SuperDEM-CFD: Open source parallel solver for non-spherical particle-fluid fluidization systems

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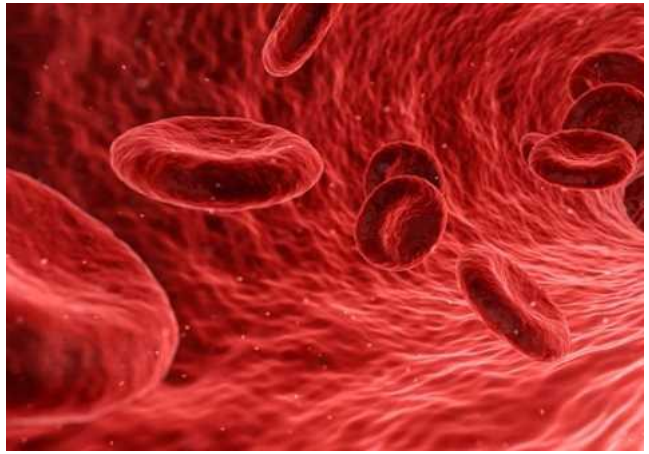
Background and motivation

- Non-spherical multibody system

Mineral industry

Civil industry

Agriculture industry



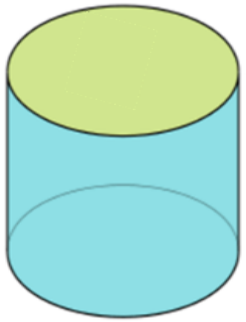
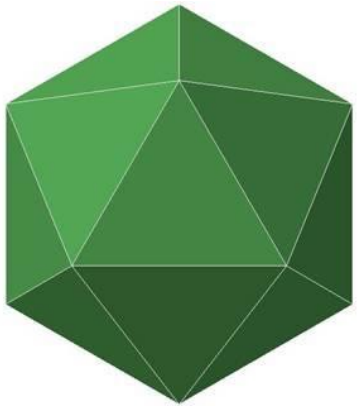
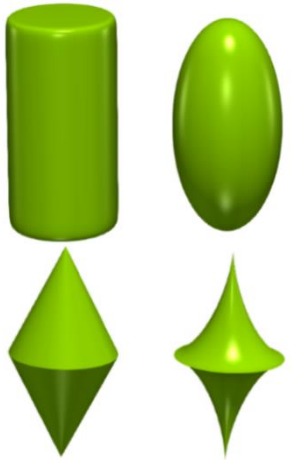
Biomedical industry

Chemical industry

Pharmaceutical industry

Bioenergy industry **(BETO CCPC projects)**

Non-spherical particle modeling methods

Method	Real geometry	Multi-sphere, Glued-sphere, bond-sphere	Polyhedron	Superquadric
Example				
Accuracy	High	Low	Medium-High (depend on resolution)	High
Computational cost	Low	Low-Medium (depend on particle numbers)	Medium-High (depend on resolution)	Medium
Shape representation	Only a few (cylinder, prolate, oblate, cubic)	Almost all	Almost all	Almost all
Contact detections, force calculation	Medium	Easy	Difficult	Difficult

Superquadric particle

- In mathematics, the superquadrics are a family of geometric shapes defined by formulas as follows (except that the squaring operations are replaced by arbitrary powers).

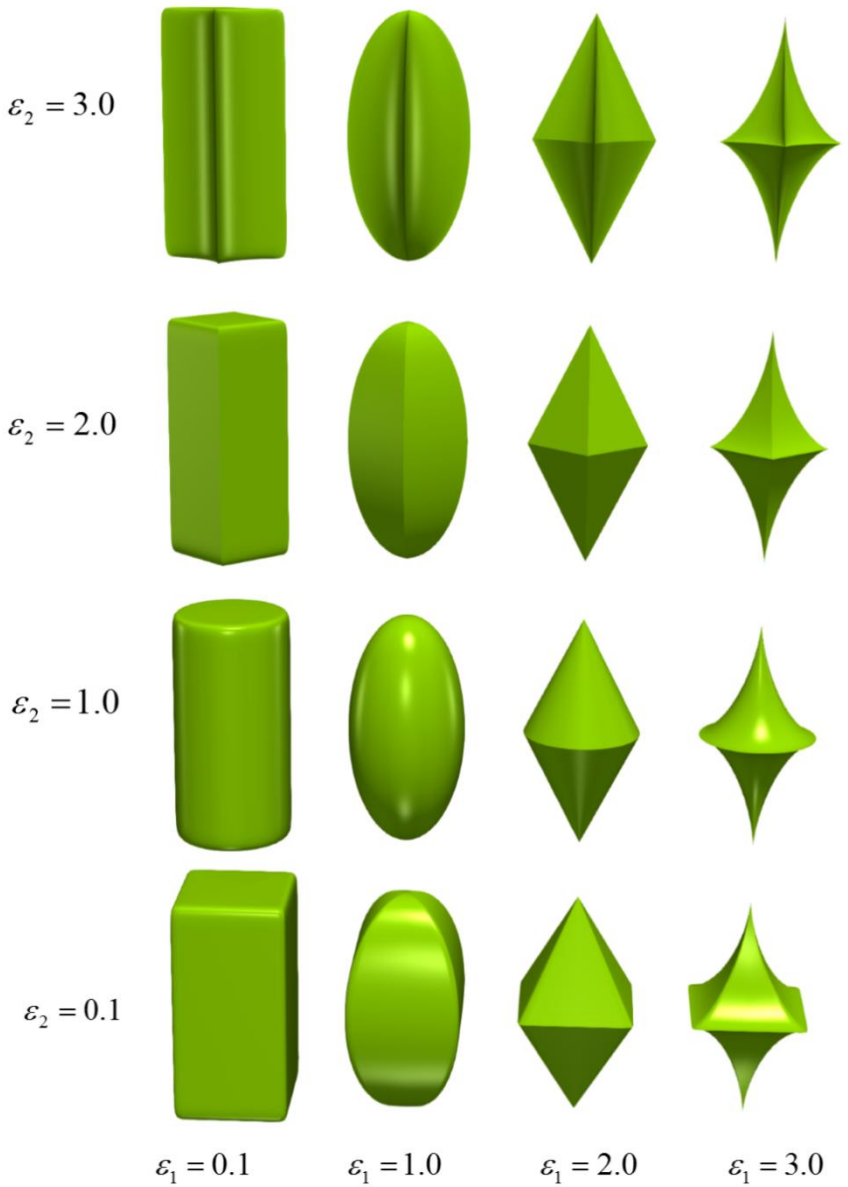
$$f(x,y,z) = \left[\left(\frac{x}{a}\right)^{\frac{2}{\varepsilon_2}} + \left(\frac{y}{b}\right)^{\frac{2}{\varepsilon_2}}\right]^{\frac{\varepsilon_2}{\varepsilon_1}} + \left(\frac{z}{c}\right)^{\frac{2}{\varepsilon 1}} - 1 = 0$$

