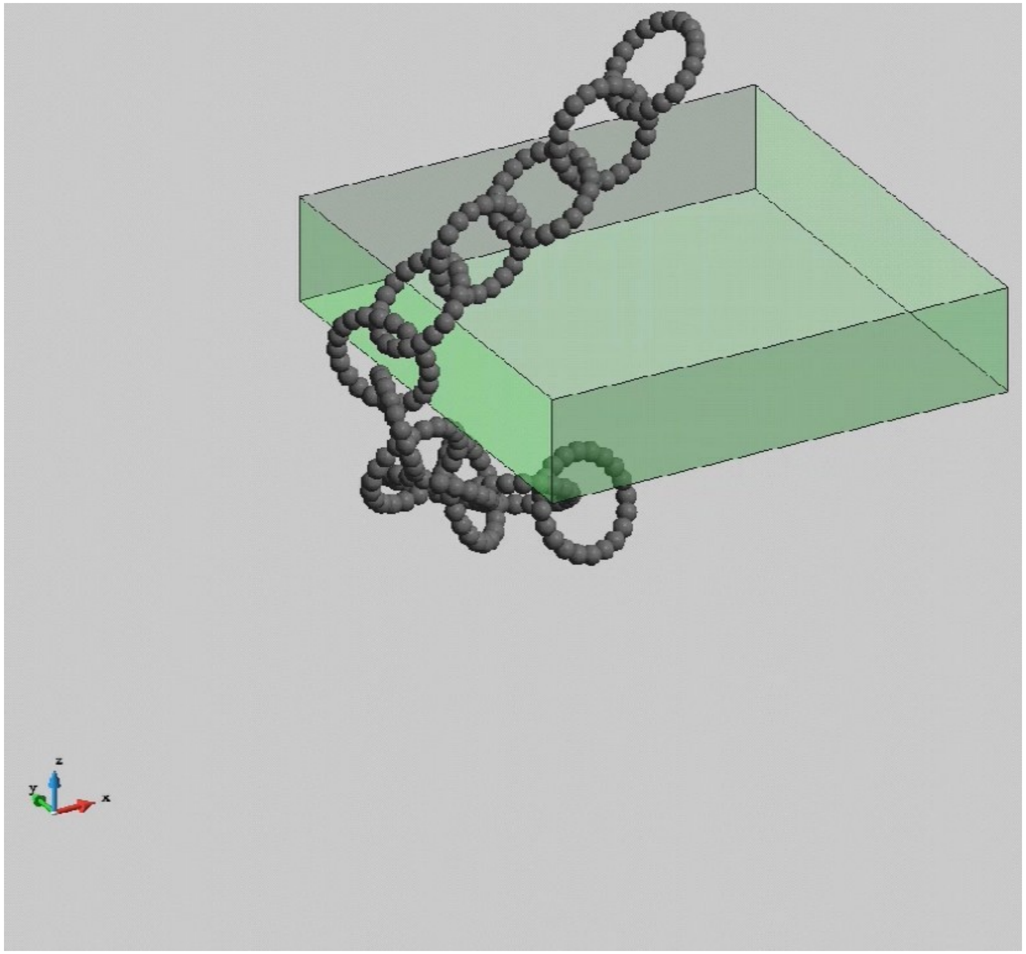
Non spherical particles: Corn seeds



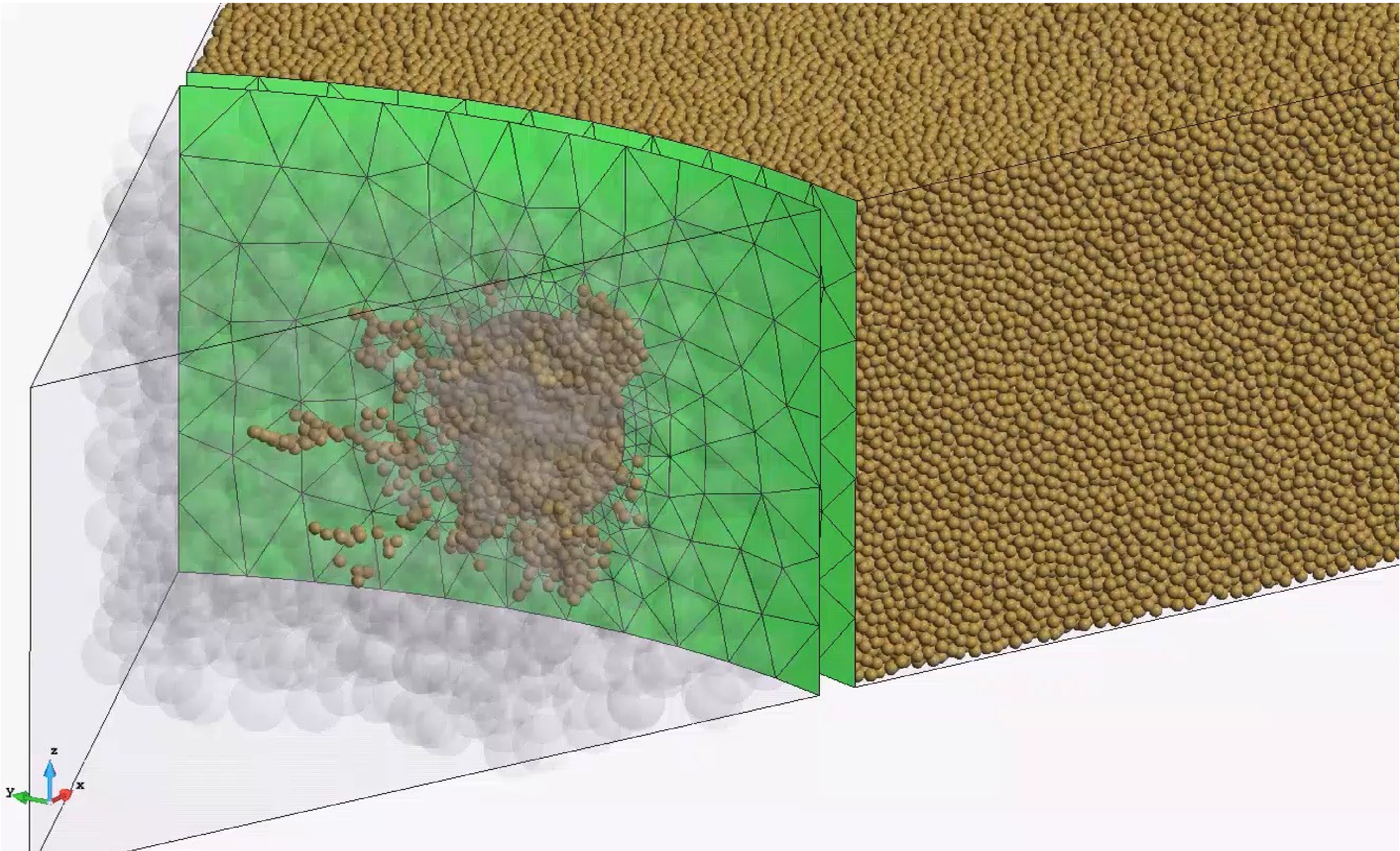
Non spherical particles: Conveyor belt with rocks of different sizes



Non spherical particles: Chain made of clusters



Sand production



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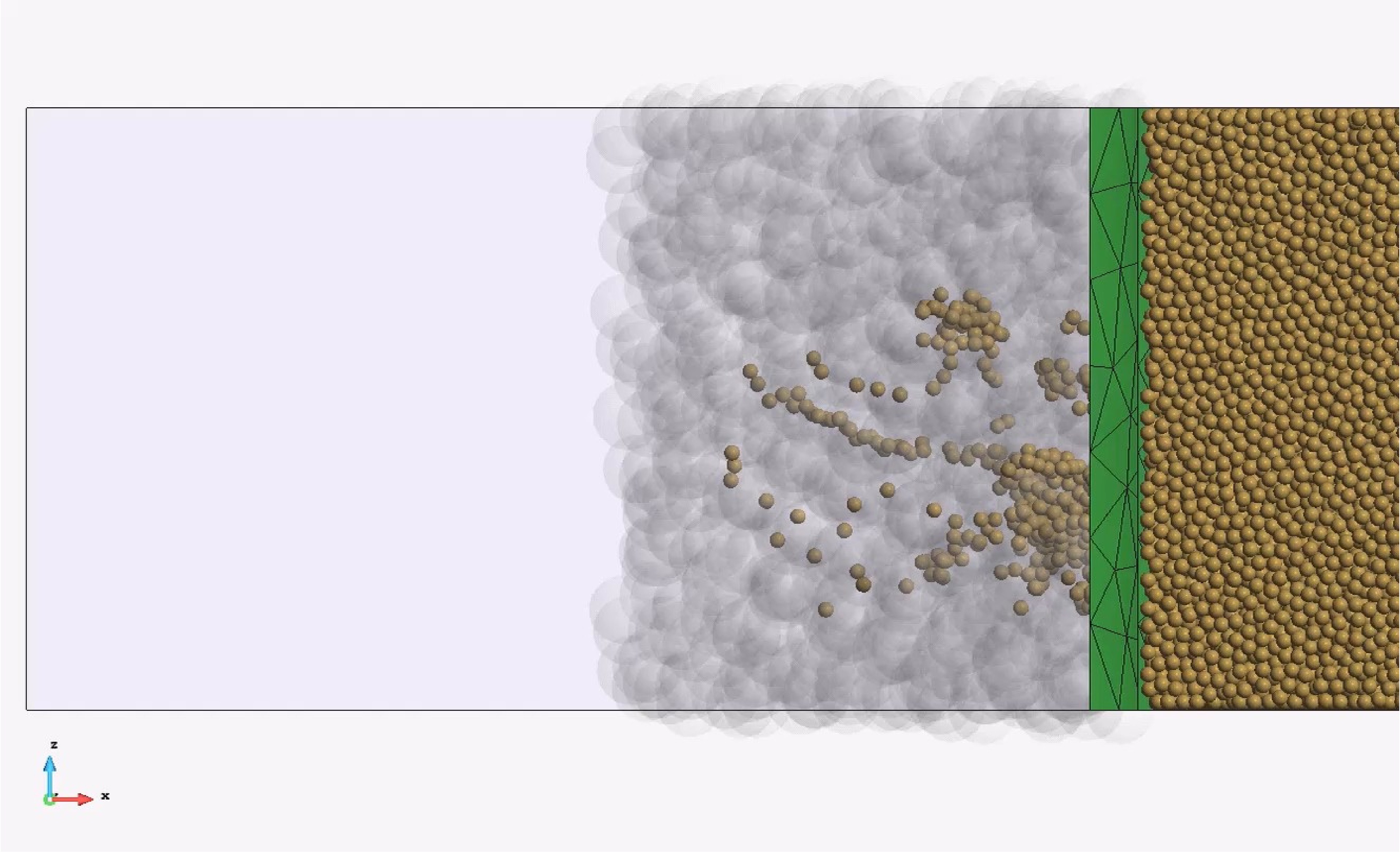
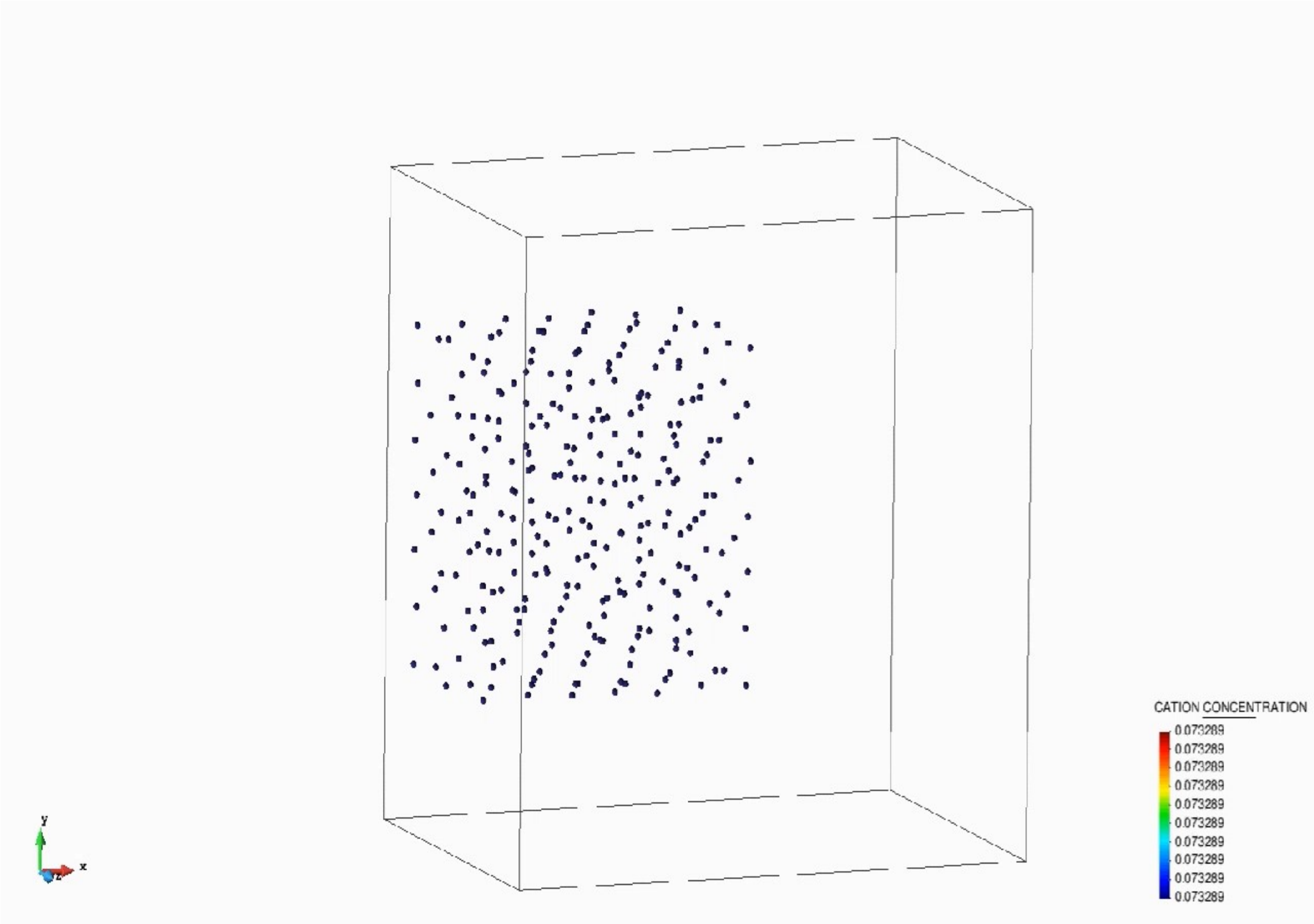


Nano particles (2e-7 m). Interaction forces are: diffuse double layer and Van der Waals



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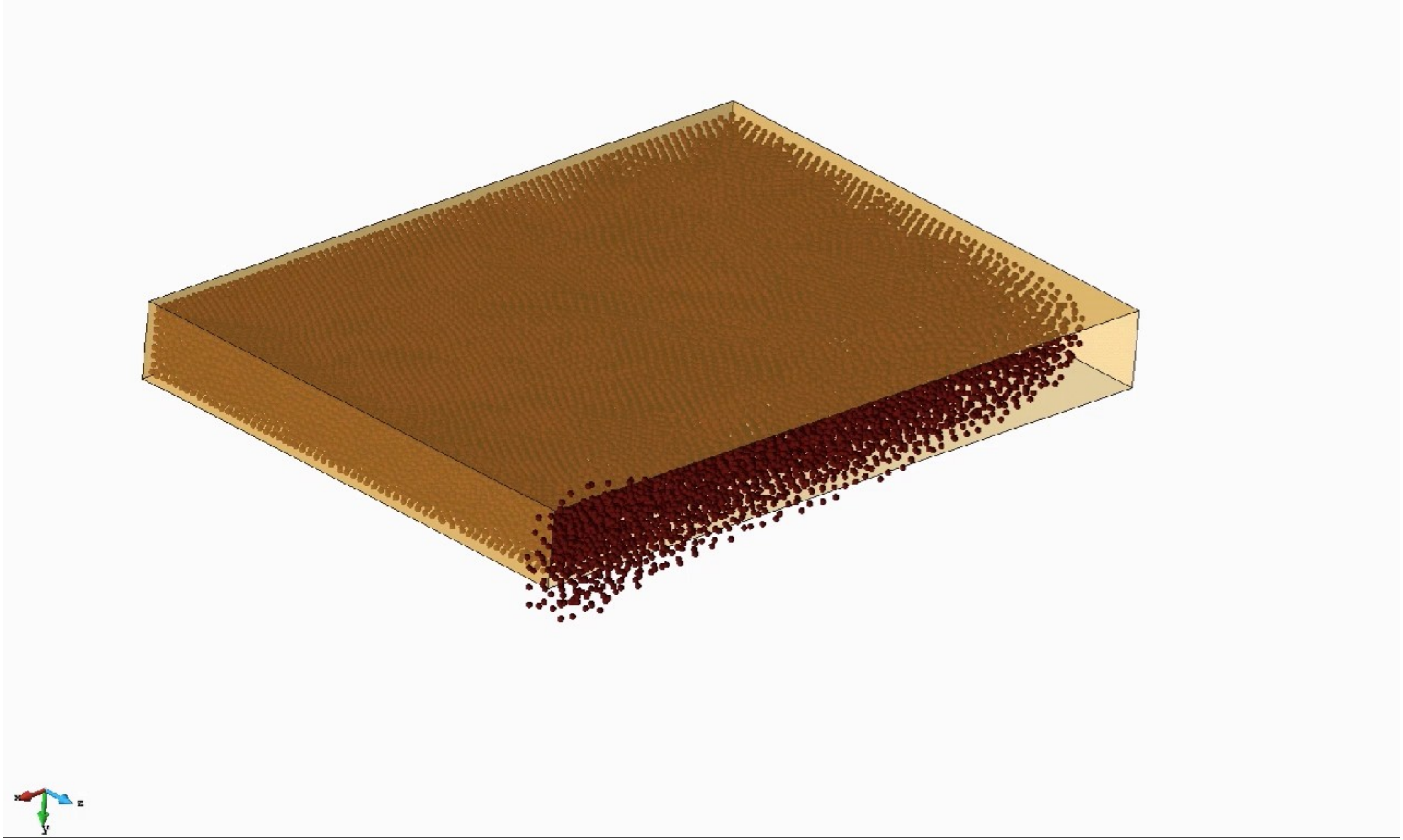
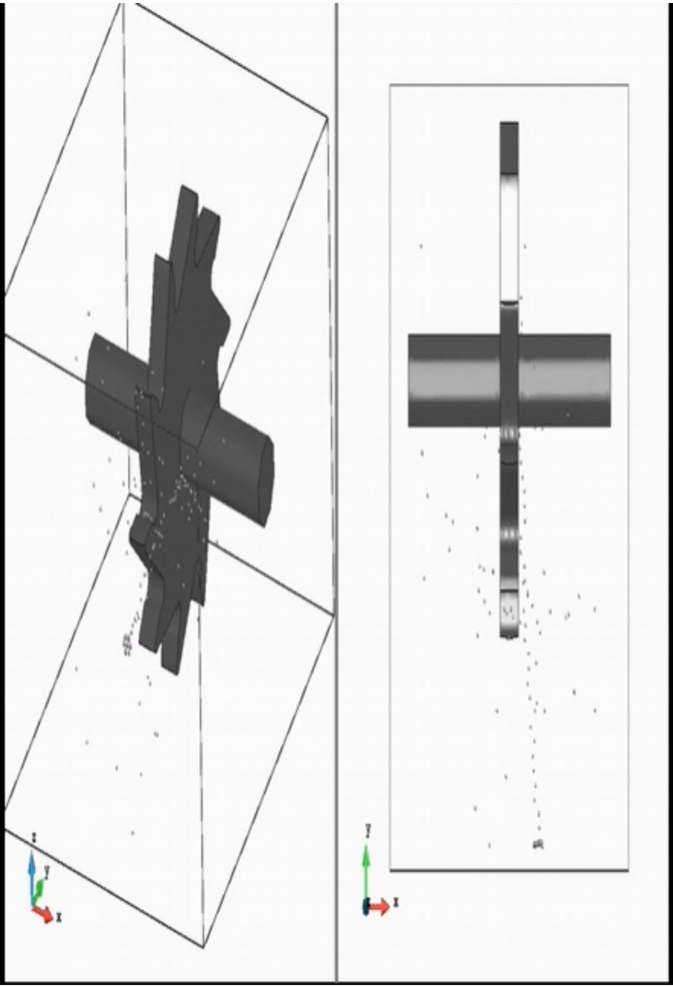
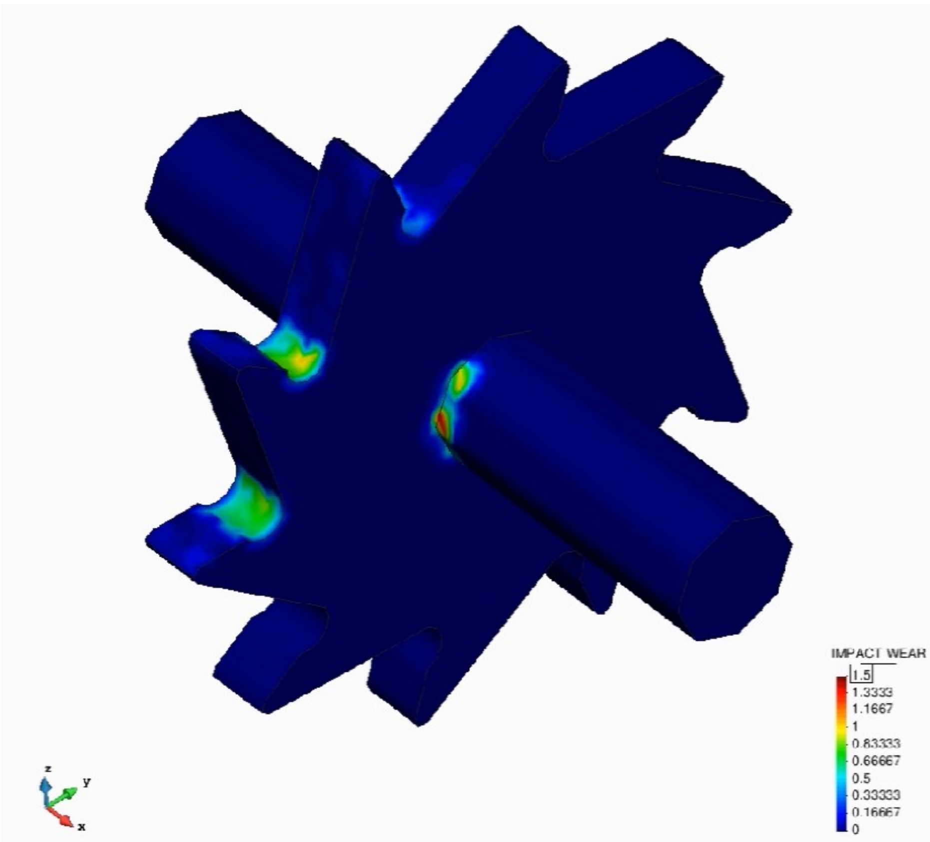