$$[a, b, c, \varepsilon_1, \varepsilon_2]^T$$

Semi-axis

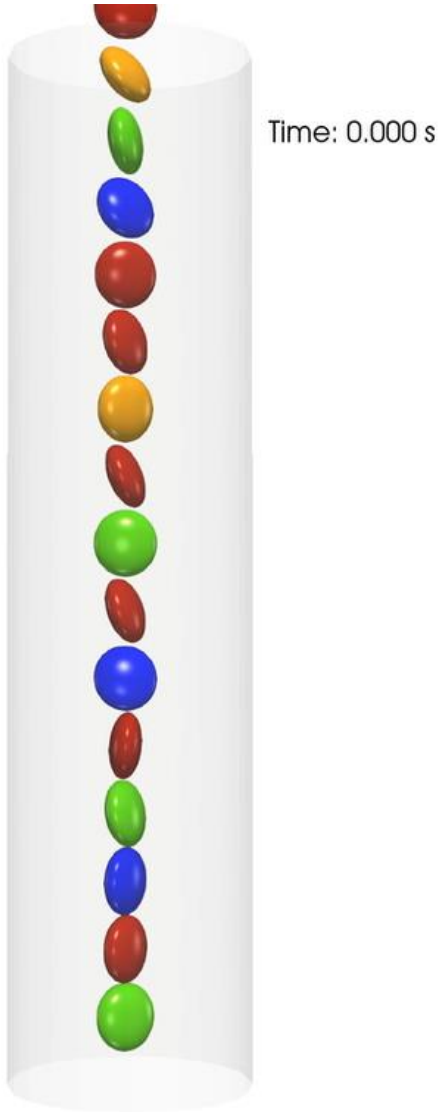
roundness parameters

- Can represent ~ 80% of all shapes by varying **five parameters**

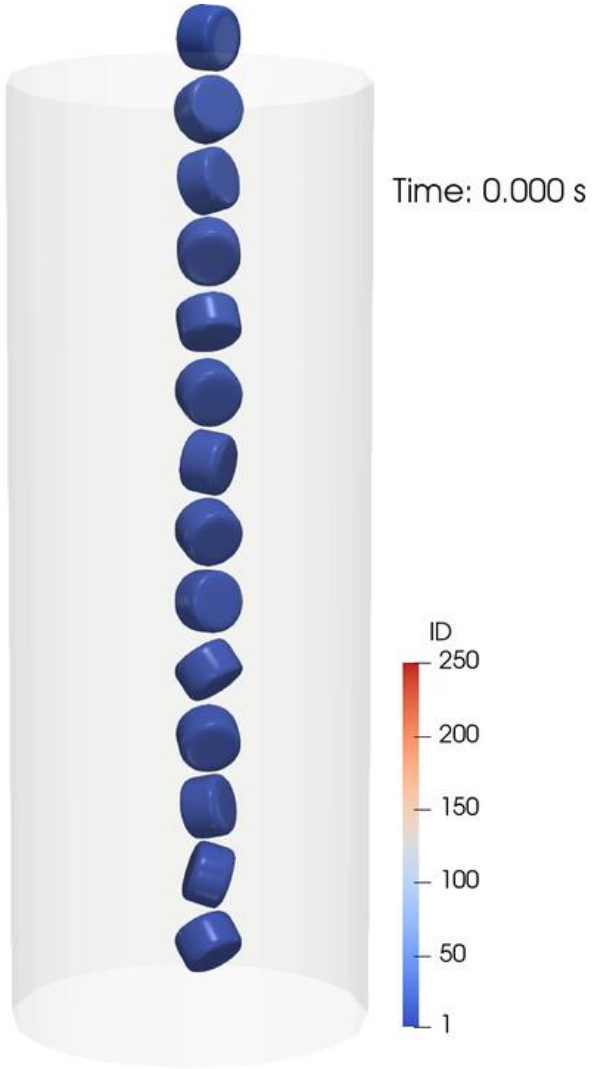


a1=2
a2=2
a3=4

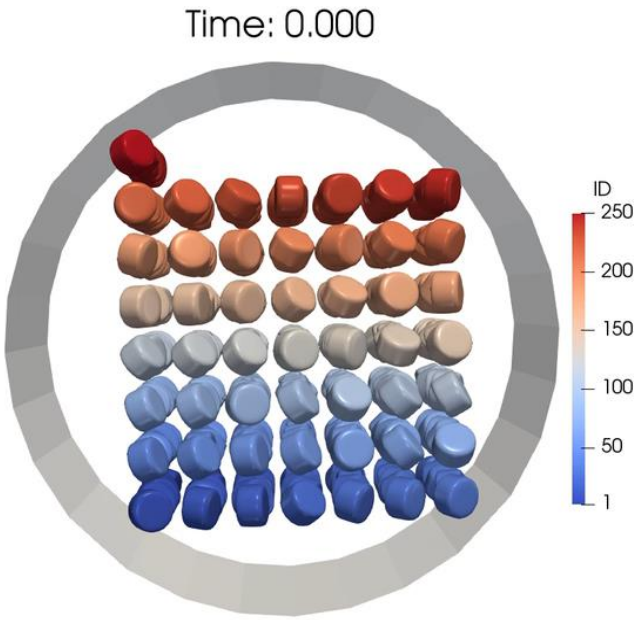
SuperDEM examples



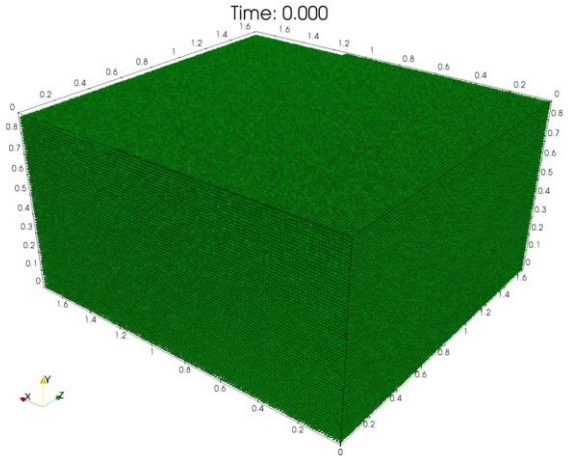
M&M candy static packing



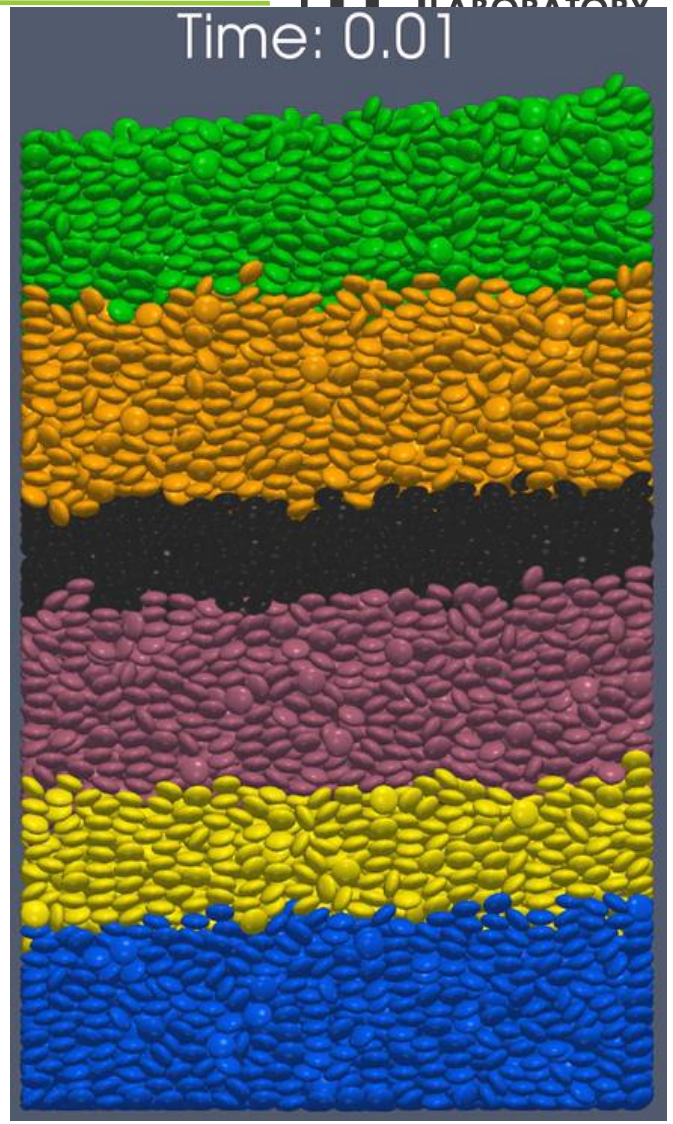
Cylinder candy static packing



Cylinder rotating drum