SHOT PEENING

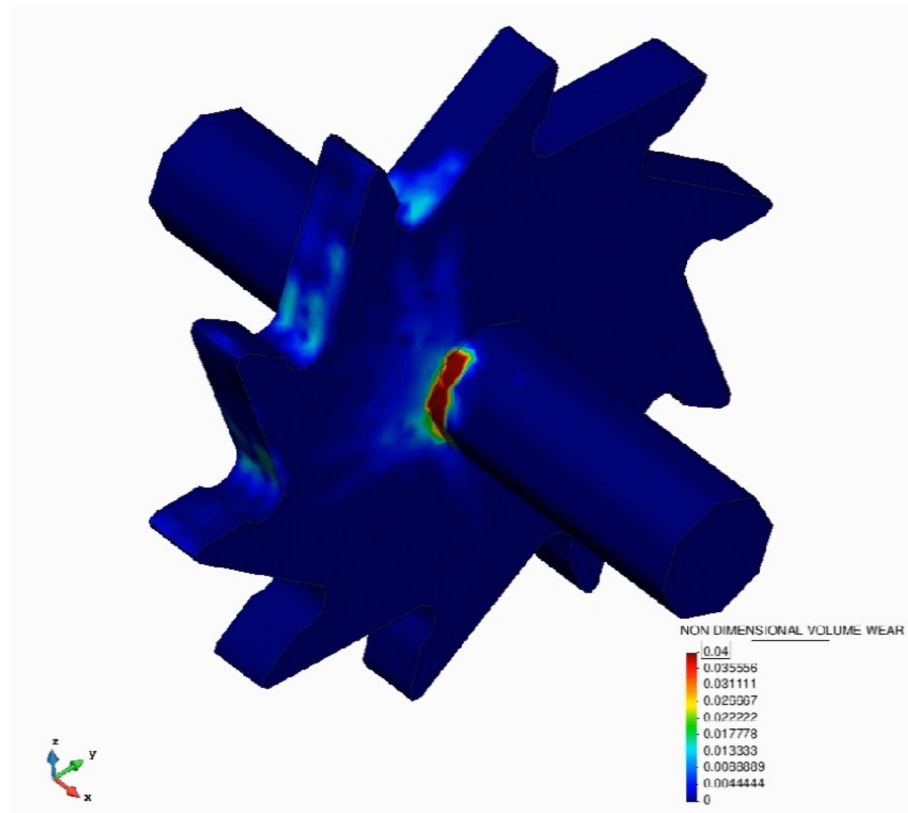


SHOT PEENING

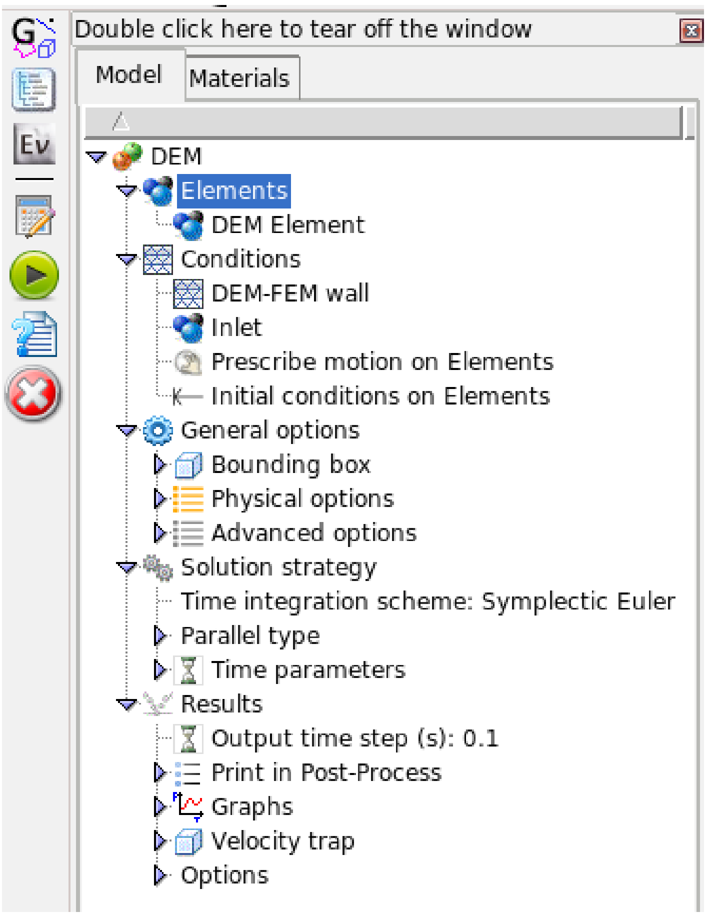
IMPACT EFFECT
(Oka et al (2005)):

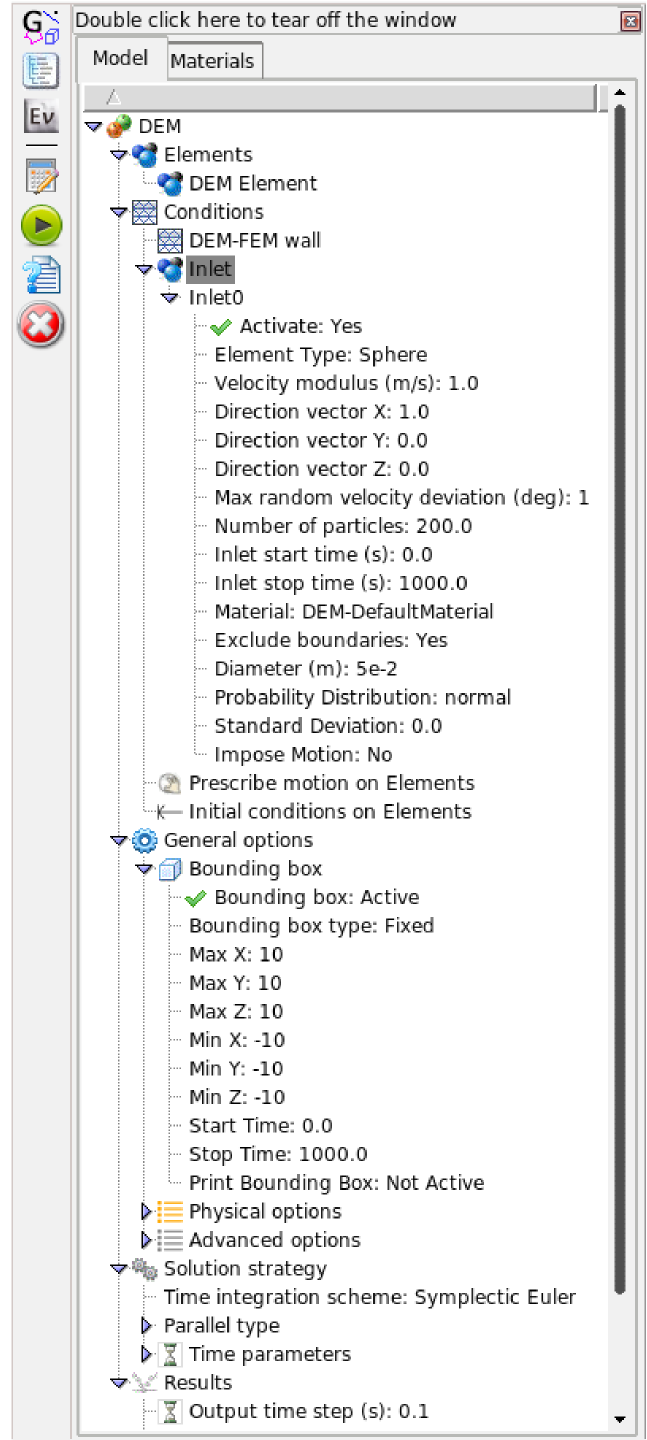


ABRASION BY FRICTION
(Archard):



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





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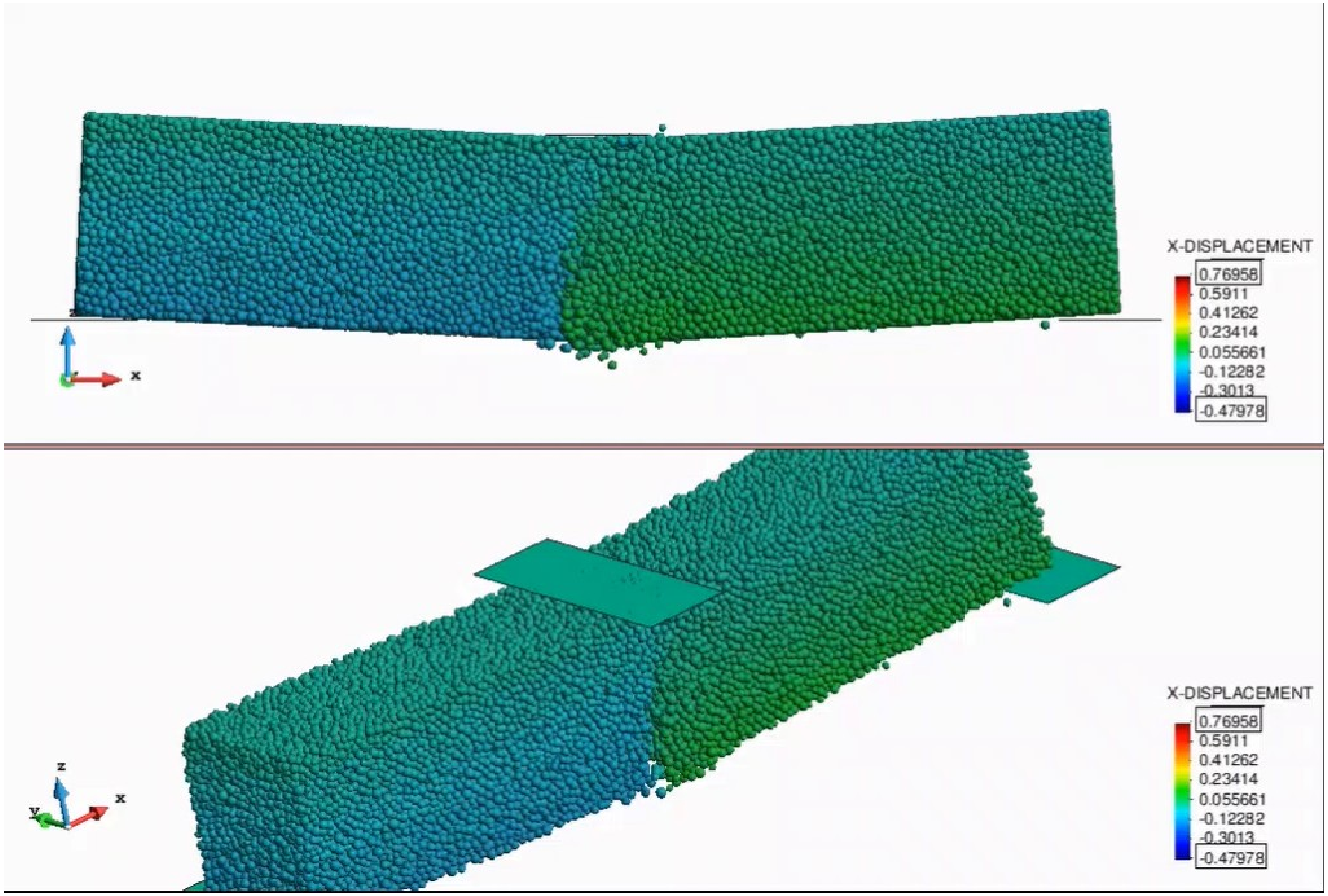
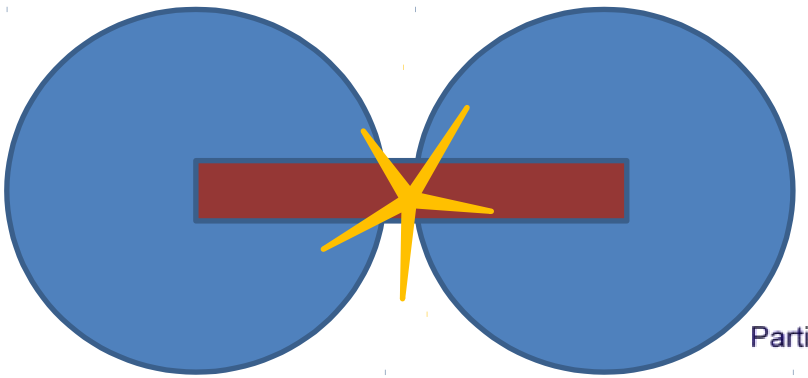
OBJECTIVE: solve relatively large domains (human size), where spheres are not micro, they can measure centimeters or meters.

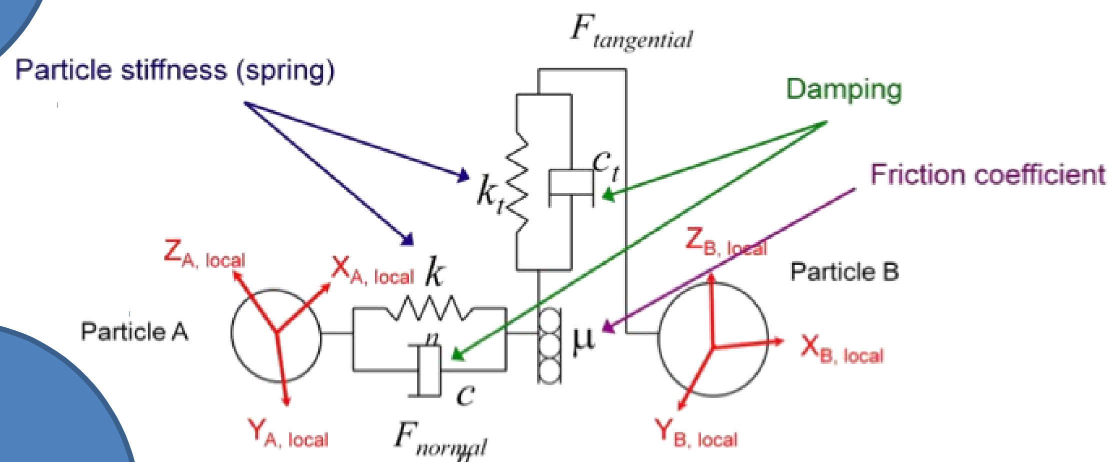


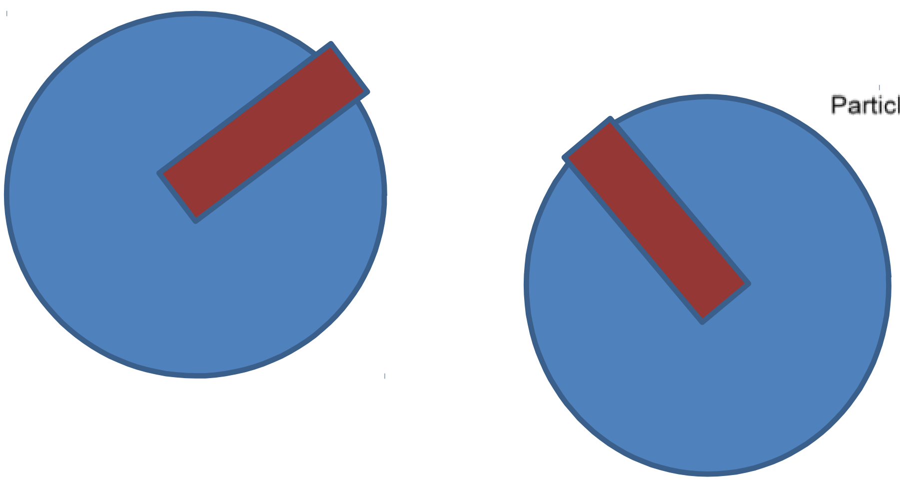
Typically, Young's Modulus and Poisson's Ratio are enough to define the elastic properties of a material. Post-elasticity requires other parameters.

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



Normal spring actuates in compression and tension

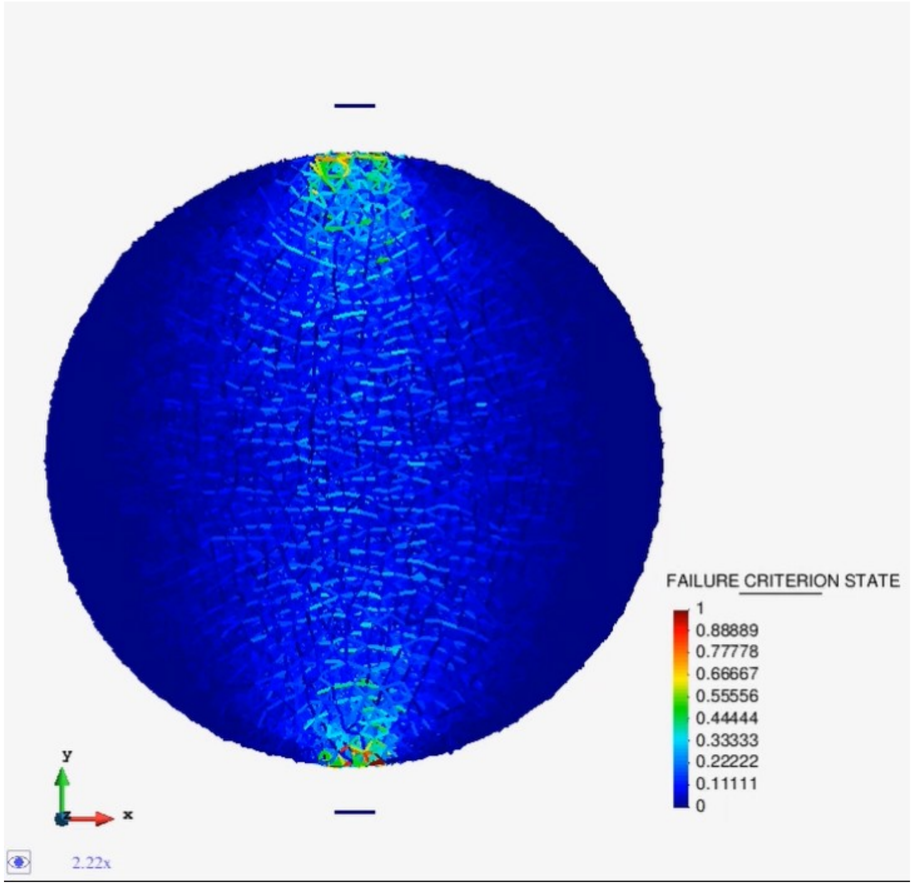


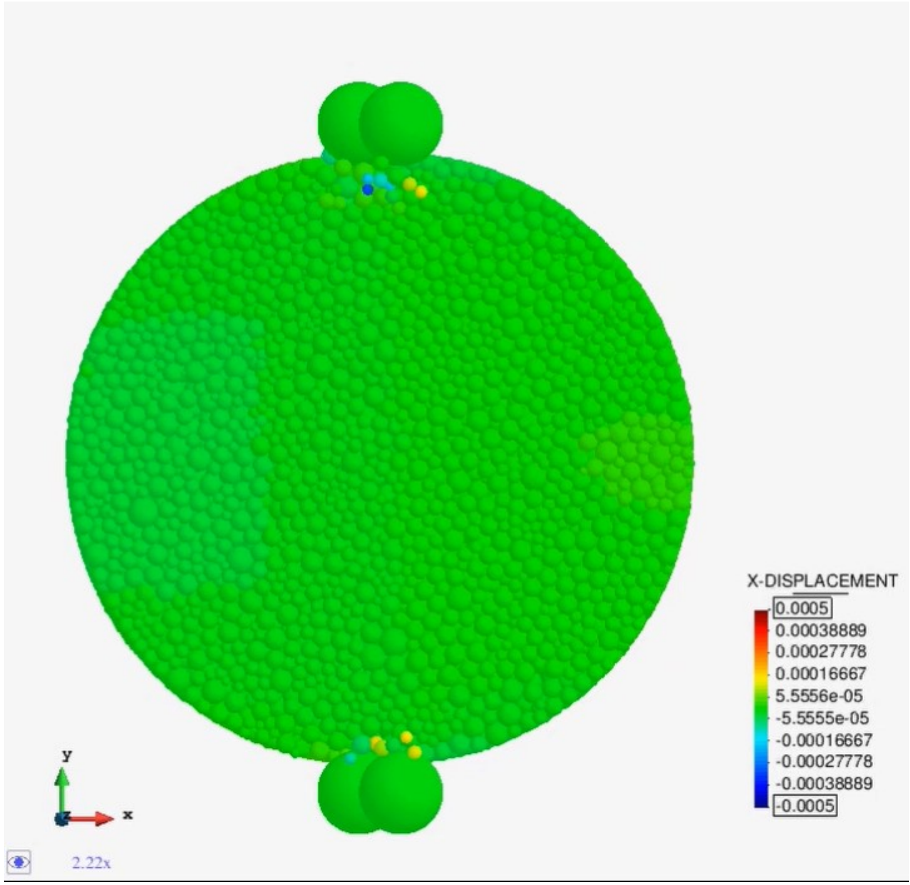


Normal spring actuates in compression only

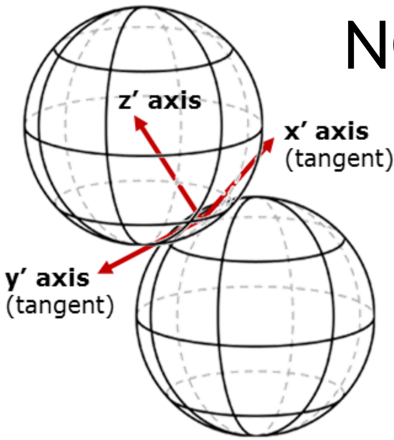
CONTINUUM SIMULATIONS WITH DEM (CONCRETE). MULTI-FRACTURE

Brazilian test





NORMAL FORCE (z' axis)



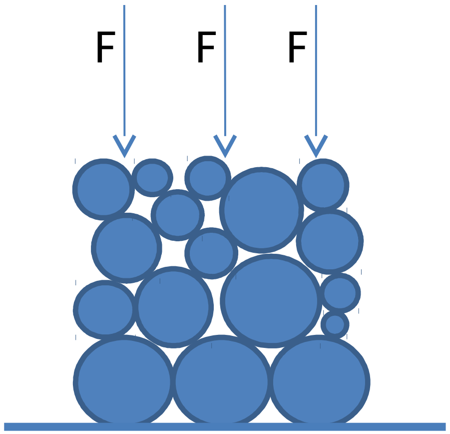
$$\sigma_{z'} = E\varepsilon_{z'}$$

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

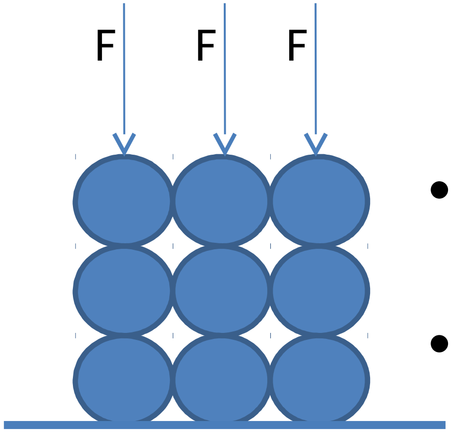
$$F_{z'} = \frac{EA^*}{R1+R2}\delta$$

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

+ Weighted Voronoi Diagram...