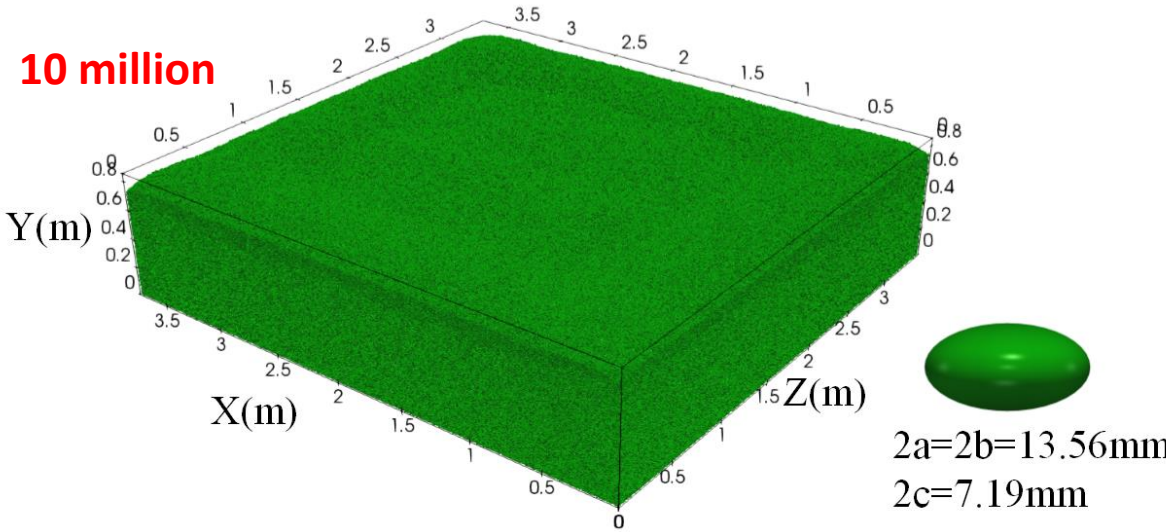
1 million non-spherical particles

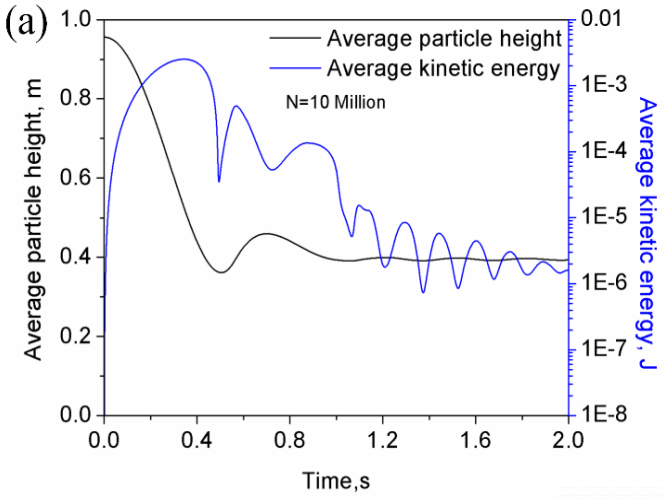


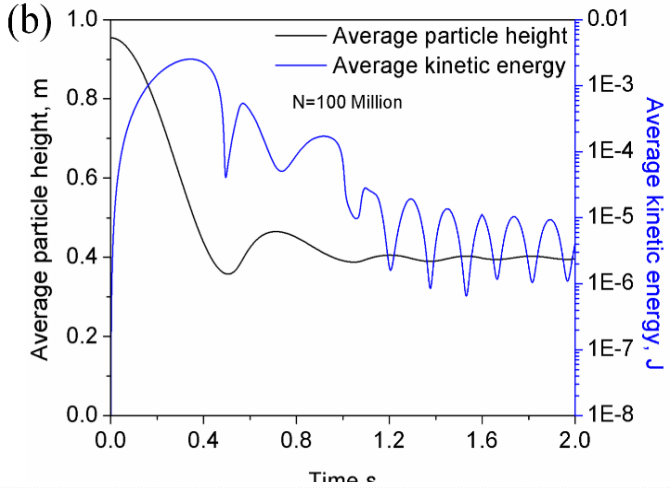
M&M candy discharging from a hopper

SuperDEM: large scale simulation example