- *Young's Modulus depends on Kt*
- *Poisson's Ratio depends on Kt*



- *Perfect Young's Modulus*
- ***Wrong Poisson's Ratio (100% error!)***

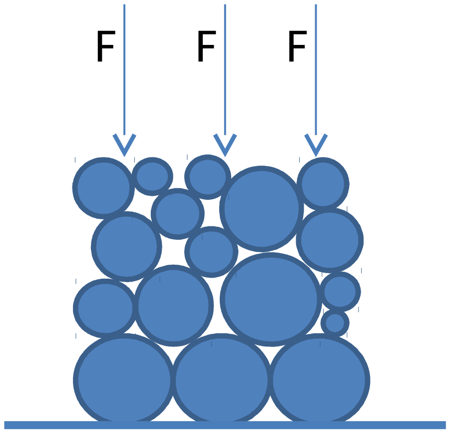
$$F_{z'} = K_n \delta + \upsilon A^{*}(\sigma_{x'} + \sigma_{y'})$$

The stress tensor is used to enrich the force computation

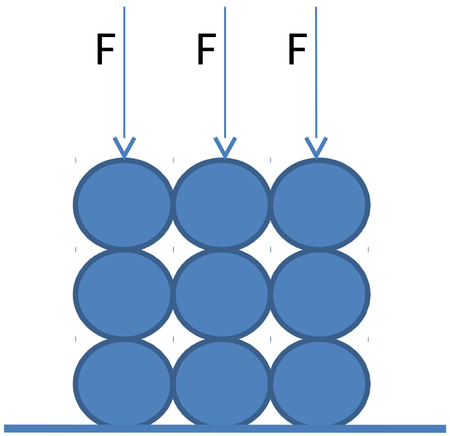
$$F_{x'_i} = k_{ti}\delta_{x'i} + A_i G \left(\frac{\tau_{z'x',i}}{G} - \frac{\delta_{x'i}}{L_i} \right)_{step}$$

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

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

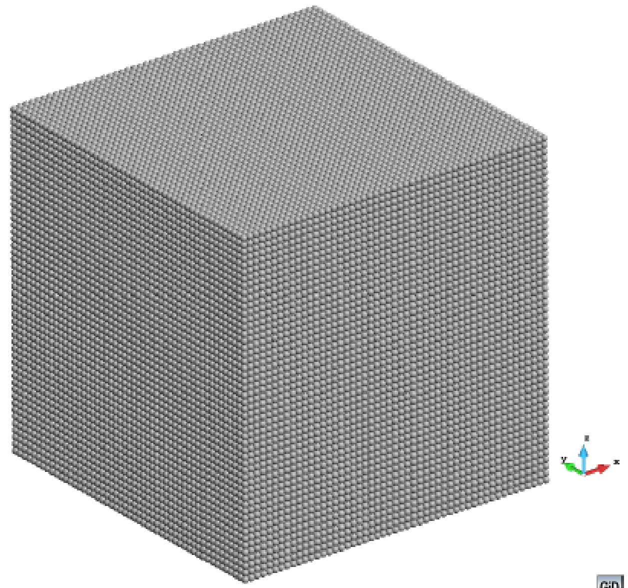


- *Good Young's Modulus*
- *Good Poisson's Ratio*

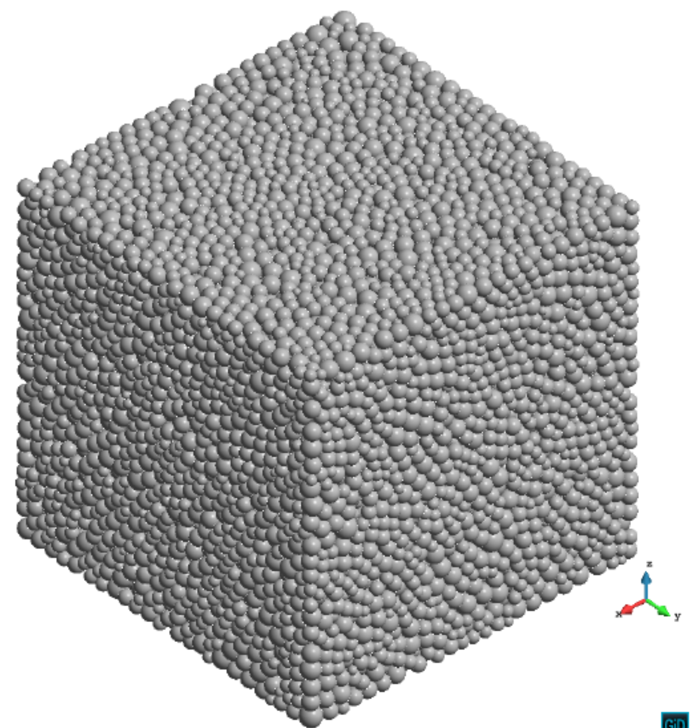


VALIDATION

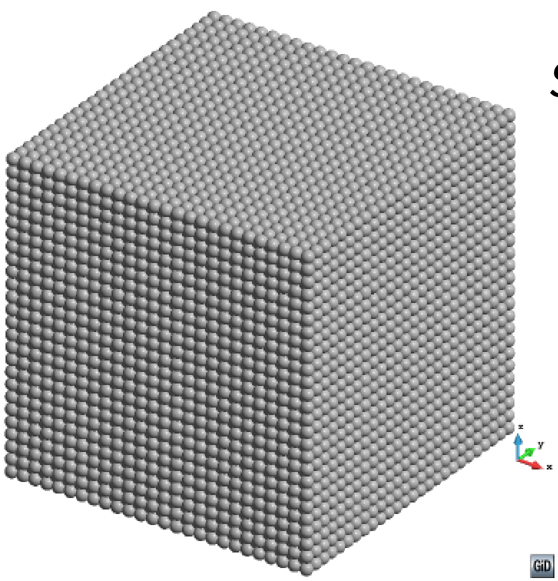
Cartesian packing

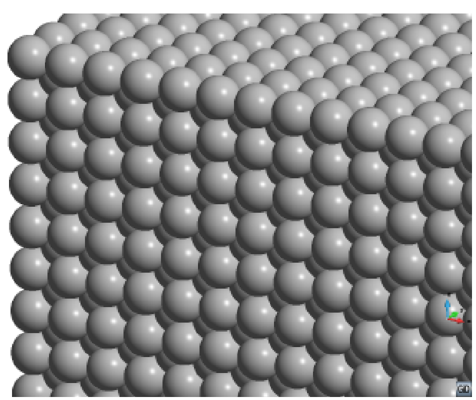


Random packing



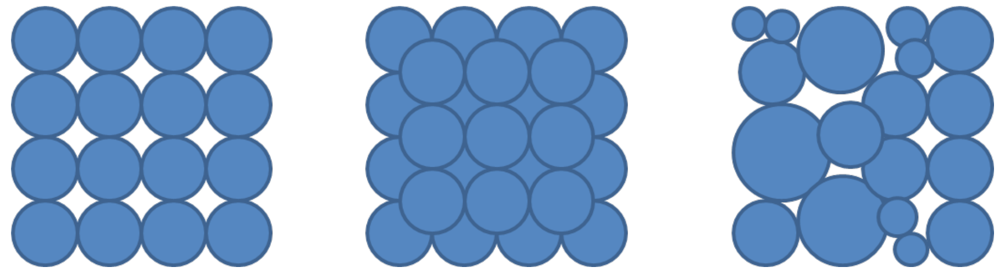
Staggered packing





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.

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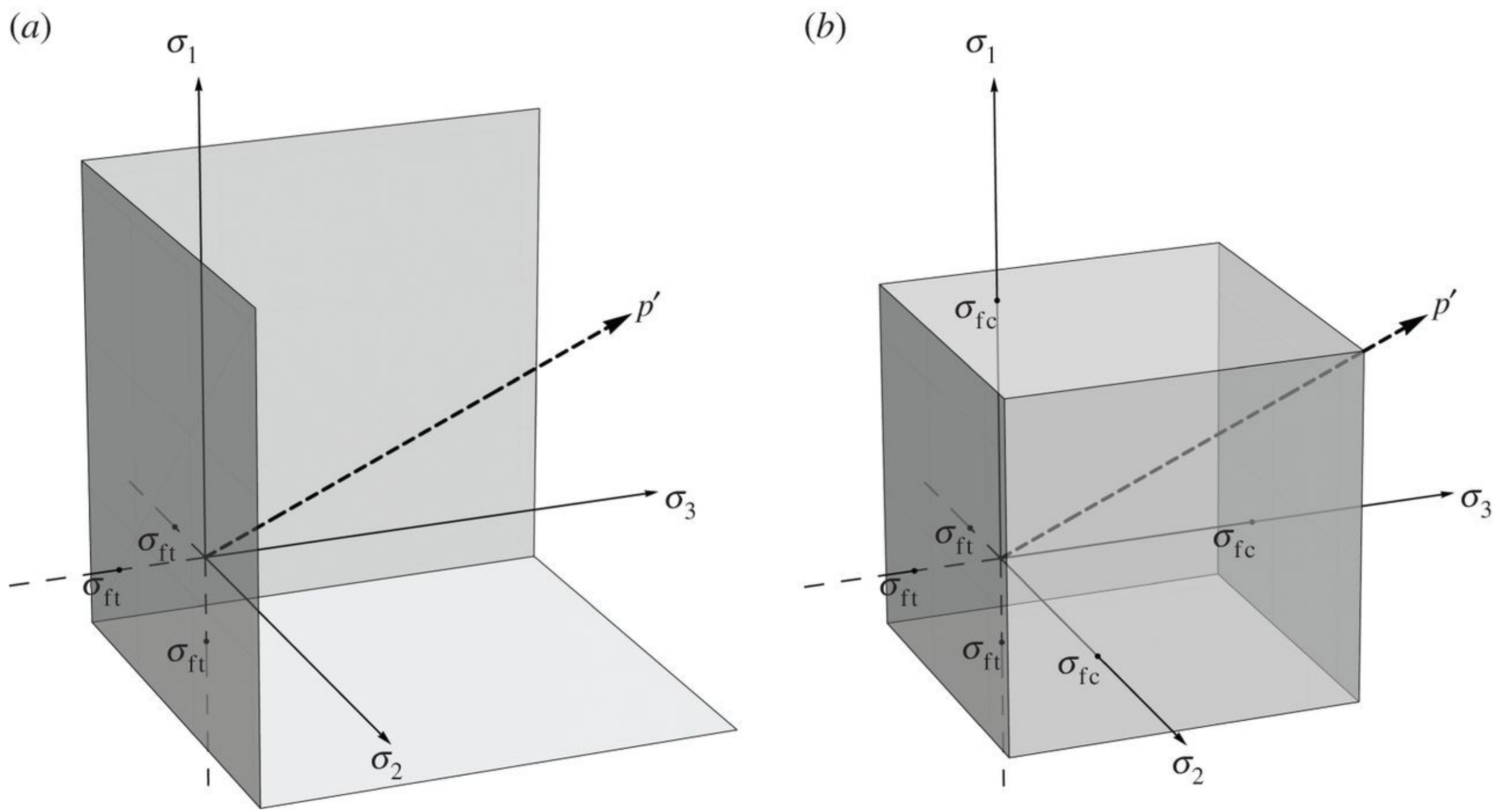
RANKINE YIELD CRITERION (FOR EXAMPLE)



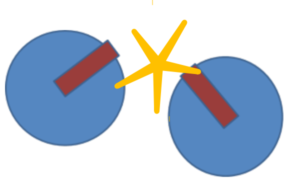
Stress tensor

$\boldsymbol{\sigma}$

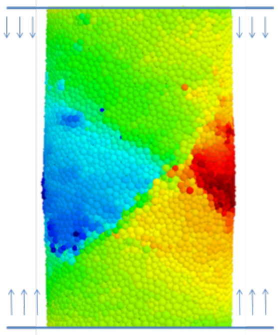
Principal Stresses

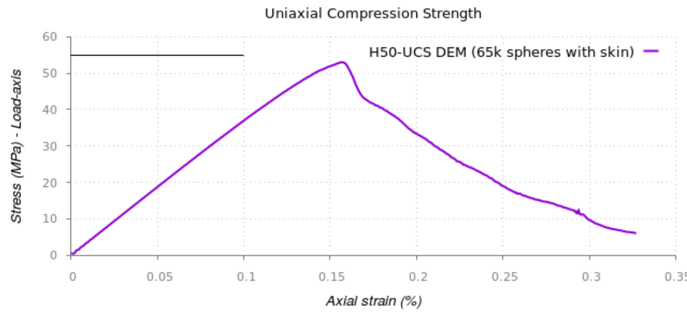
$\sigma_1, \sigma_2, \sigma_3$

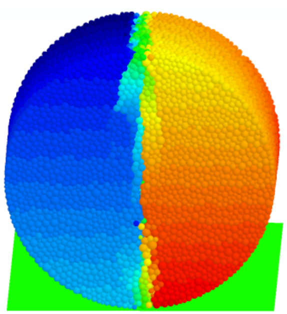
Bond breakage

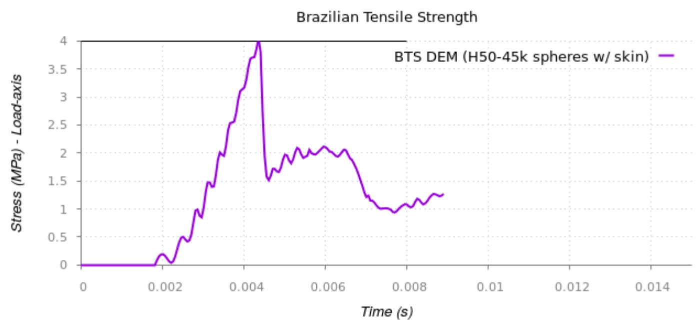


50 MPa Concrete

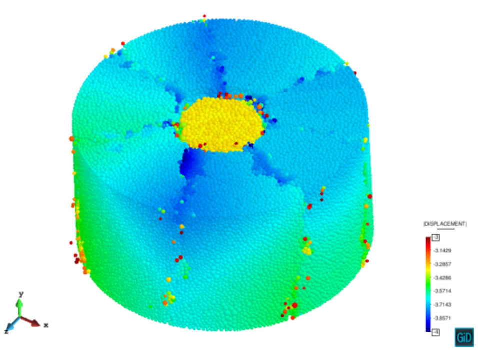


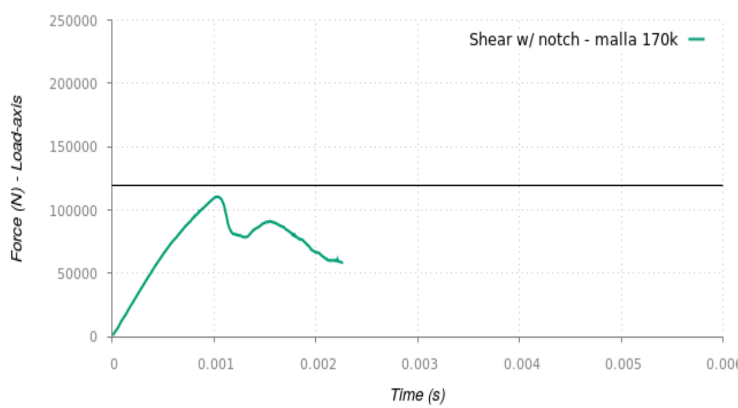






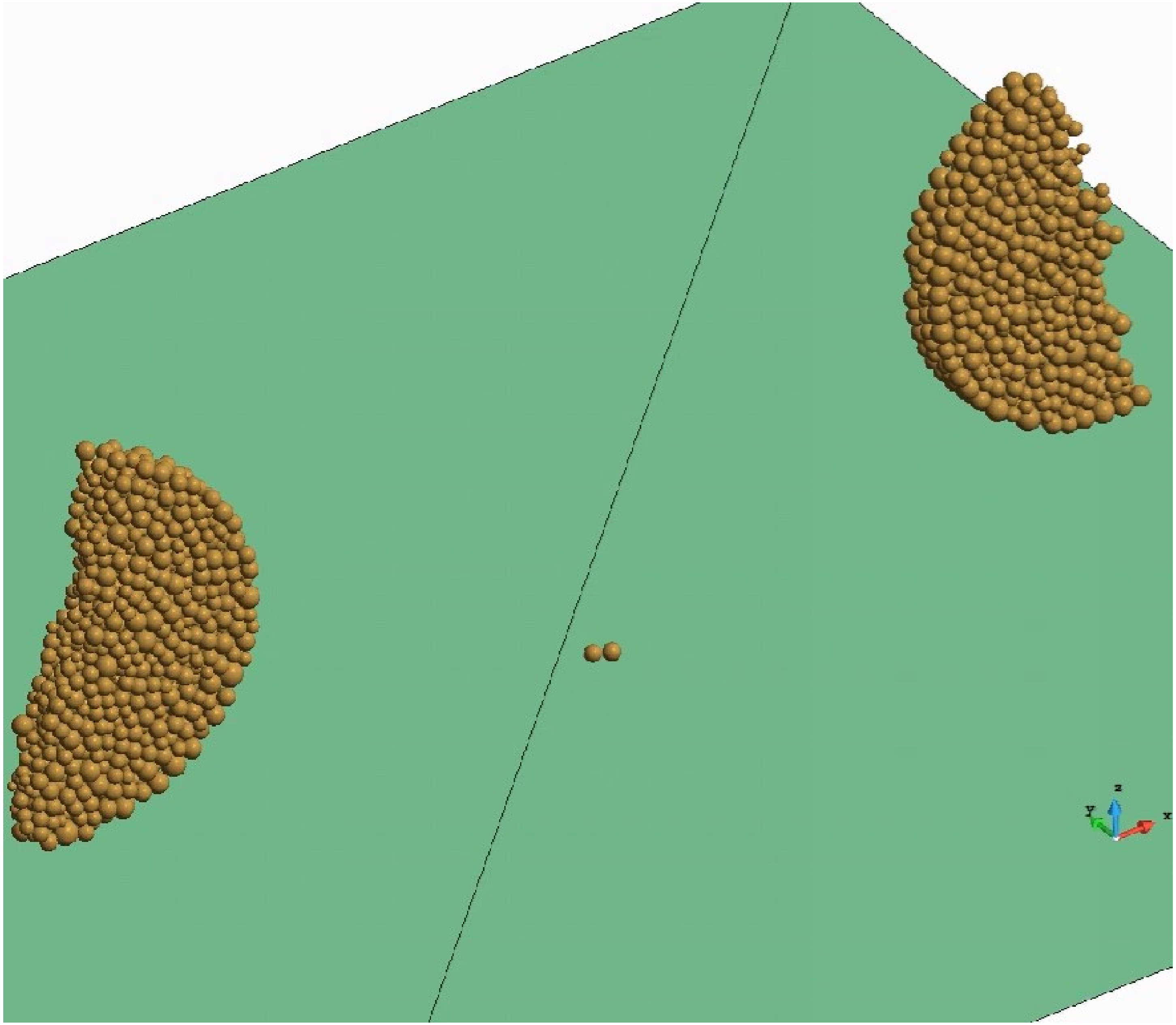
Just **one** micro parameter was calibrated (σ_{ft})



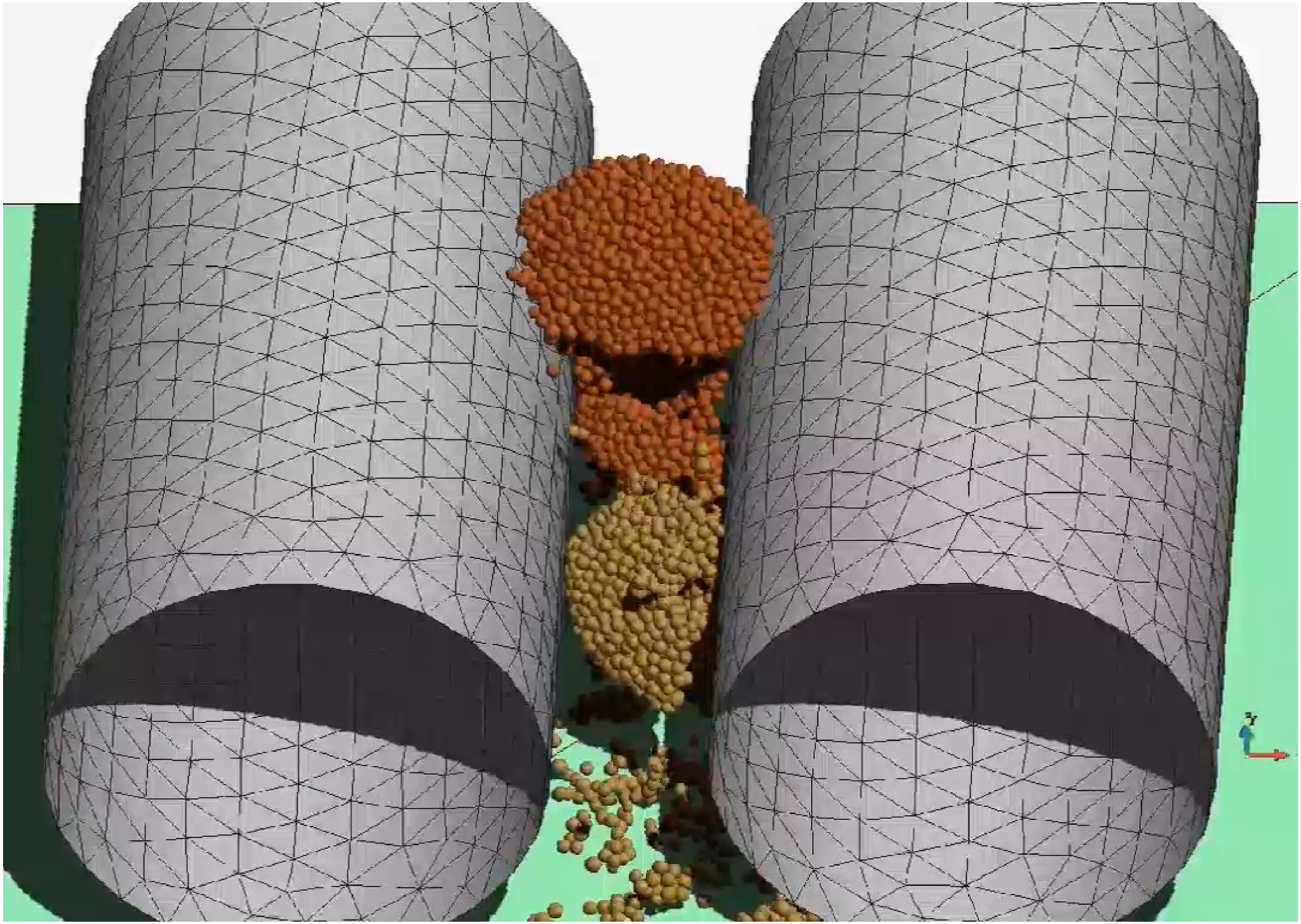


Just **two** micro parameters were calibrated (plus)
(same σ_{ft} plus μ)