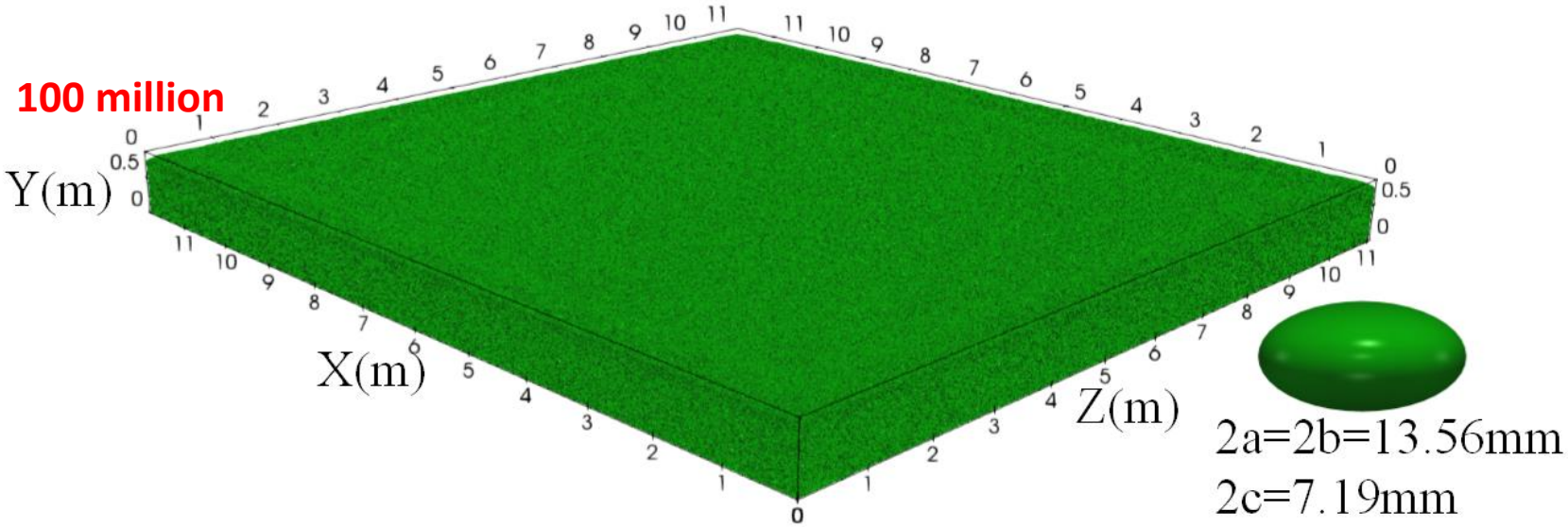
10 million

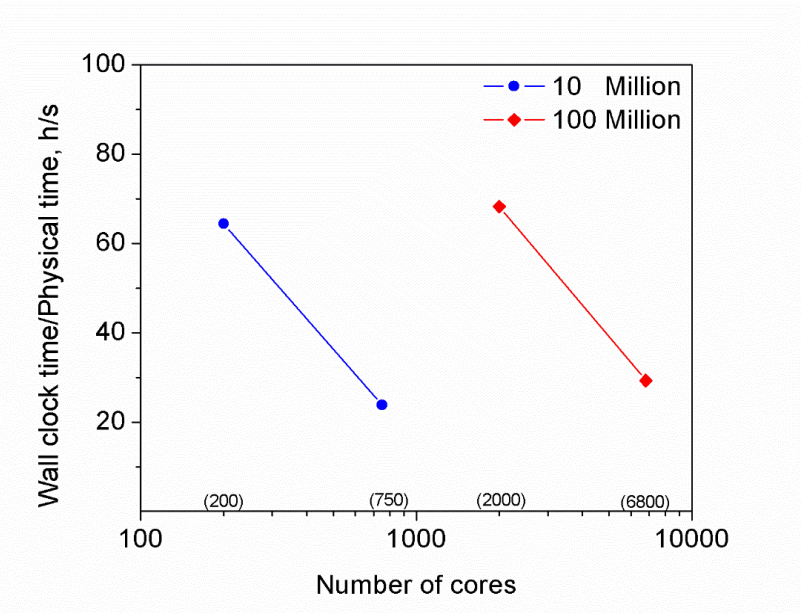




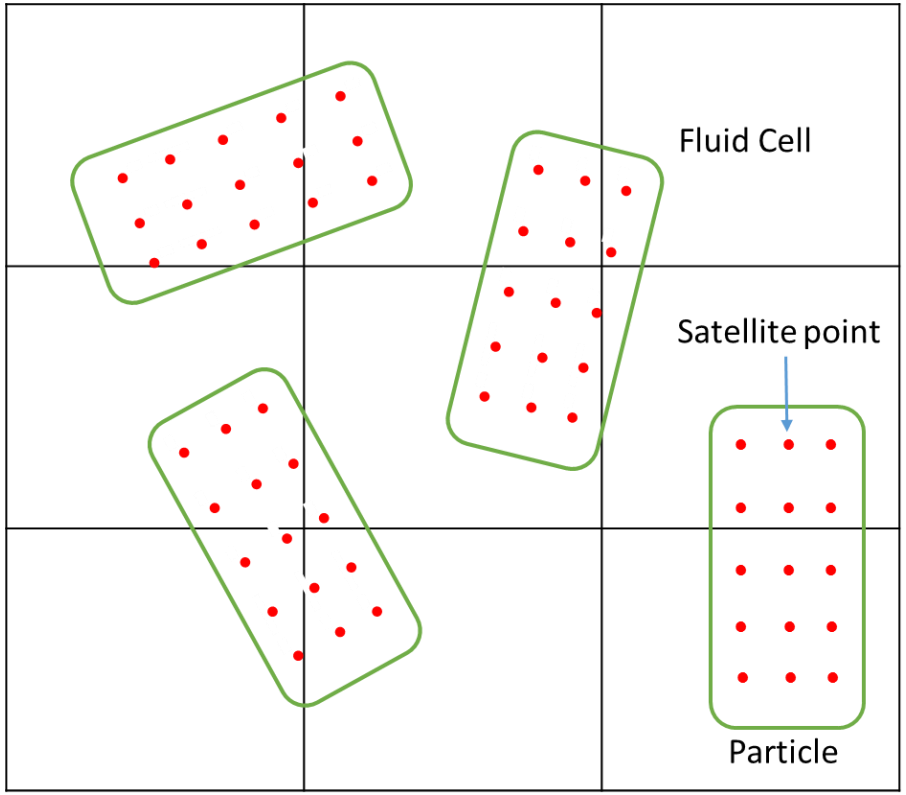


100 million

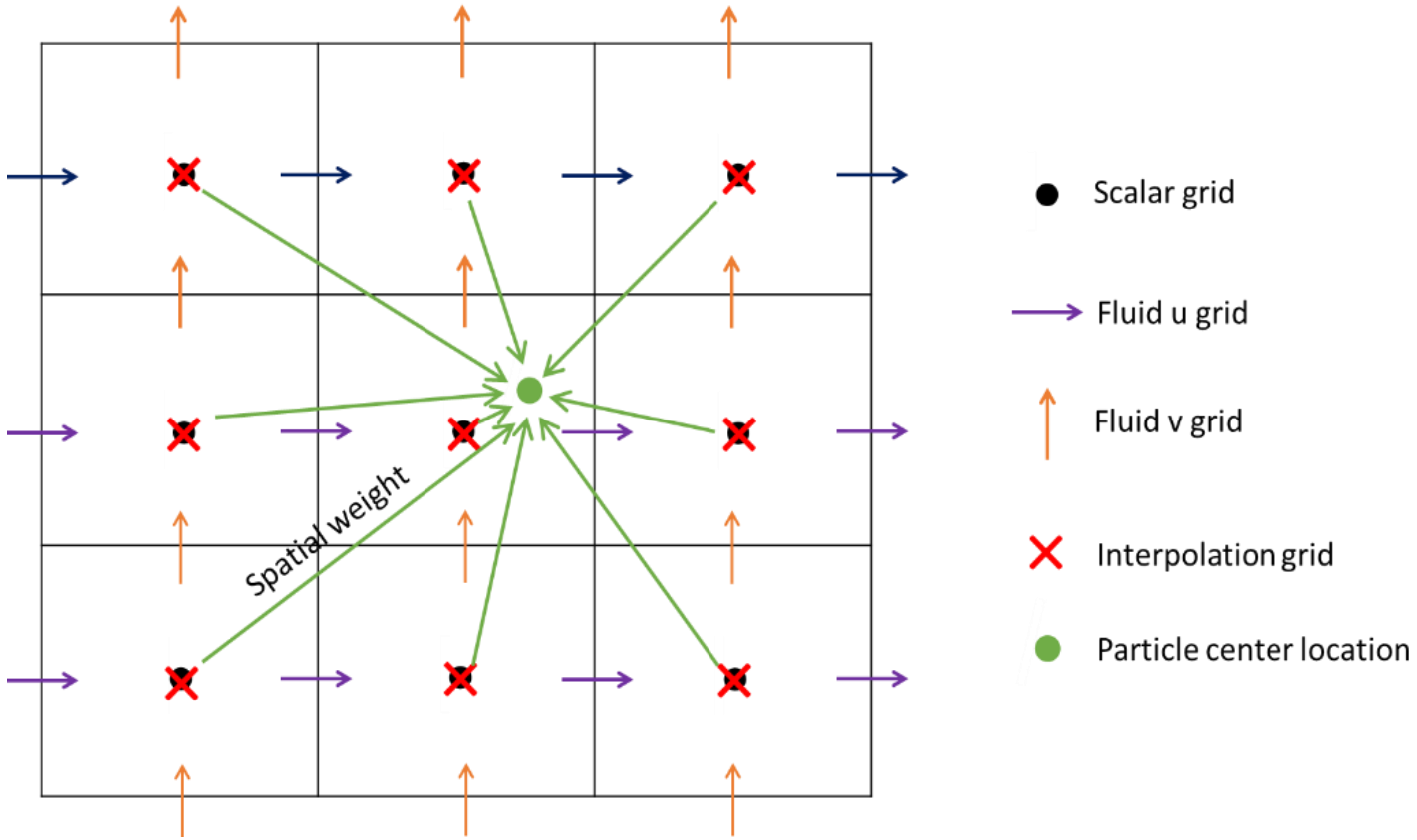




SuperDEM-CFD coupling: Non-spherical particles interpolation

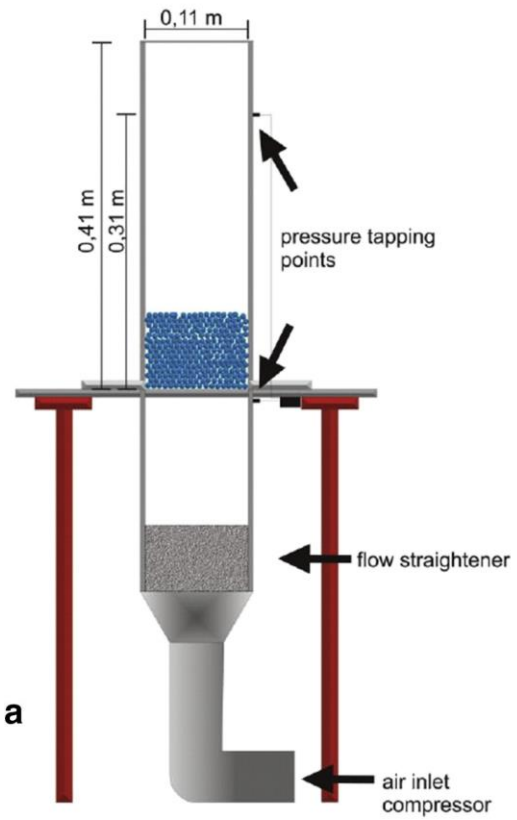


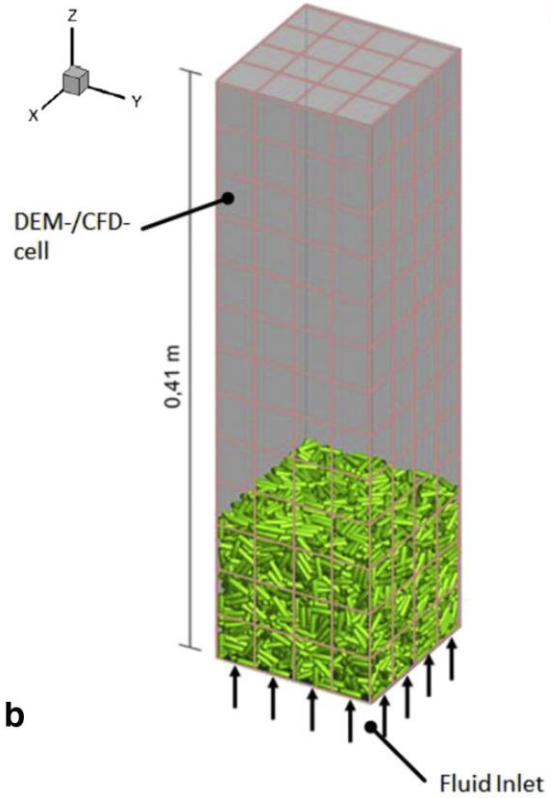
DPVM-satellites: Divided particle volume method for non-spherical particles based on a satellite point approach.