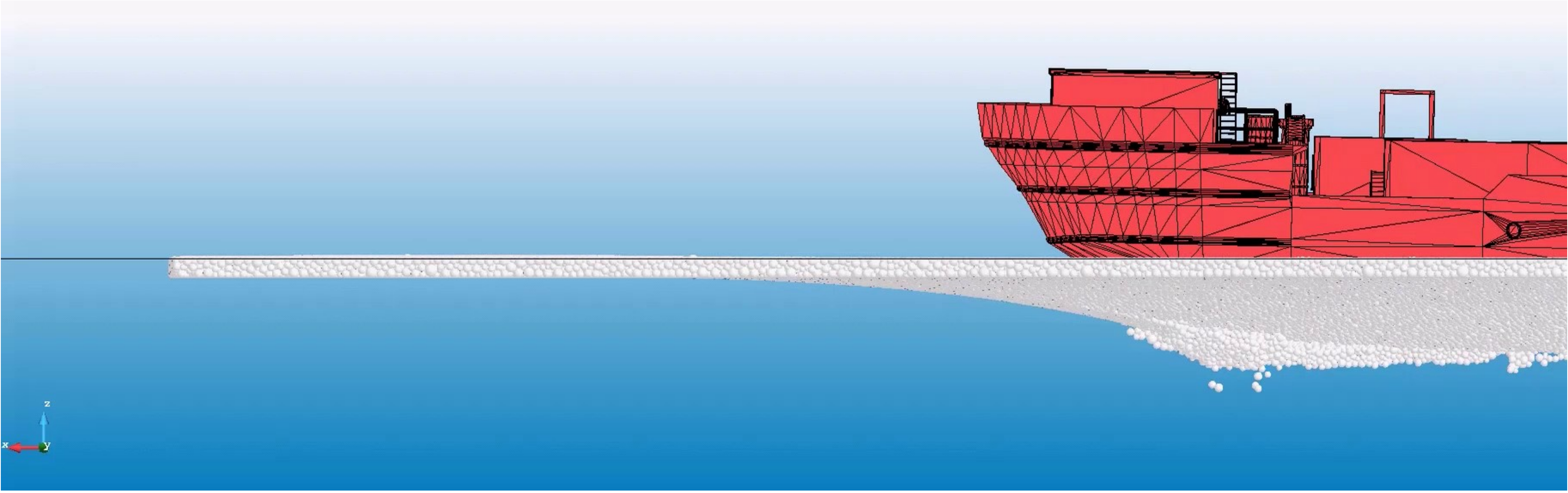
Large displacements and rotations are allowed



Fragments can break again

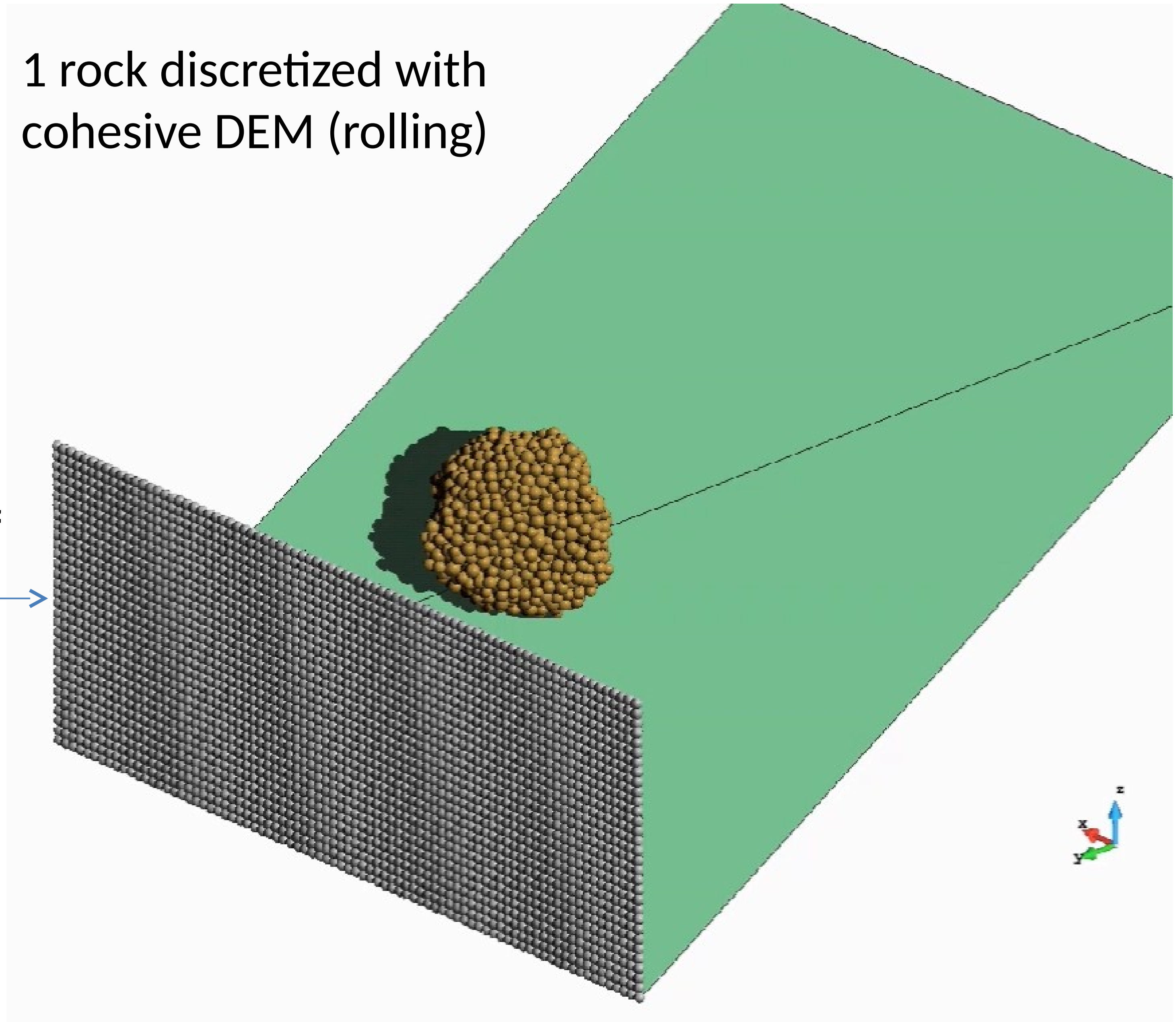


Icebreakers (understanding ice-ship interactions)



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

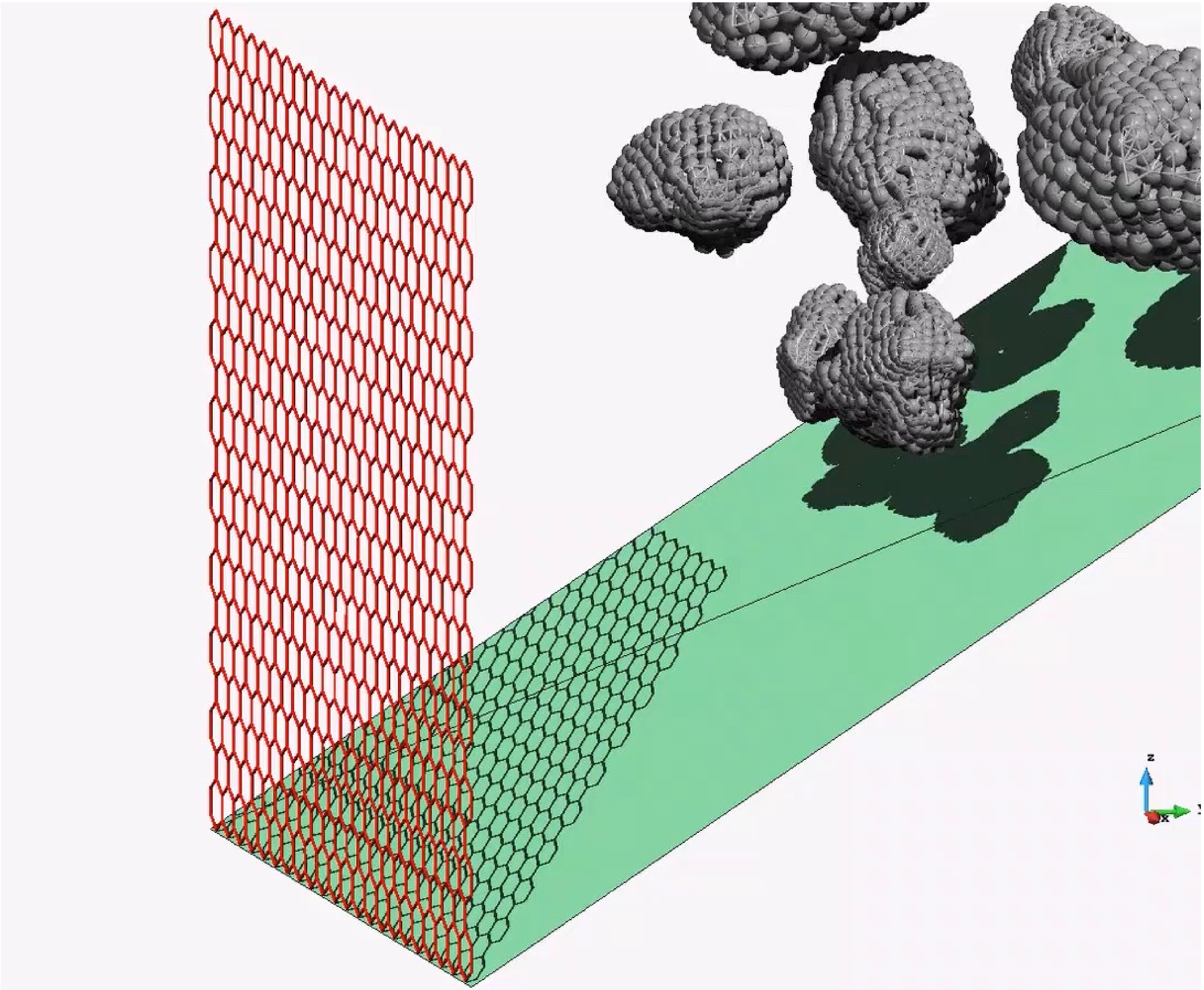
1 rock discretized with cohesive DEM (rolling)



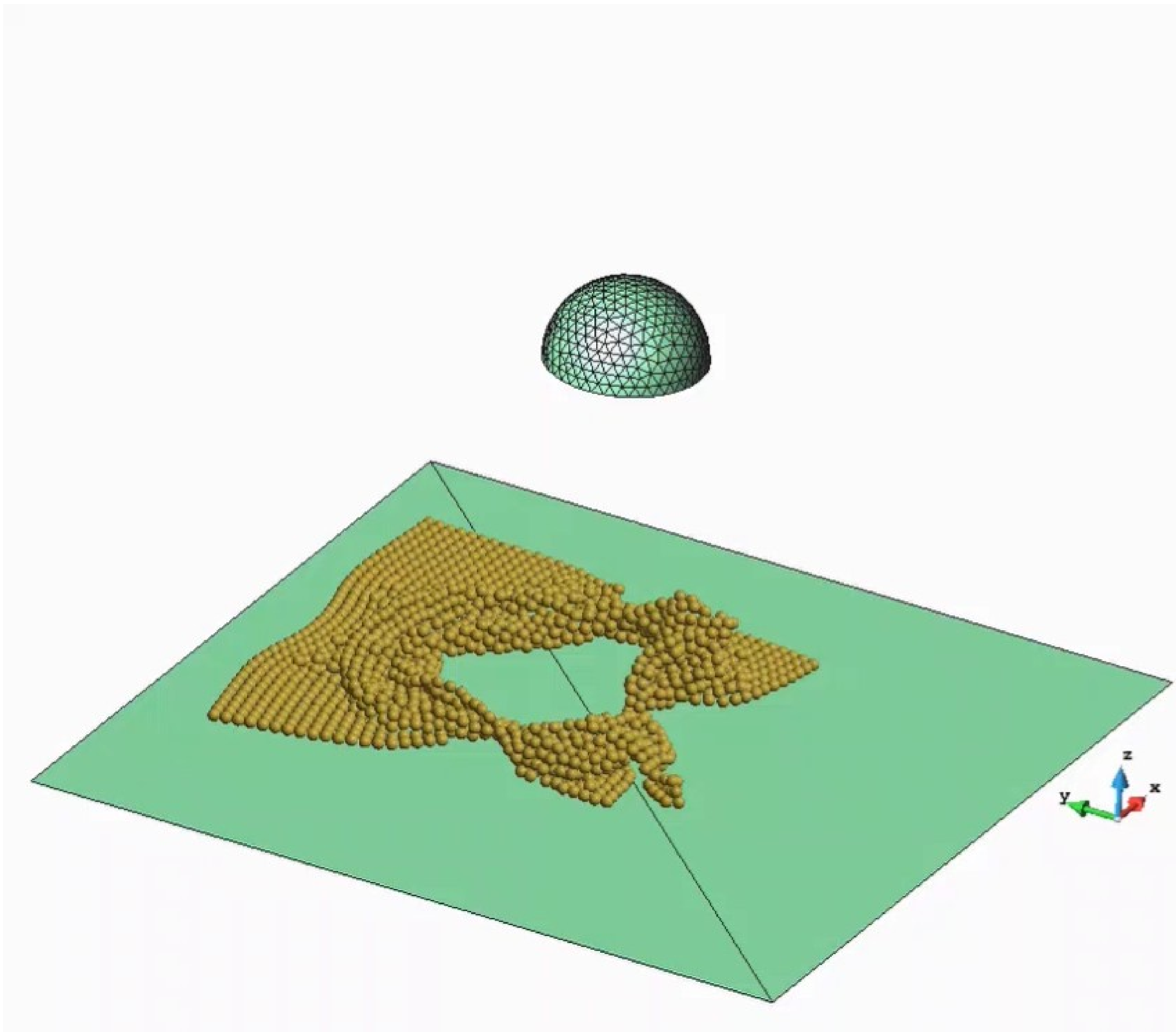
1 single layer of bonded DEM

Rockfall protection nets (roads safety)

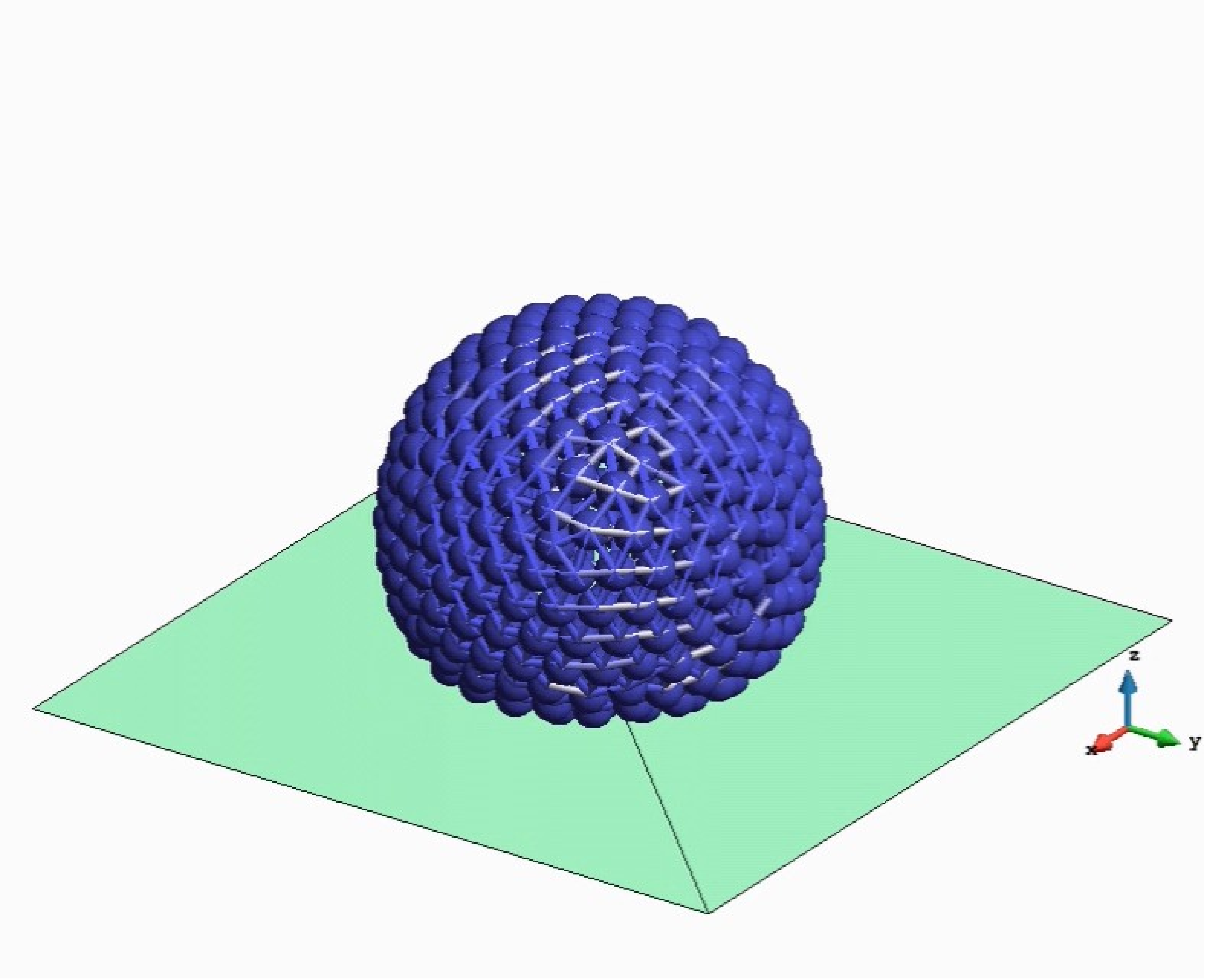
(hidden spheres)



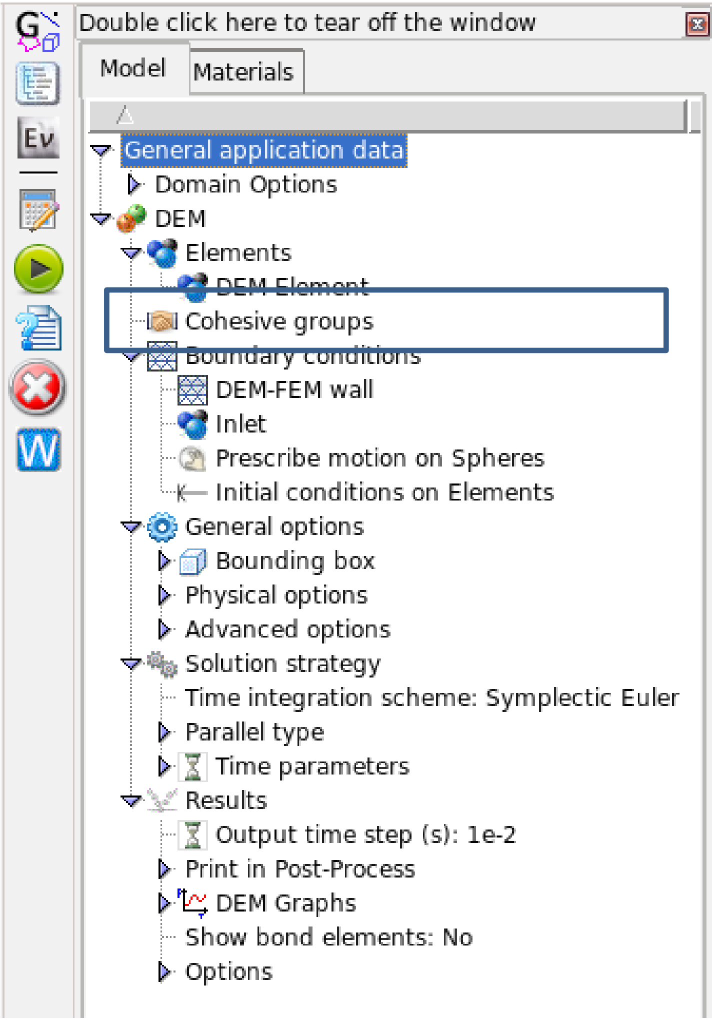
Fabrics breakage.