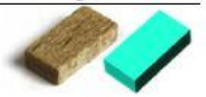
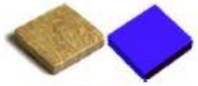
Schematic of the staggered grid scheme (only show 2-D for simplification). The fluid fields of neighboring 9 (2D) or 27 (3D) cells are interpolated to the particle center location to calculate particle drag force.

Validation experiment





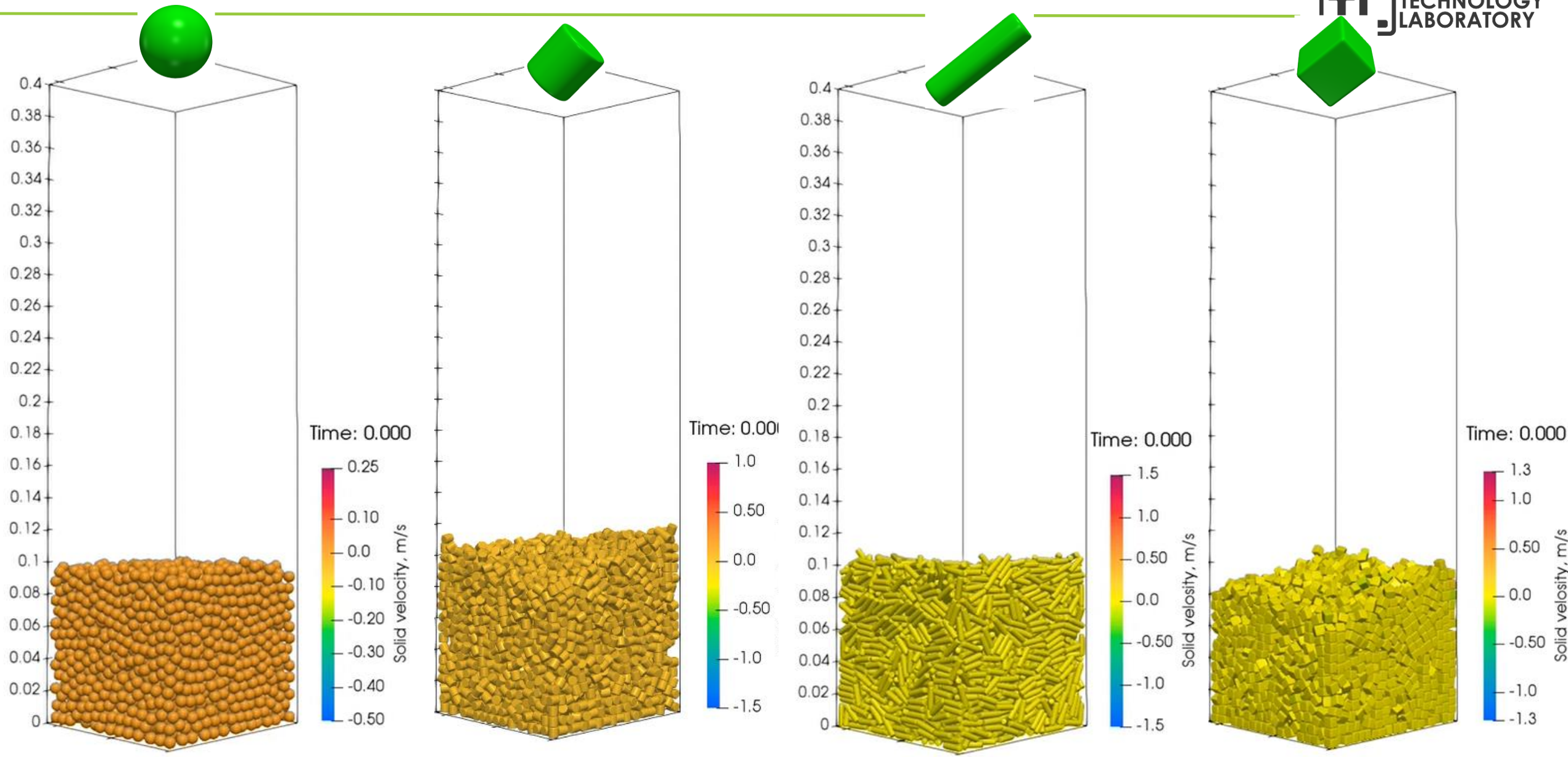
Particle properties including the volume equivalent diameter d_ε-*class*, the particle dimensions, the sphericity ϕ, the particle density ρ_p, the bed height L and the averaged porosity ε for the initial, unfluidized setup.