Bending stiffness in fabrics



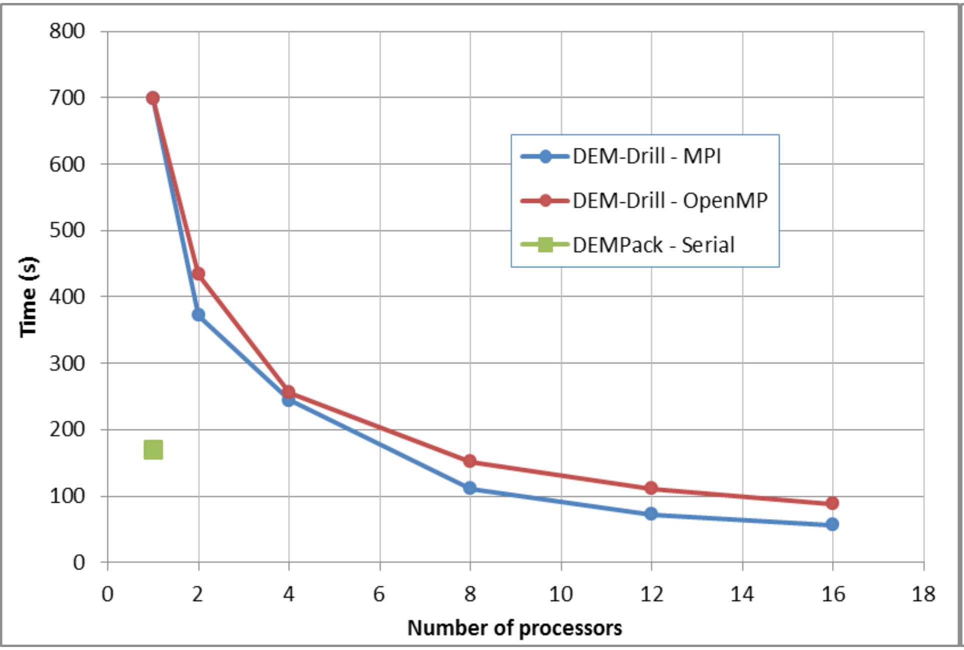
GUI (for **GiD**, a pre- and post- processor developed at CIMNE)

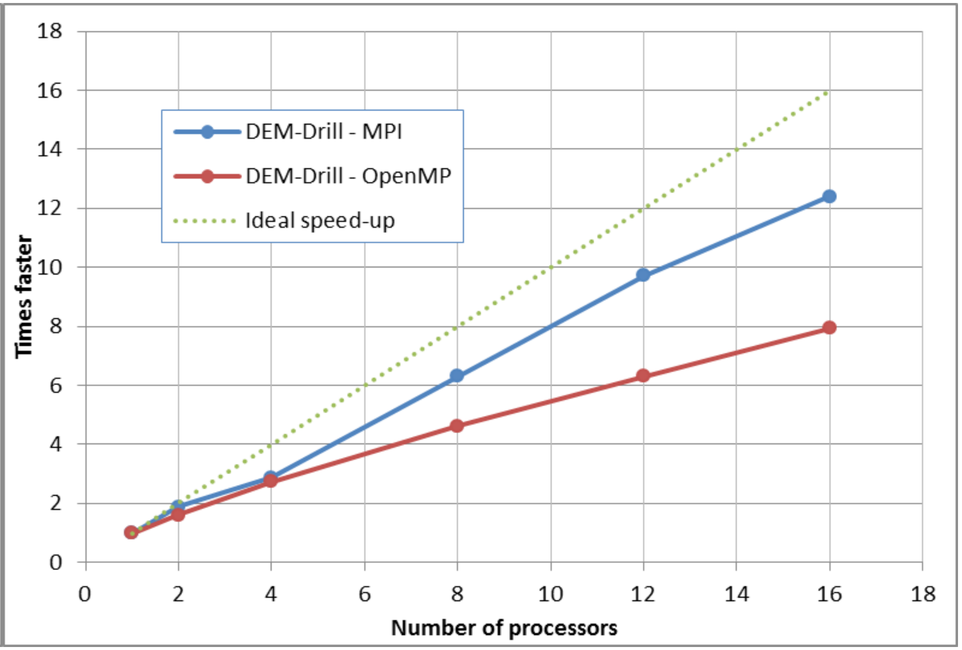


CONTINUUM SIMULATIONS WITH DEM (CONCRETE). MULTI-FRACTURE

SPEED-UP

Number of processors	DEMPack-serial Time (s)	DEM-Drill Time (s) OpenMP	DEM-Drill Speed-up OpenMP	DEM-Drill Time (s) MPI	DEM-Drill 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

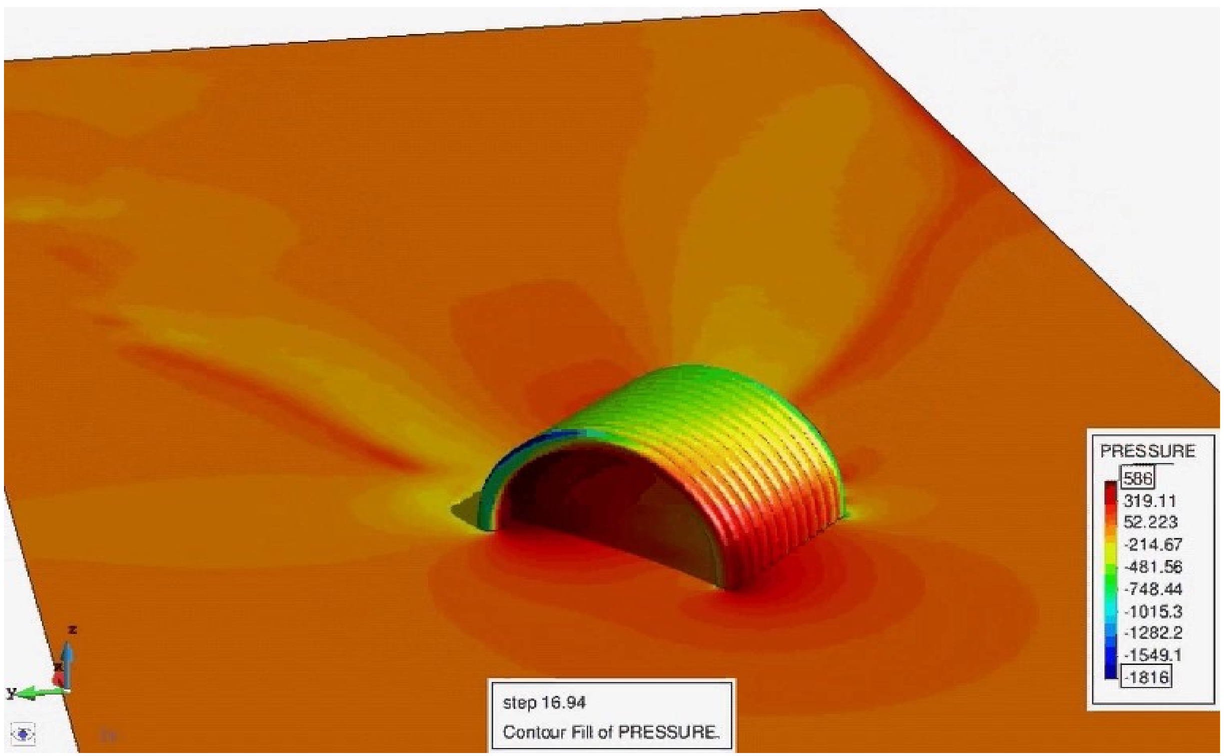




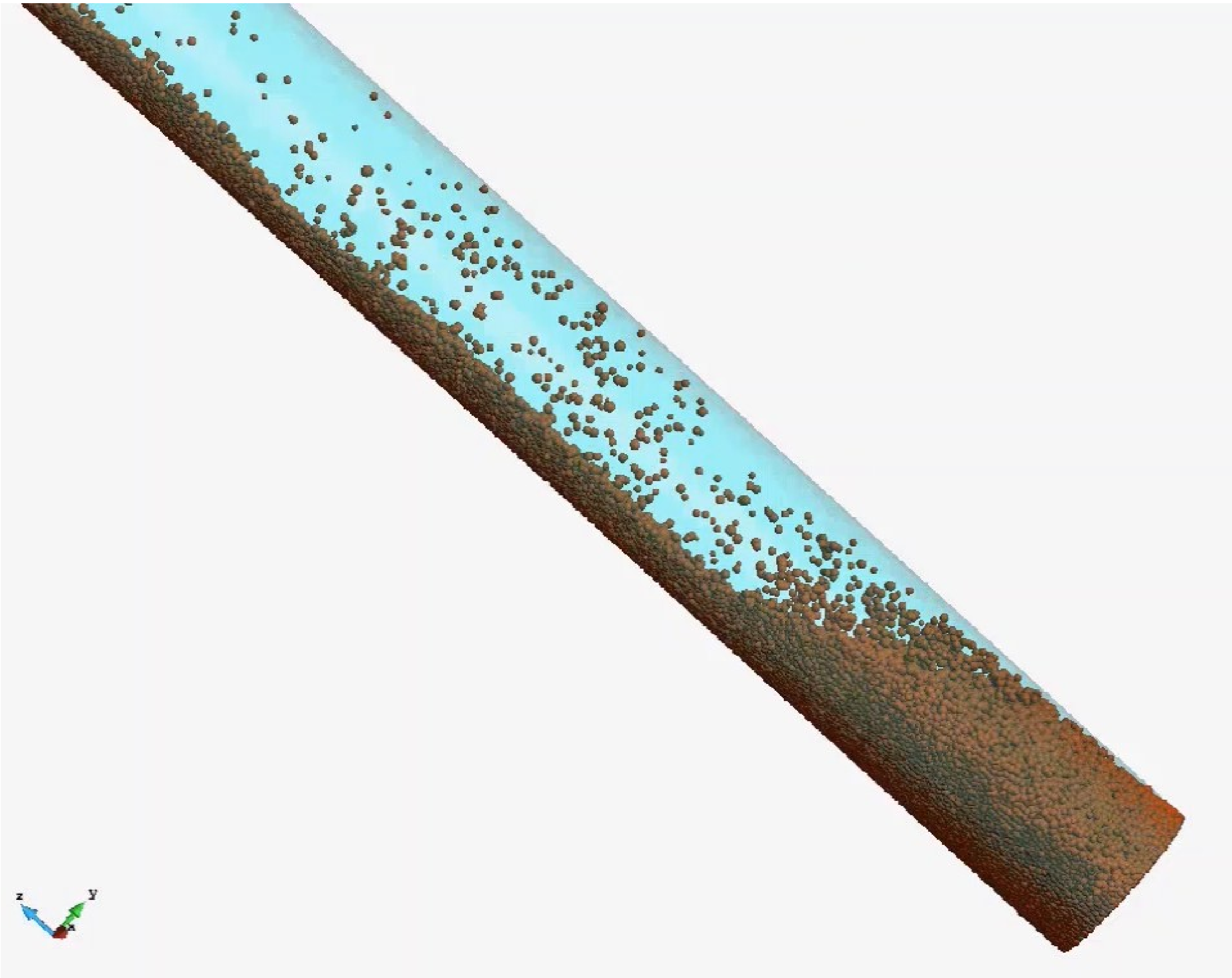
- What is Kratos - DEMpack?
- DEMpack – non-cohesive (granular materials, slightly cohesive soils)
- DEMpack – cohesive (rocks, concrete, fabrics)
- **DEMpack – CFD (strong 2-way coupling)**
- DEMpack – CSD (plasticity, damage)
- Wizards

FLUID CODES: KRATOS CFD AND PFEM

KRATOS MULTI-PHYSICS CFD



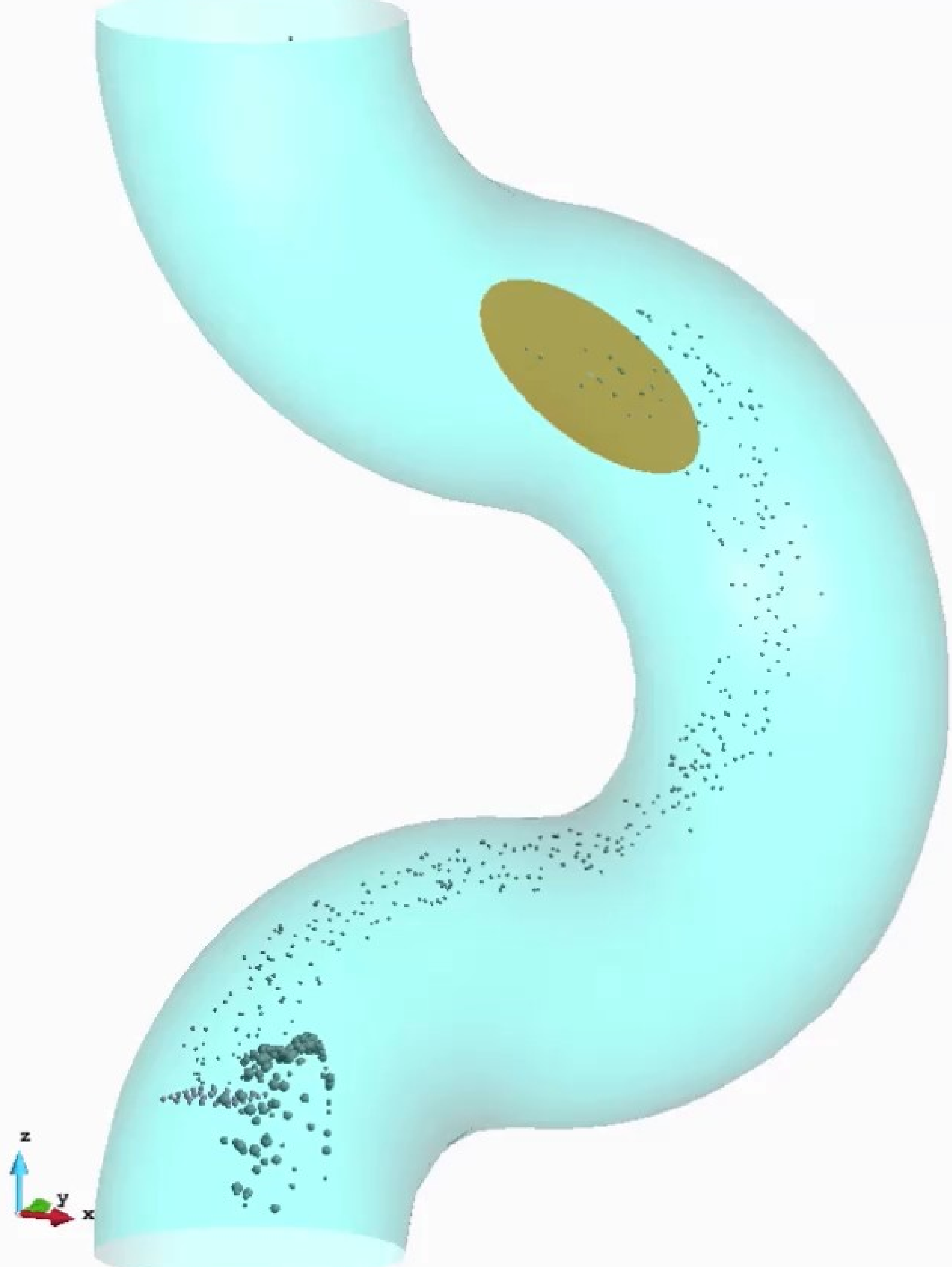
KRATOS Multi-Physics CFD + KRATOS Multi-Physics DEMpack



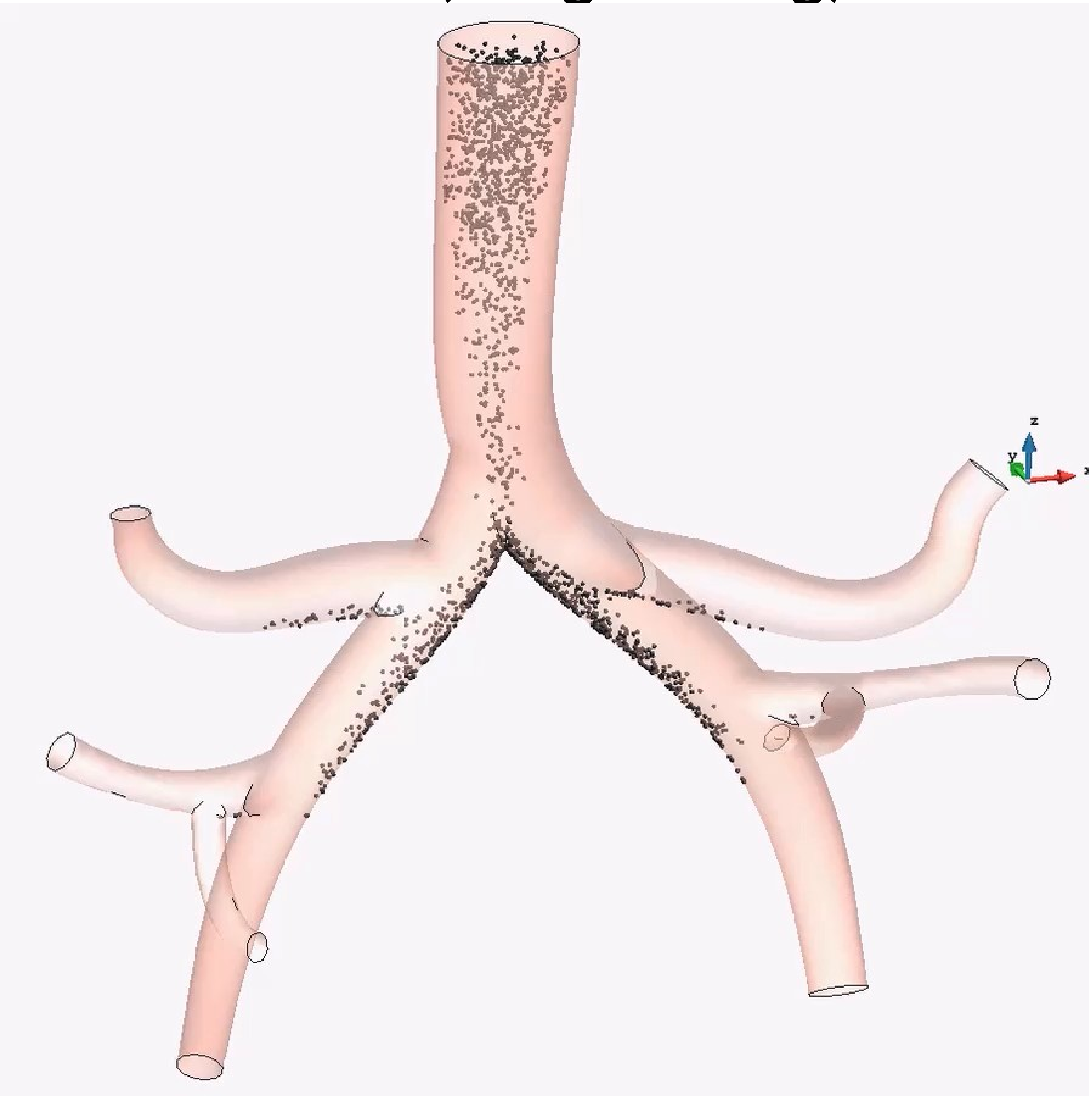
Fluidized bed

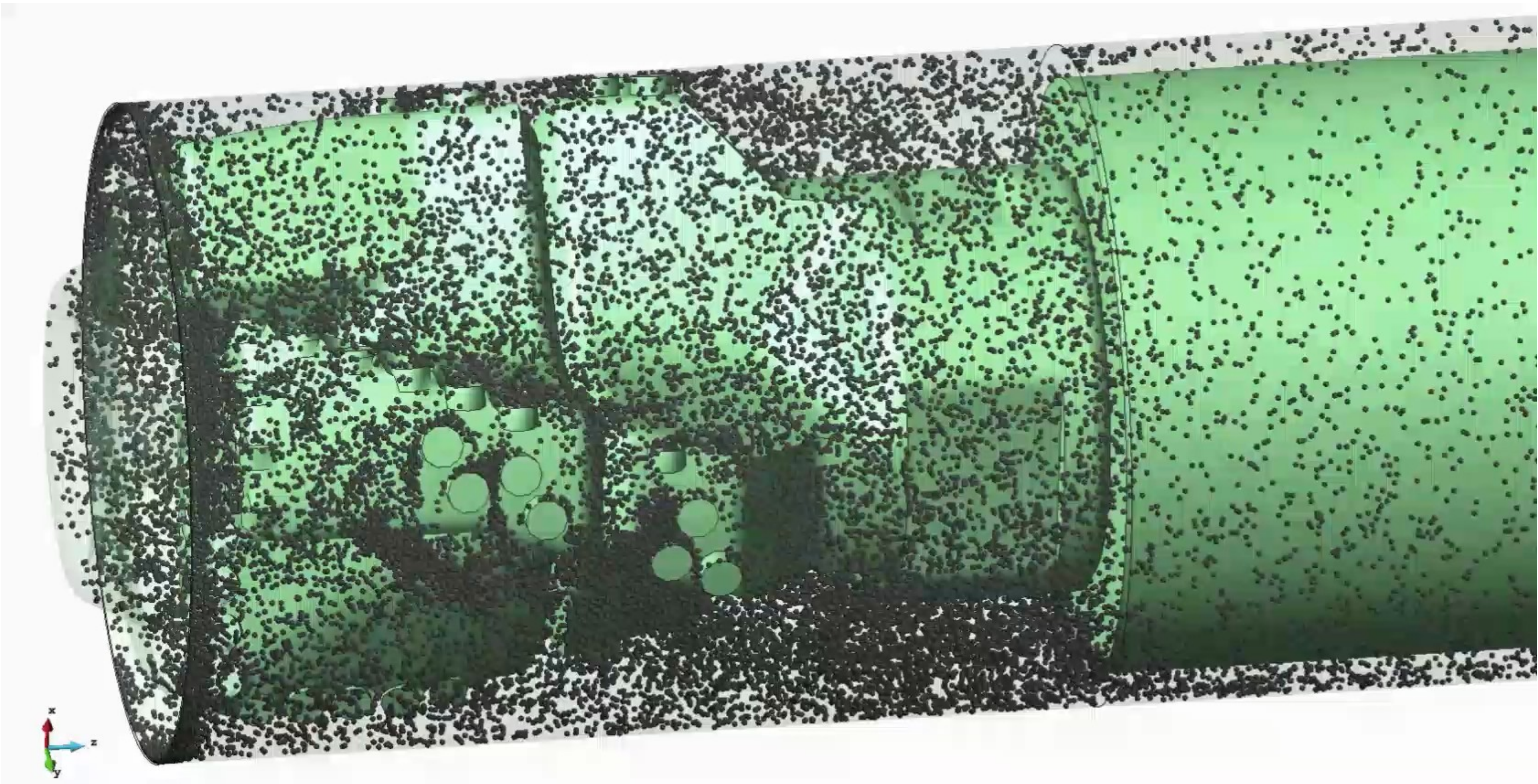
KRATOS MULTI-PHYSICS DEMpack
+ KRATOS MULTI-PHYSICS CFD

Ascending fluid


z
y
x

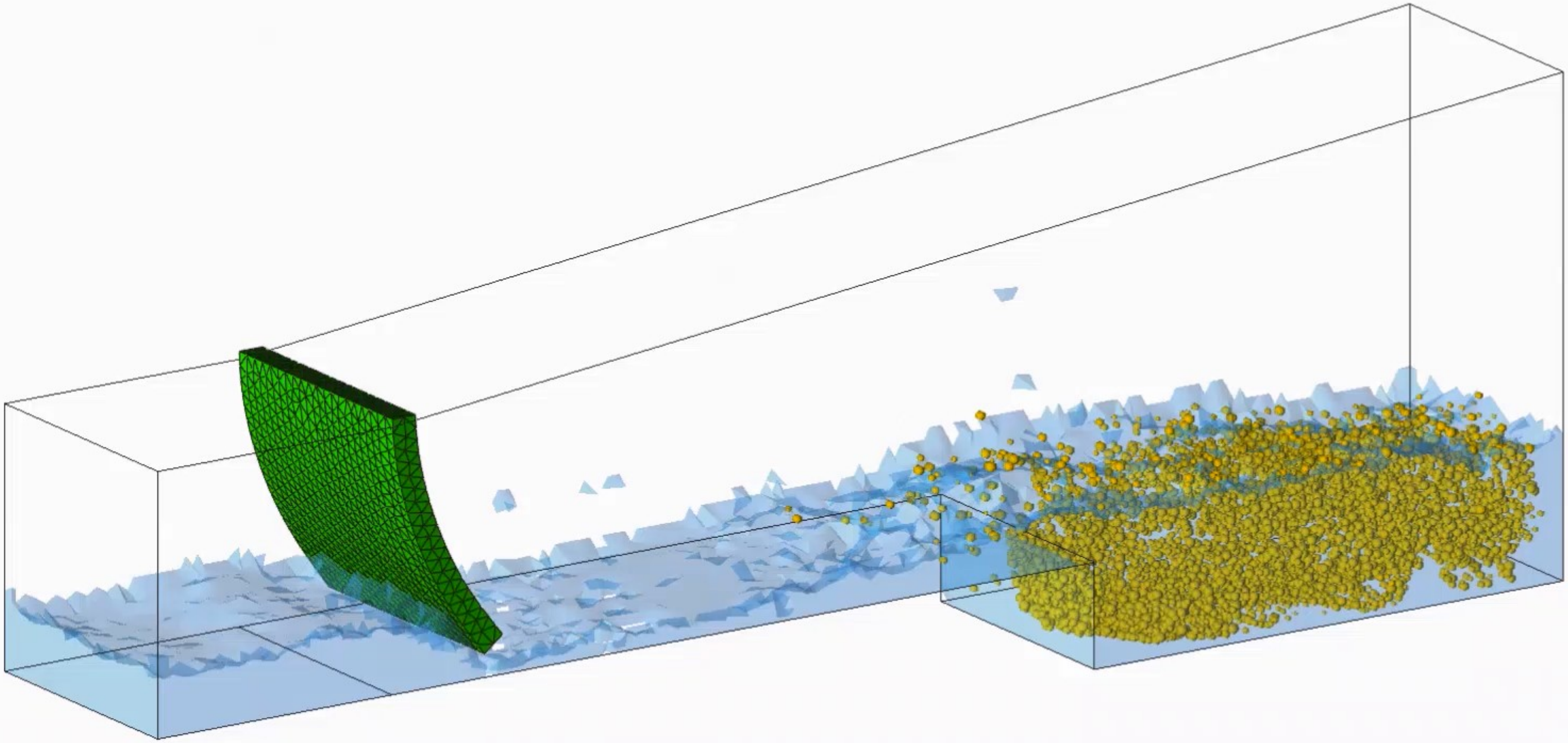
Biomedical studies (lung soiling)



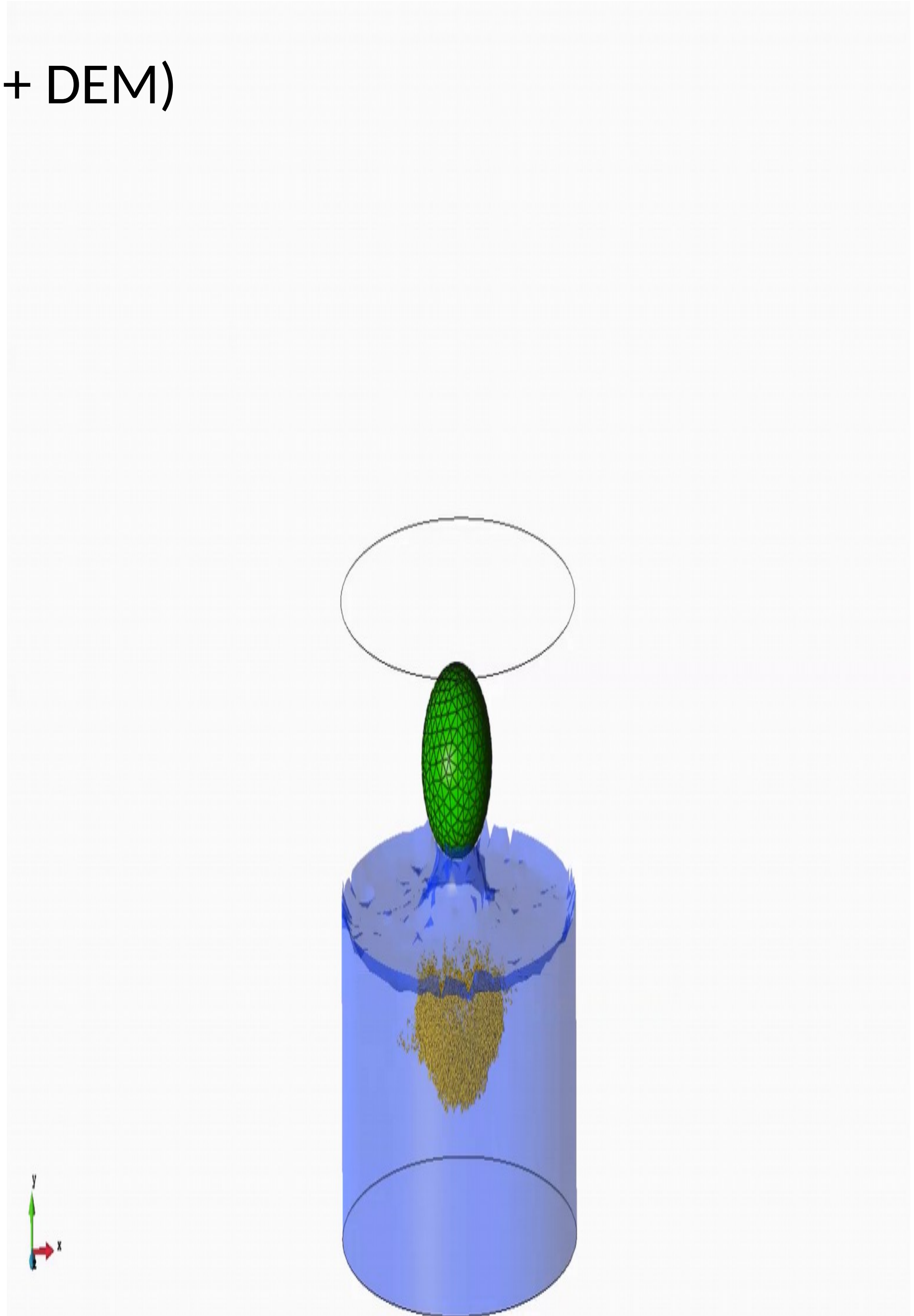


x
z
y

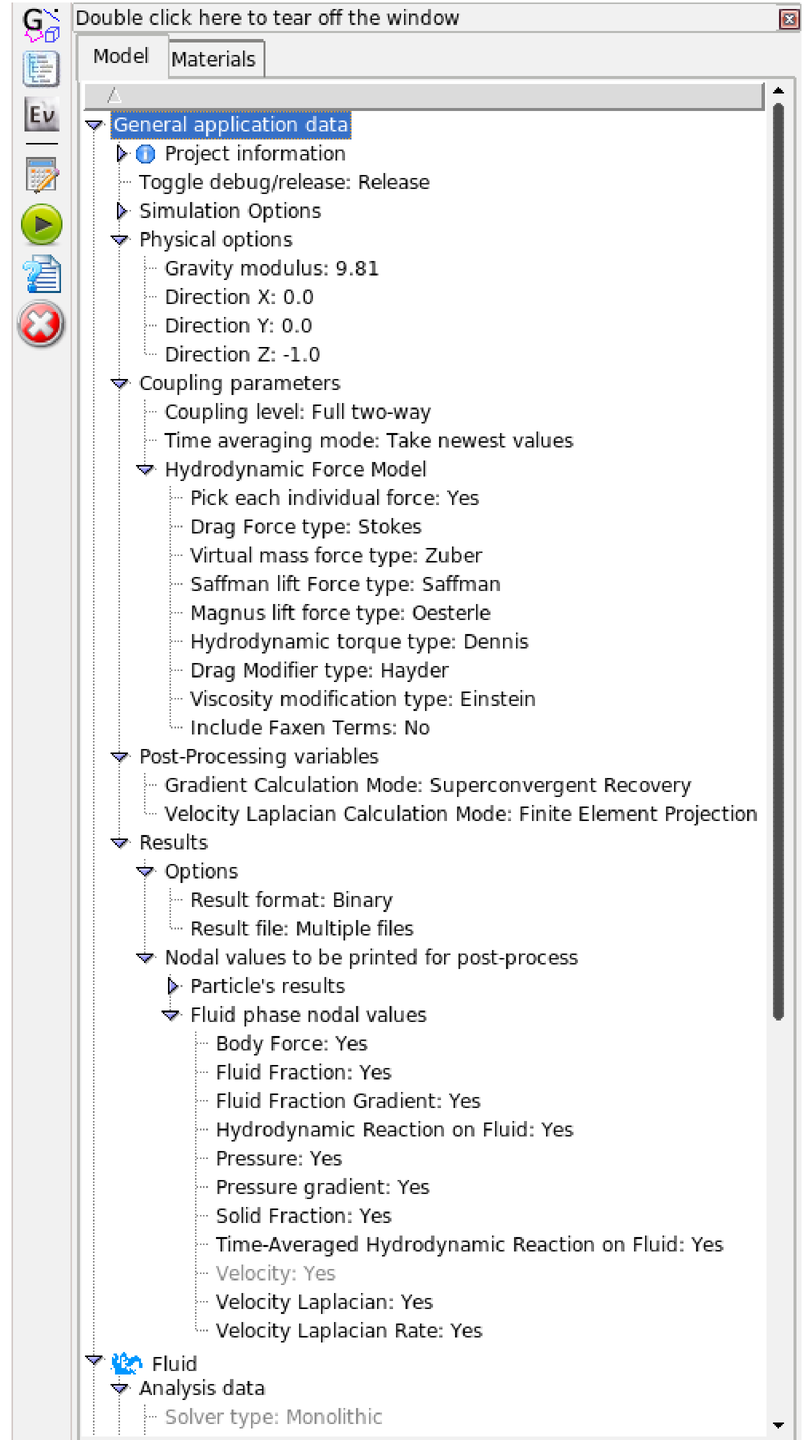
Free surface flows (PFEM + DEM)



Free surface flows (PFEM + DEM)



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



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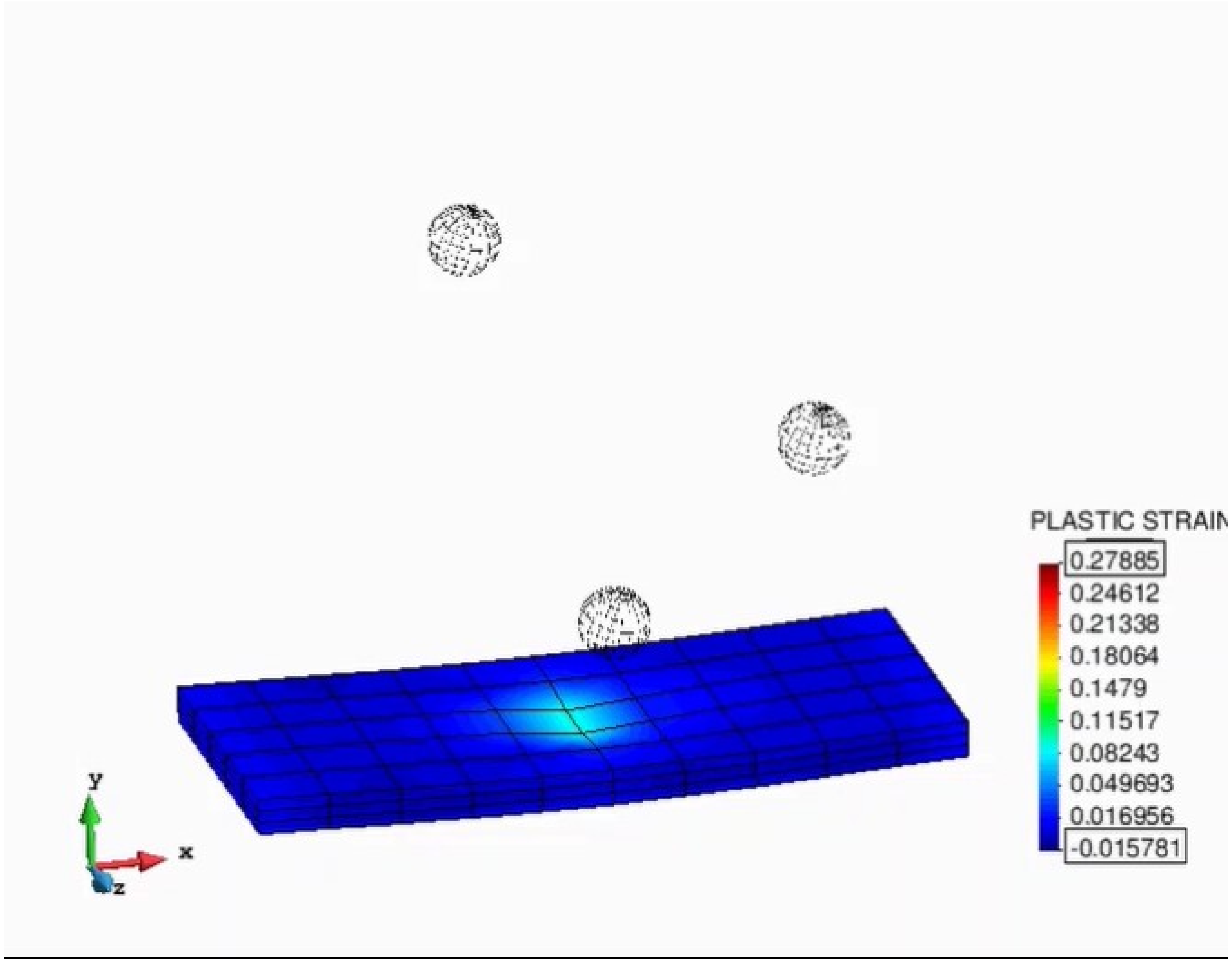
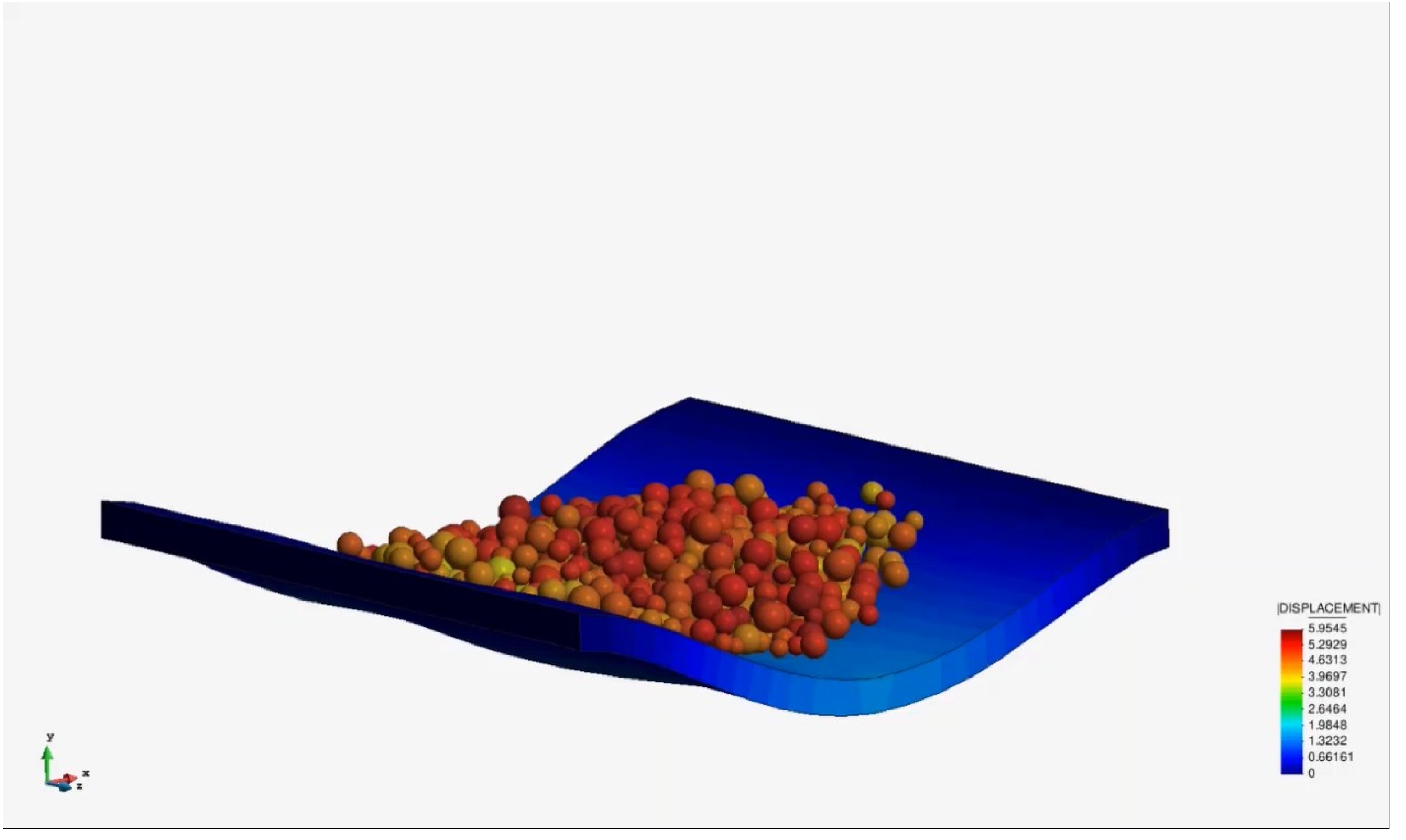
- Wizards

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.

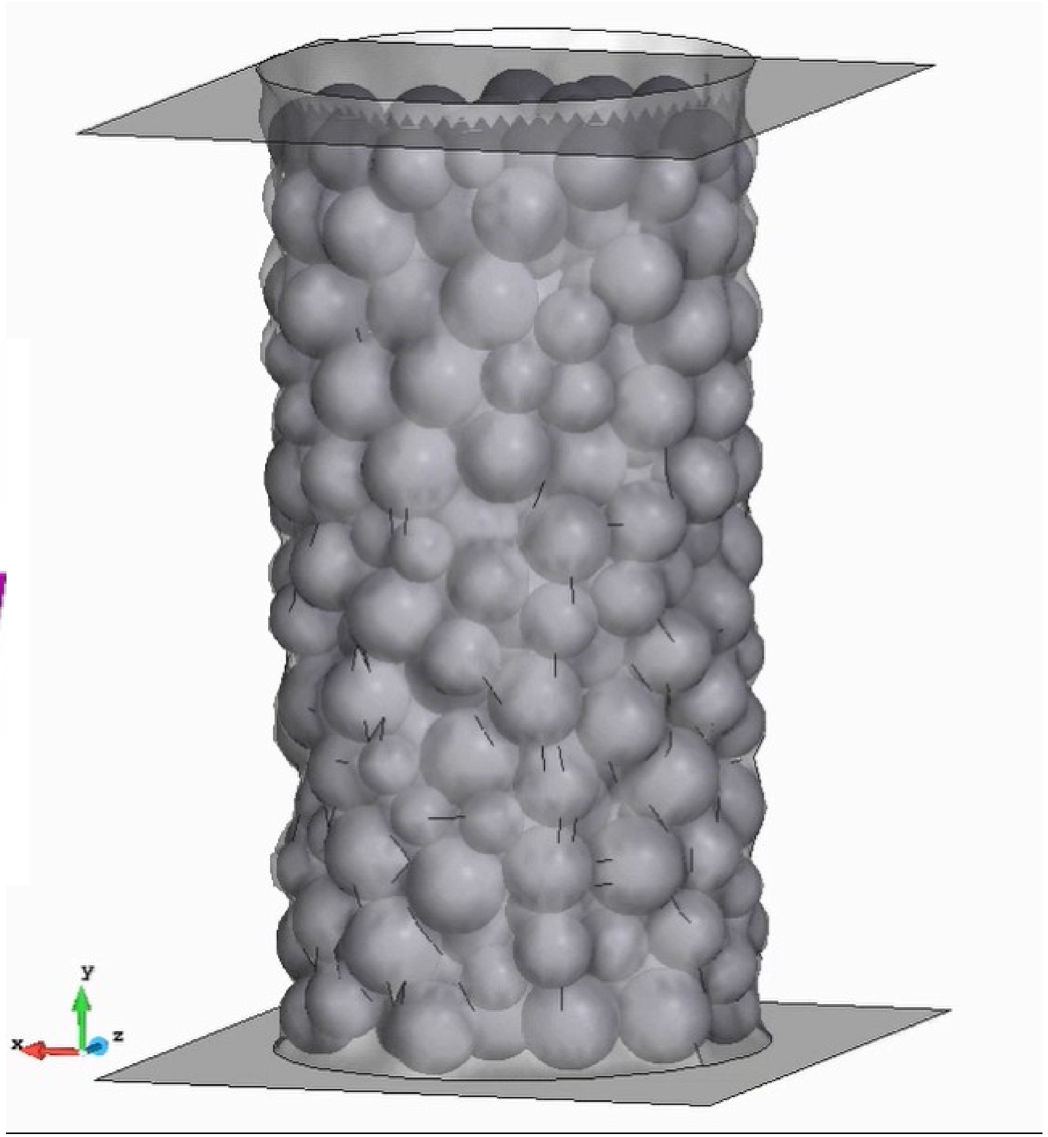


Interaction between particles and elastic plate

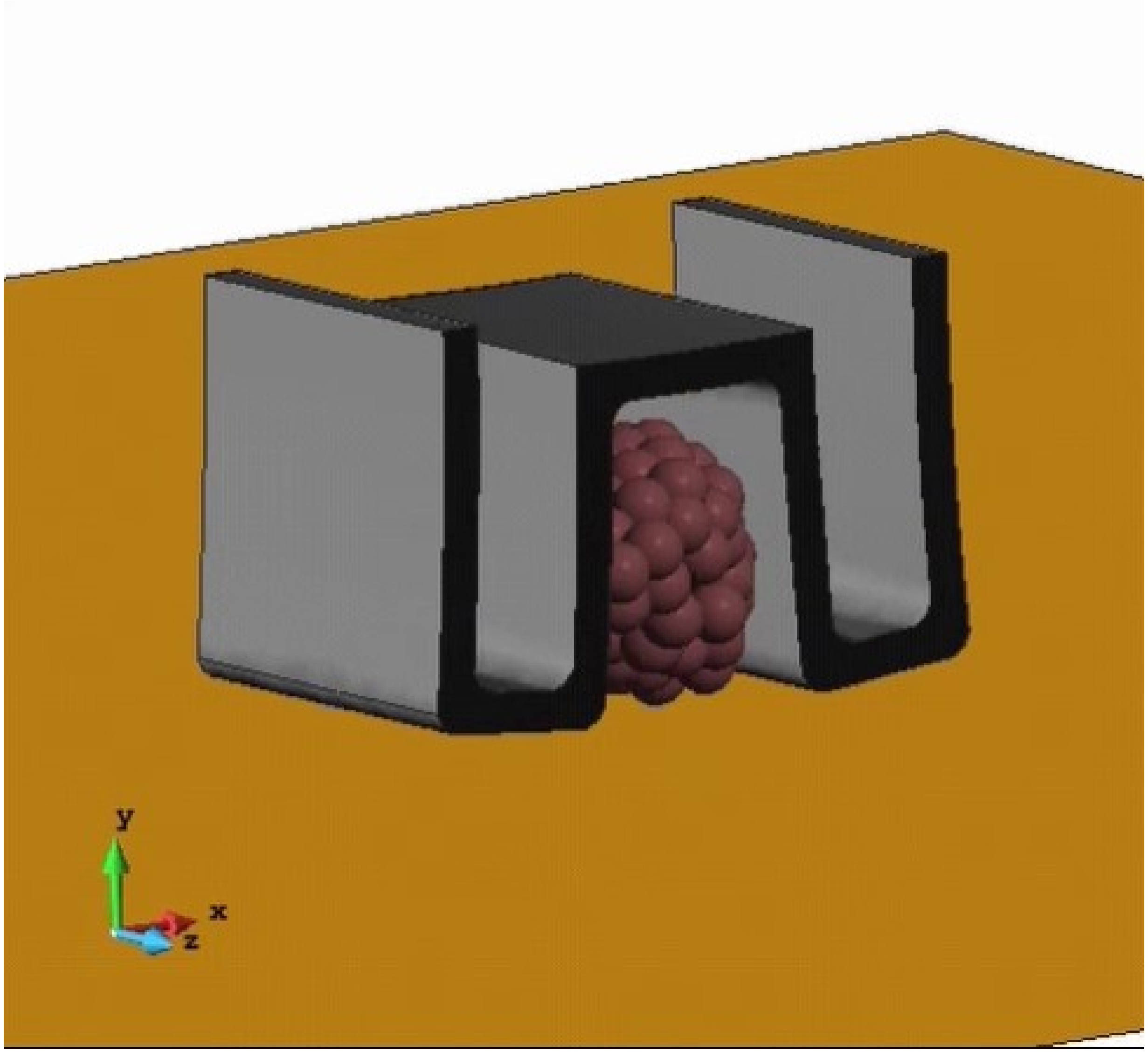


Santasusana, M., Irazábal, J., Oñate, E., Carbonell, J.M. The Double Hierarchy Method. A parallel 3D contact method for the interaction of spherical particles with rigid FE boundaries using the DEM.
DOI:10.1007/s40571-016-0109-4

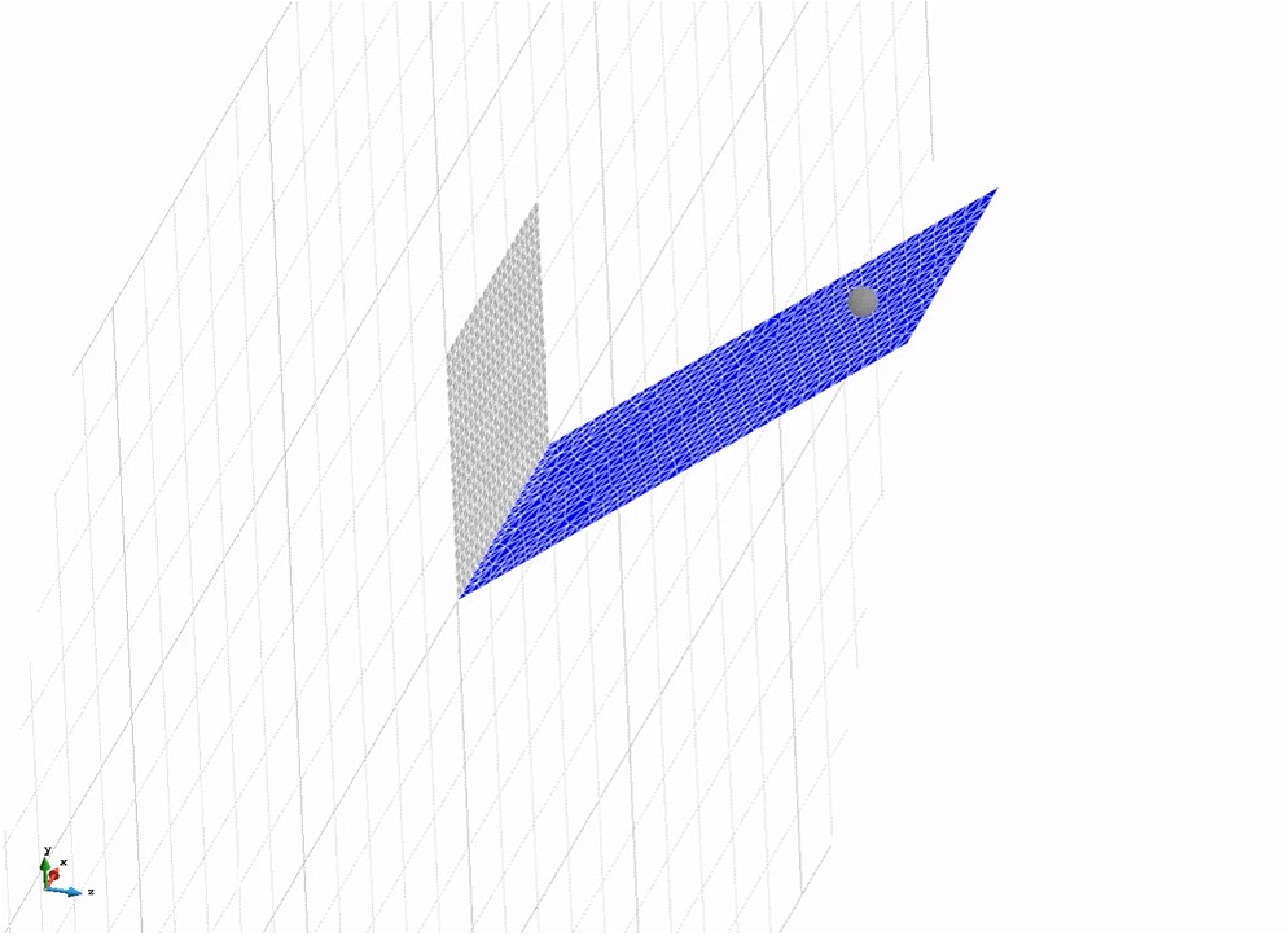
Triaxial test (wrapper structural membrane):



Truck tyre and stone



Coupling DEM-Structure (beams) – WIP in TUM



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- DEMpack – CFD (strong 2-way coupling)
- DEMpack – CSD (plasticity, damage)
- **Wizards**

Features of a ‘Wizard’:

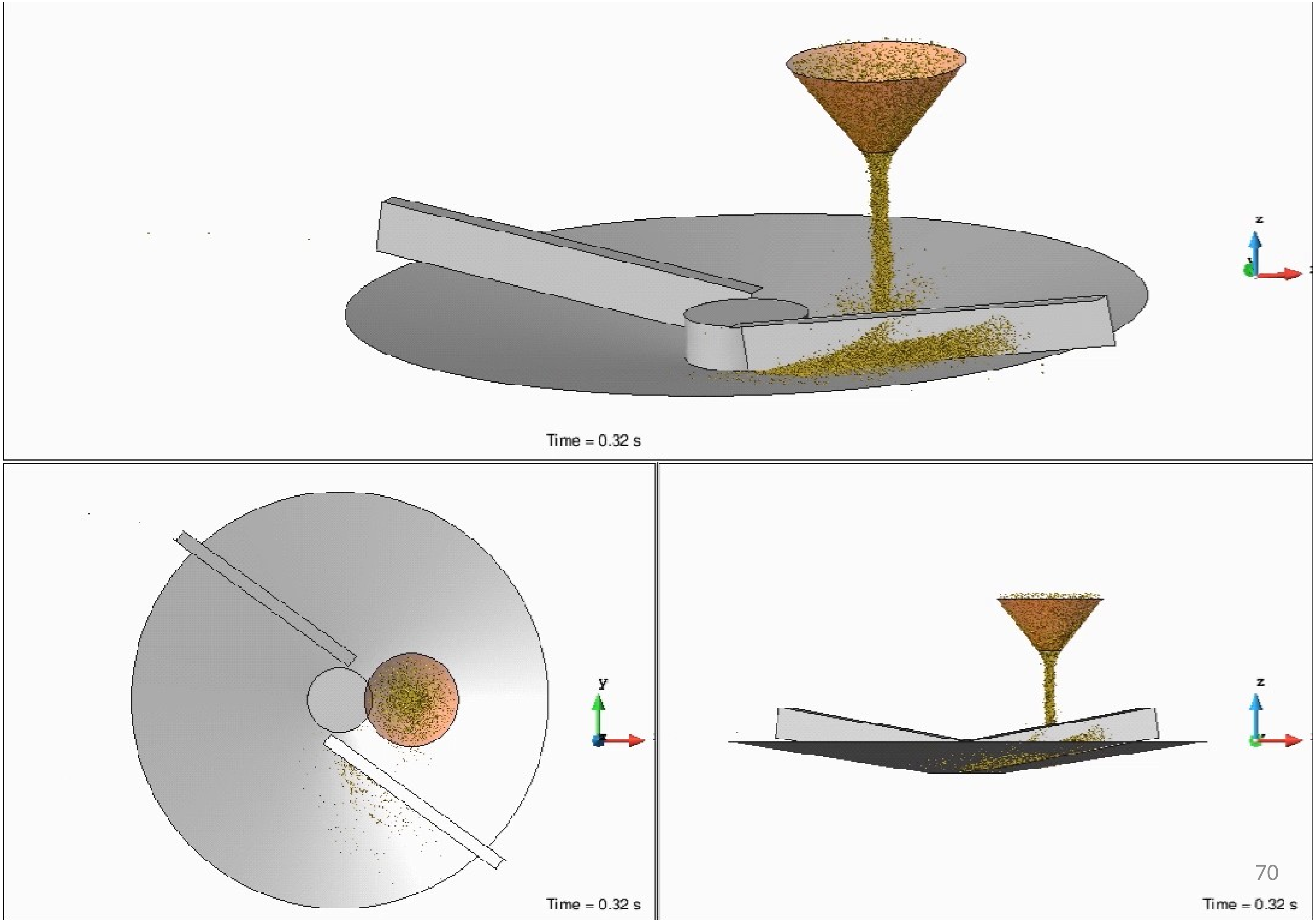
- A Graphical User Interface which allows to launch a computation in a very short time (computation might take hours or more, though)
- Little or no effort in creating geometries or meshes
- Limited and very specific capabilities and output
- Optimized for a specific task

SpreadDEM v1.0

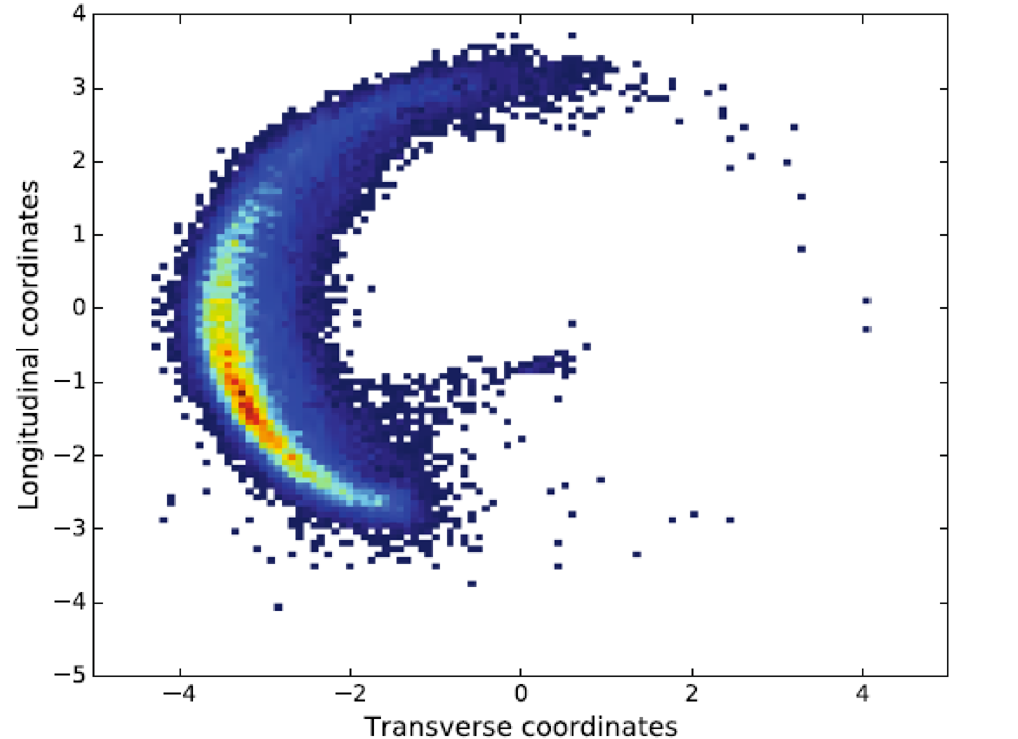
(presented in Gid Workshop 2018)

CIMNE

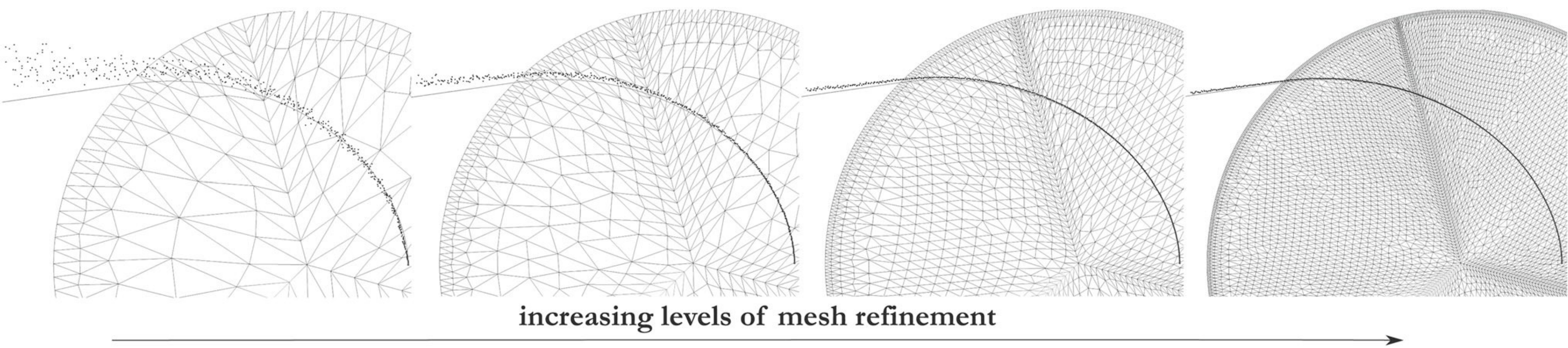
Fertilizer (or seeds) spreader


Time = 0.32 s
Time = 0.32 s
Time = 0.32 s

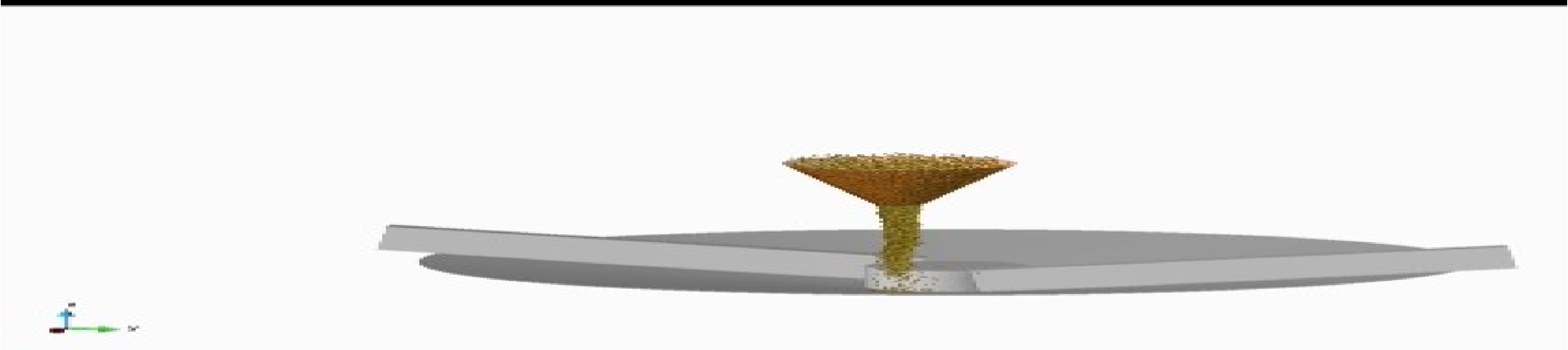
Dispersion patterns:



Accuracy assessment:

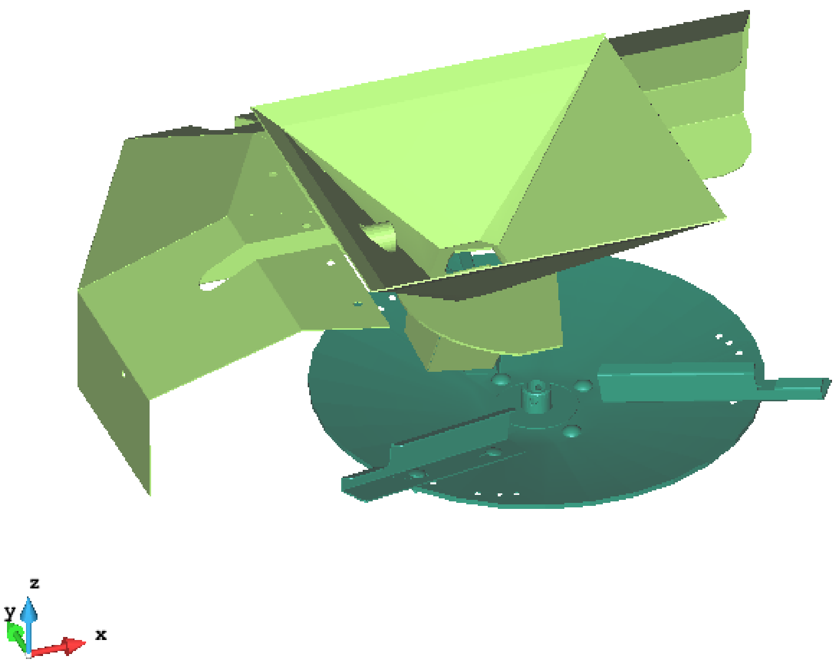


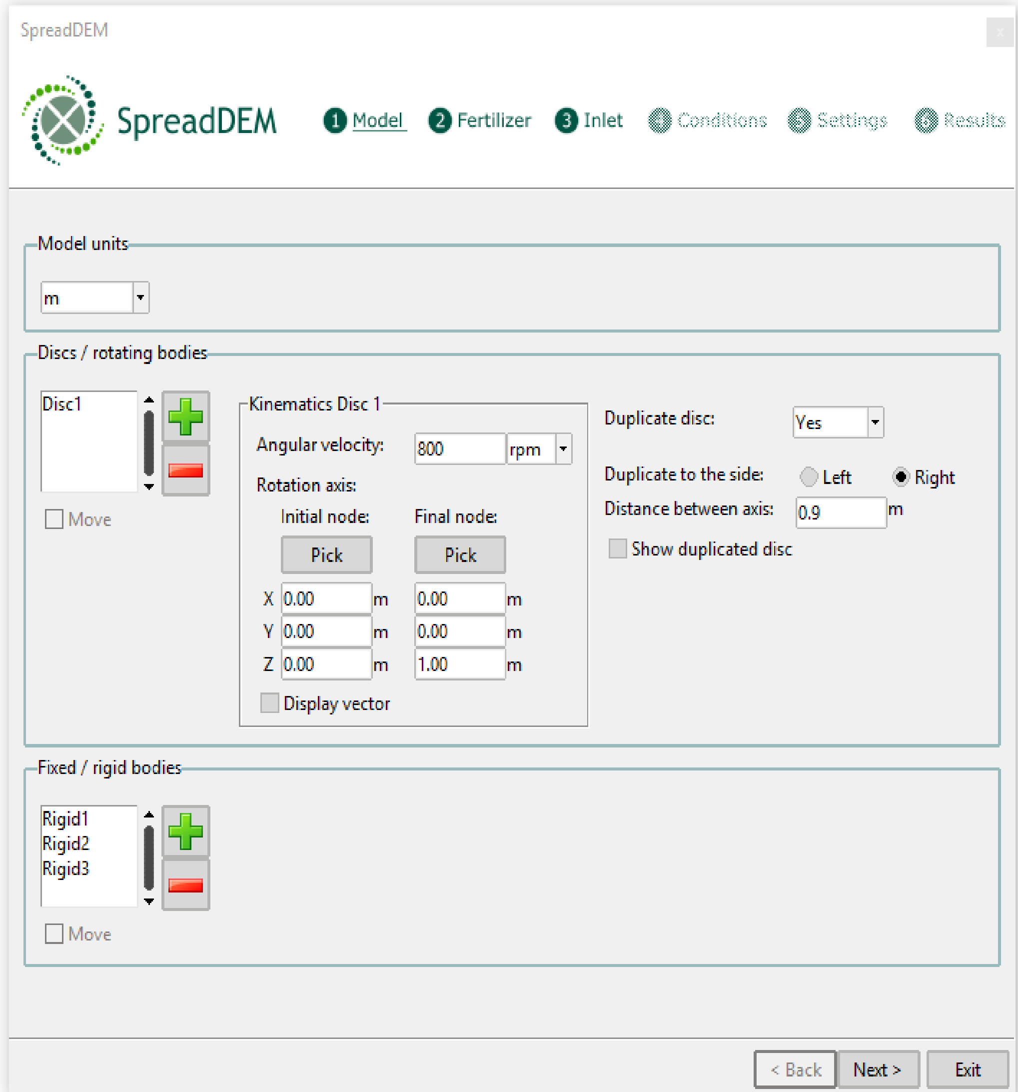
G Casas, D Mukherjee, MA Celigueta, TI Zohdi, E Onate . A modular, partitioned, discrete element framework for industrial grain distribution systems with rotating machinery. Computational Particle Mechanics, 1-18, 2015



STEP 1. Model

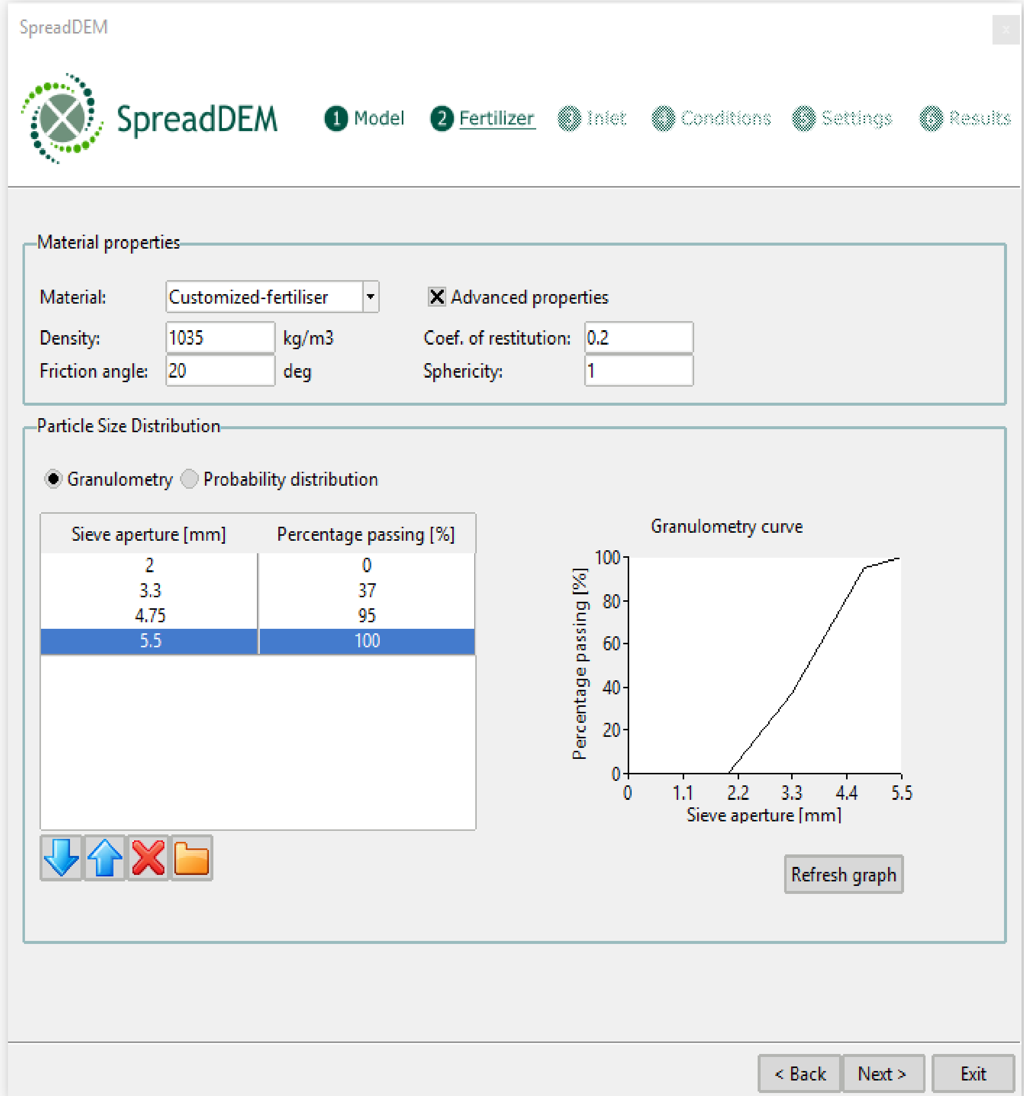
- Rotative parts imported
  - Angular velocity of the discs
  - Rotation axis
- Fixed parts imported





STEP 2. Fertilizer

Fertilizer properties
- Density
- Friction angle
- Granulometry



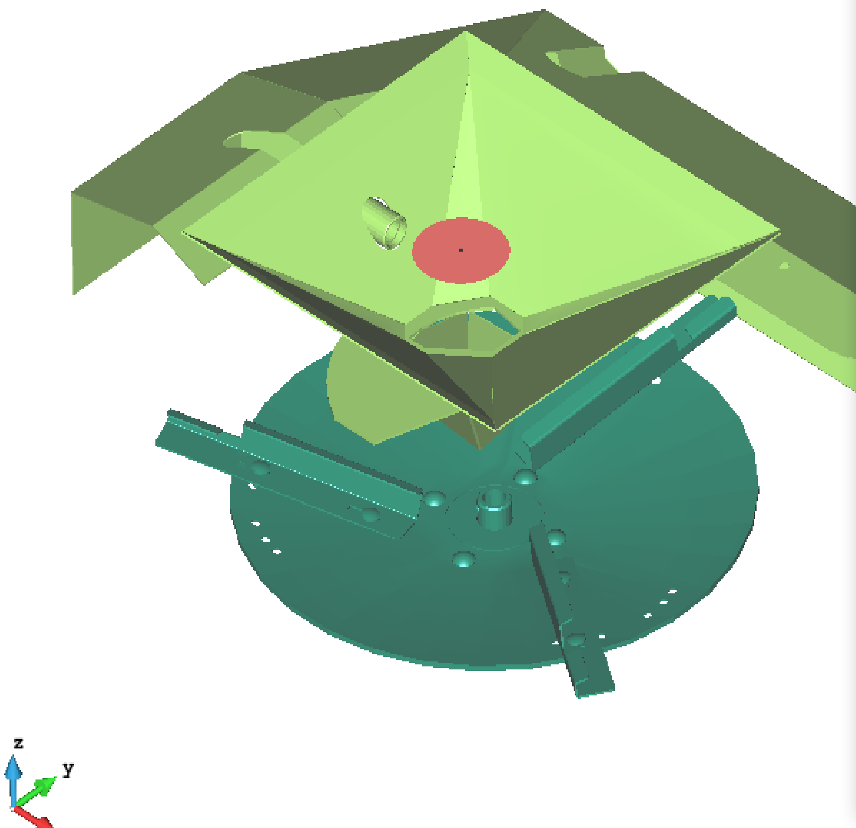
CIMNE

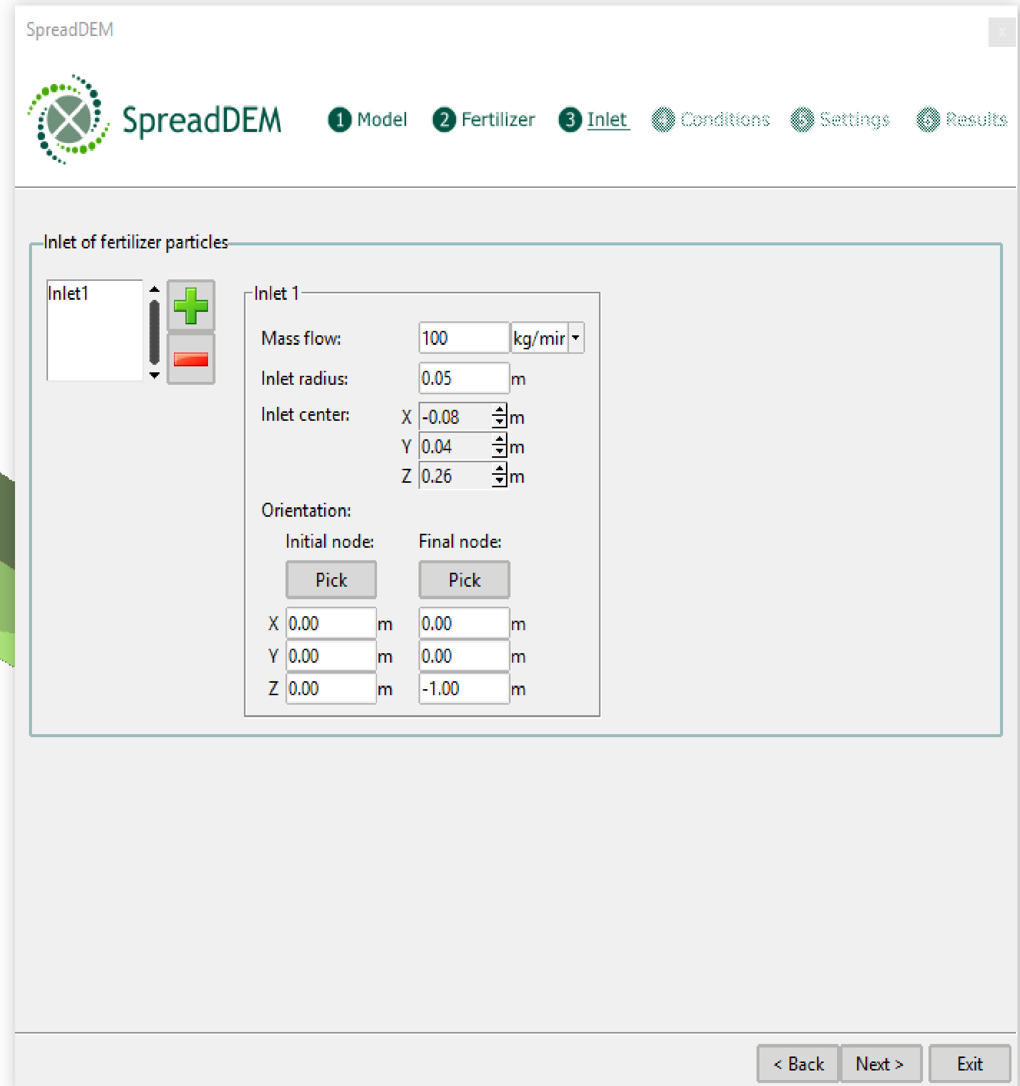
SpreadDEM v1.0

STEP 3. Inlet

Inlet of fertilizer particles

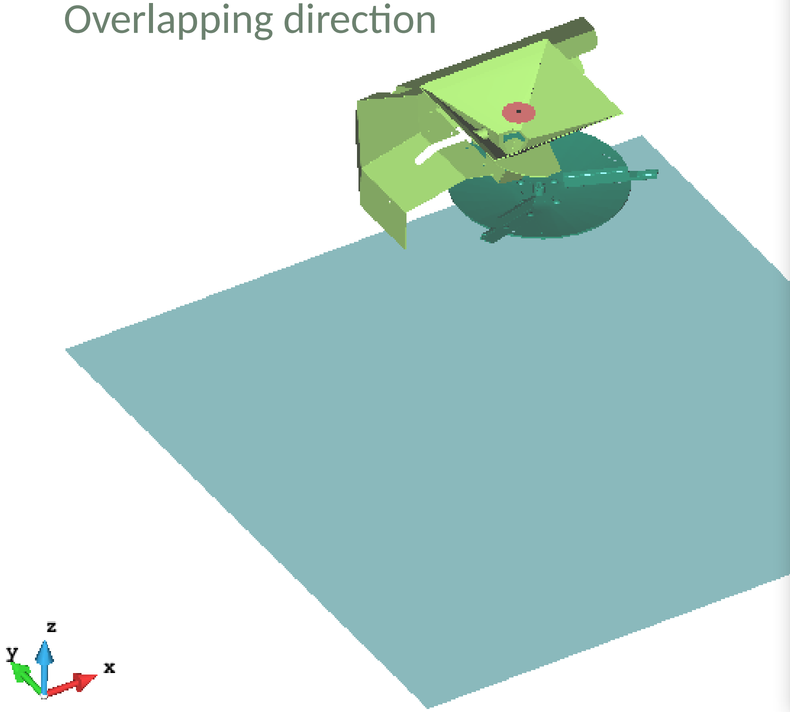
- Mass flow
- Inlet geometry and position

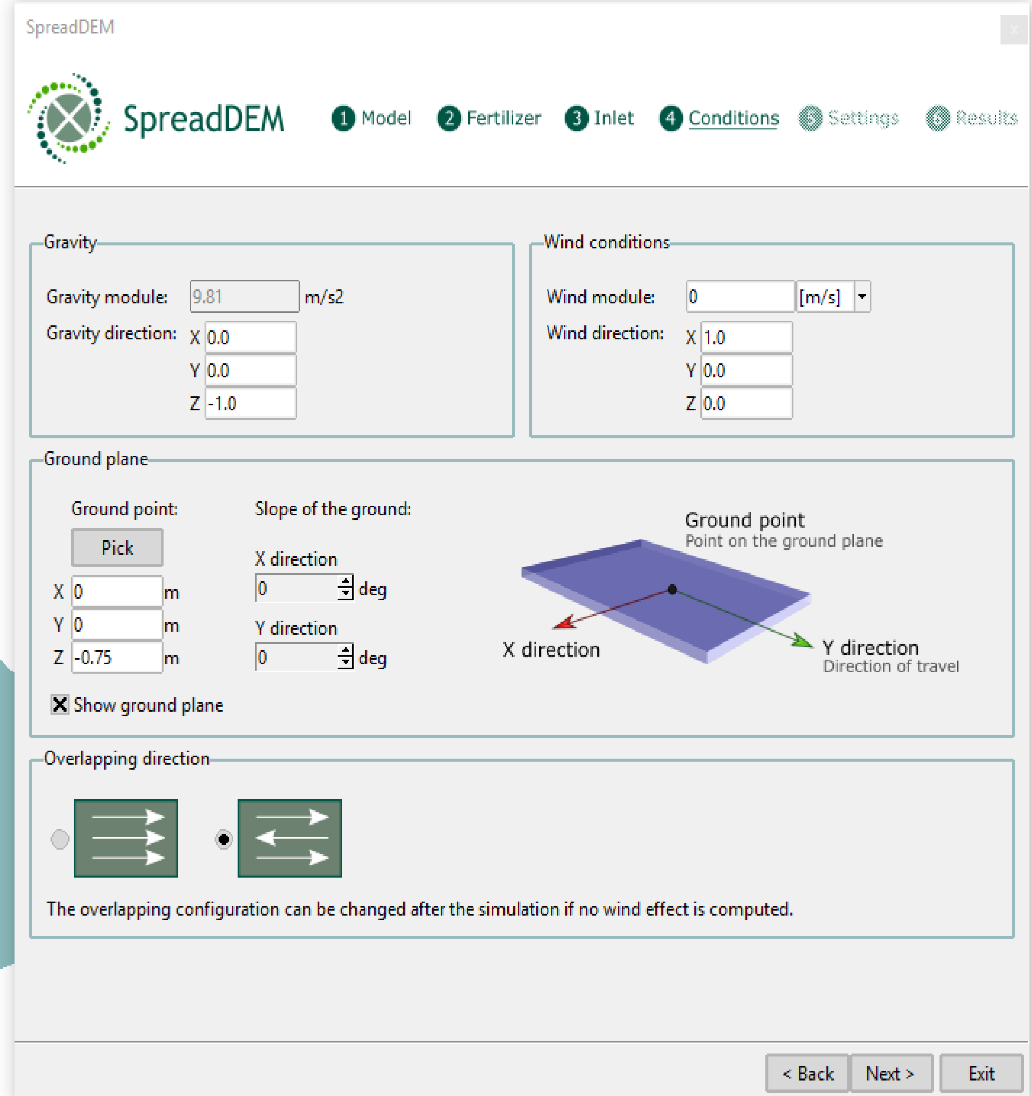




STEP 4. Conditions

- Gravity
- Wind conditions
- Ground plane
    - Distance to floor
    - Slope of the ground
- Overlapping direction

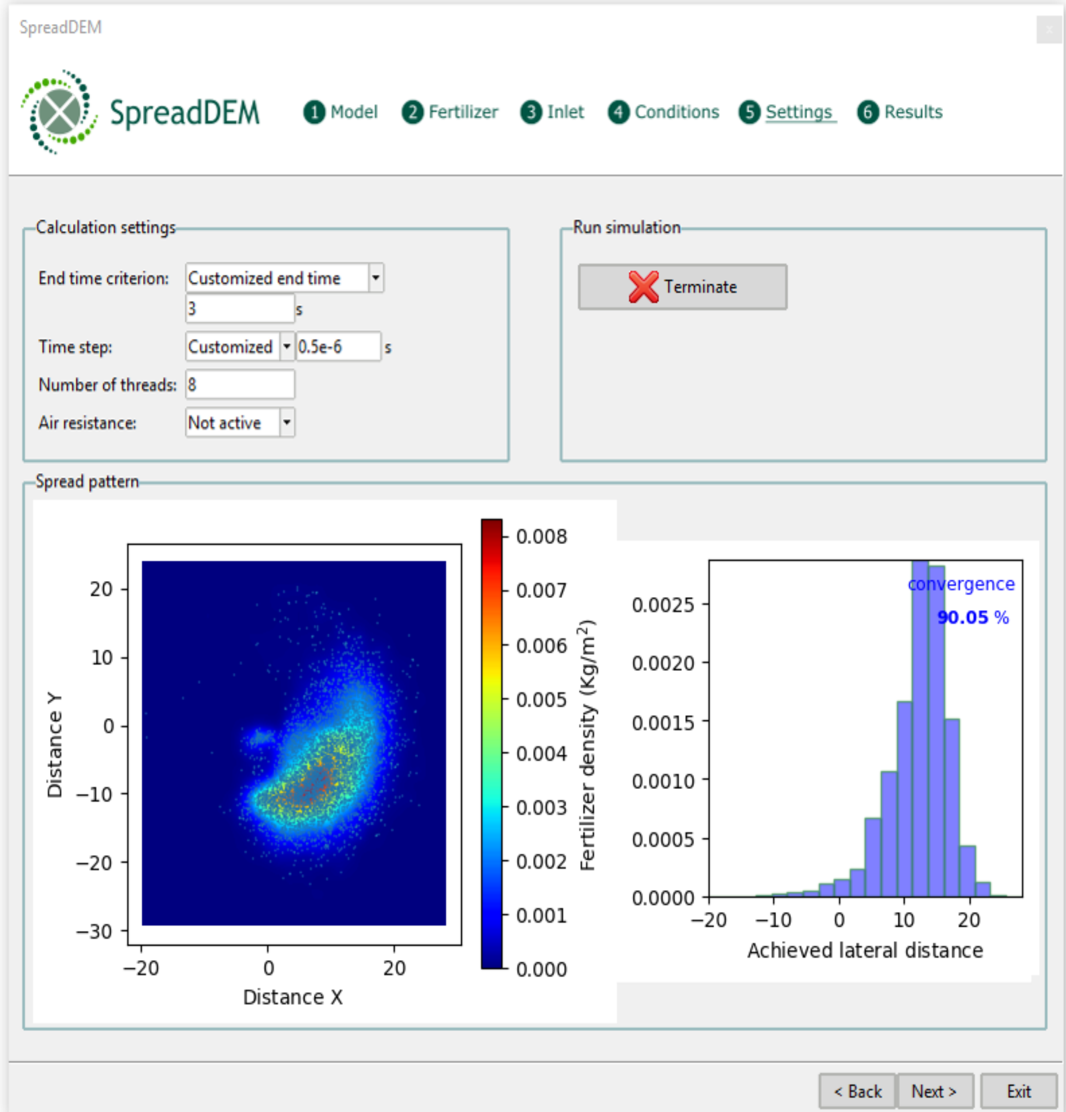





SpreadDEM v1.0
CIMNE

STEP 5. Settings

Calculation settings
Spread pattern during simulation

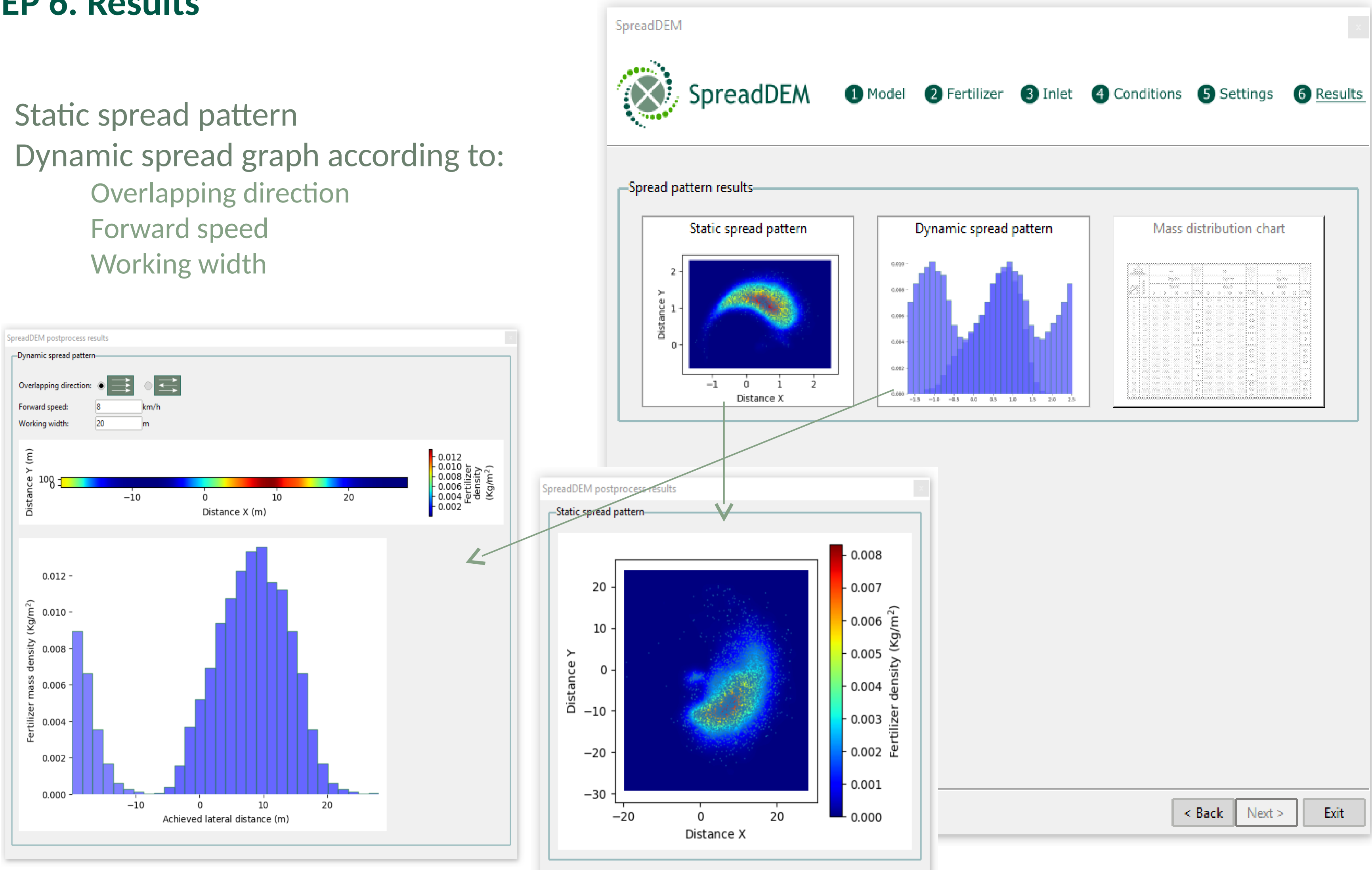


STEP 6. Results

Static spread pattern

Dynamic spread graph according to:

- Overlapping direction
- Forward speed
- Working width



An overview on the main features of

KRATOS MULTI-PHYSICS DEMpack

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

gcasas@cimne.upc.edu
maceli@cimne.upc.edu
spreaddem@cimne.upc.edu

CIMNE UPC