Shape	Sphere	Sphere	Ideal Cylinder	Cube	Cube
d_ε–class [mm]	7	5	7	5	7
Size [mm]	7.2	5	6.1 6.2	4.2 4.3 4.5	5.2 6.3 6.3
ϕ [–]	1.00	1.00	0.87	0.81	0.80
ρ_p [kg/m³]	772.5	823.0	708.5	639.7	746.9
L_{fb} [mm] / $\bar{\varepsilon}$ [–]	95 0.40	88 0.40	98 0.36	98 0.37	103 0.43
Shape	Elongated Cylinder	Elongated Cuboid	Elongated Cuboid	Plate	Elongated Plate
					
d_ε–class [mm]	7	5	7	5	5
Size [mm]	3.9 14.0	3.0 3.0 7.1	4.2 4.2 11.4	2.0 4.9 6.0	2.0 4.0 8.0
ϕ [–]	0.75	0.75	0.73	0.71	0.69
ρ_p [kg/m³]	764.4	745.6	639.7	754.1	756.6
L_{fb} [mm] / $\bar{\varepsilon}$ [–]	103 0.44	103 0.42	115 0.40	102 0.43	108 0.46
Shape	Elongated Cuboid	Plate	Elongated Plate		
					
d_ε–class [mm]	5	7	7		
Size [mm]	2.0 3.0 11.0	2.2 9.0 9.8	2.0 6.0 14.9		
ϕ [–]	0.64	0.63	0.58		
ρ_p [kg/m³]	728.1	672.8	721.7		
L_{fb} [mm] / $\bar{\varepsilon}$ [–]	117 0.48	121 0.46	124 0.51		

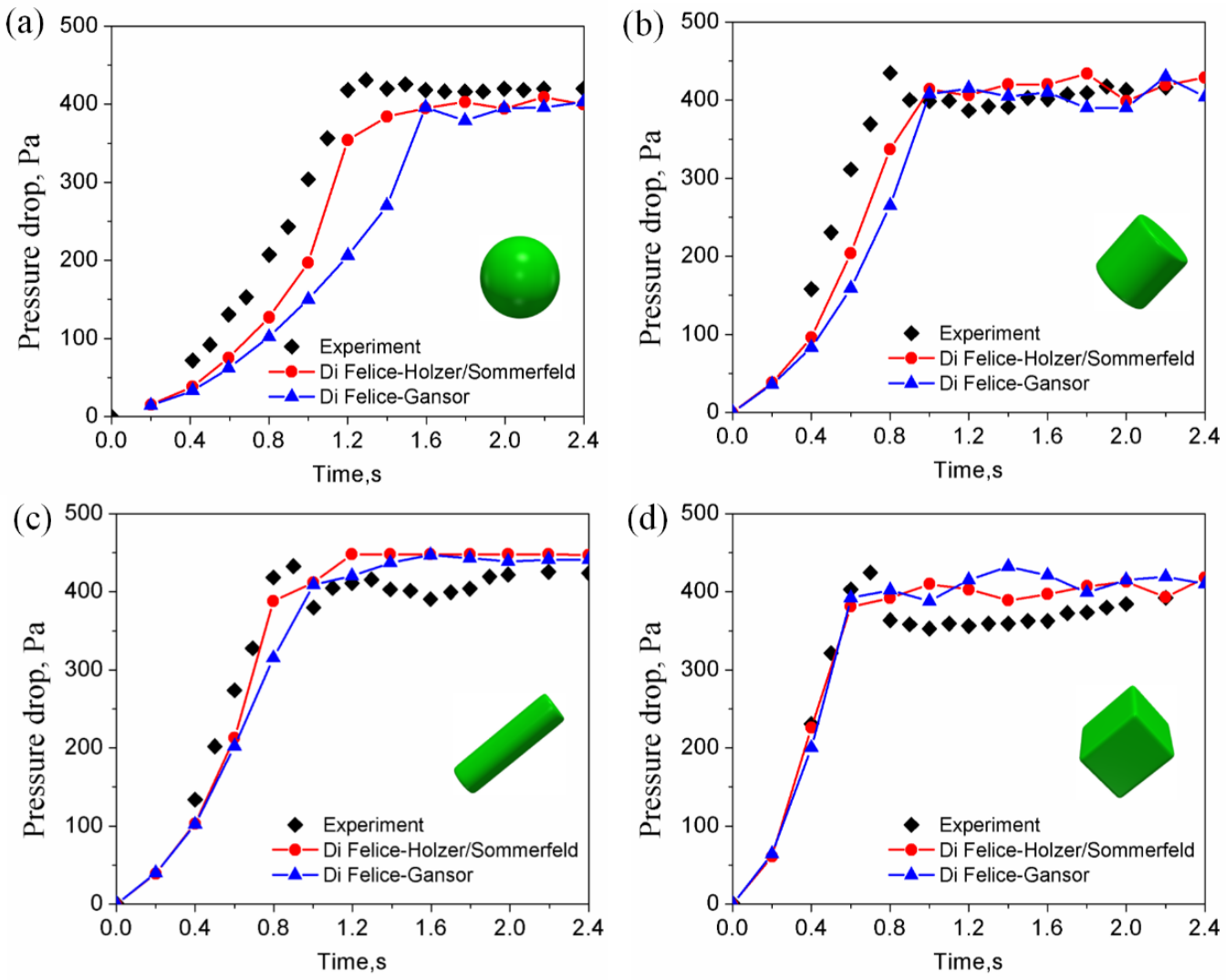
Experiment: Vollmari K, Jasevičius R, Kruggel-Emden H. Experimental and numerical study of fluidization and pressure drop of spherical and non-spherical particles in a model scale fluidized bed. Powder Technology. 2016;291:506-521.

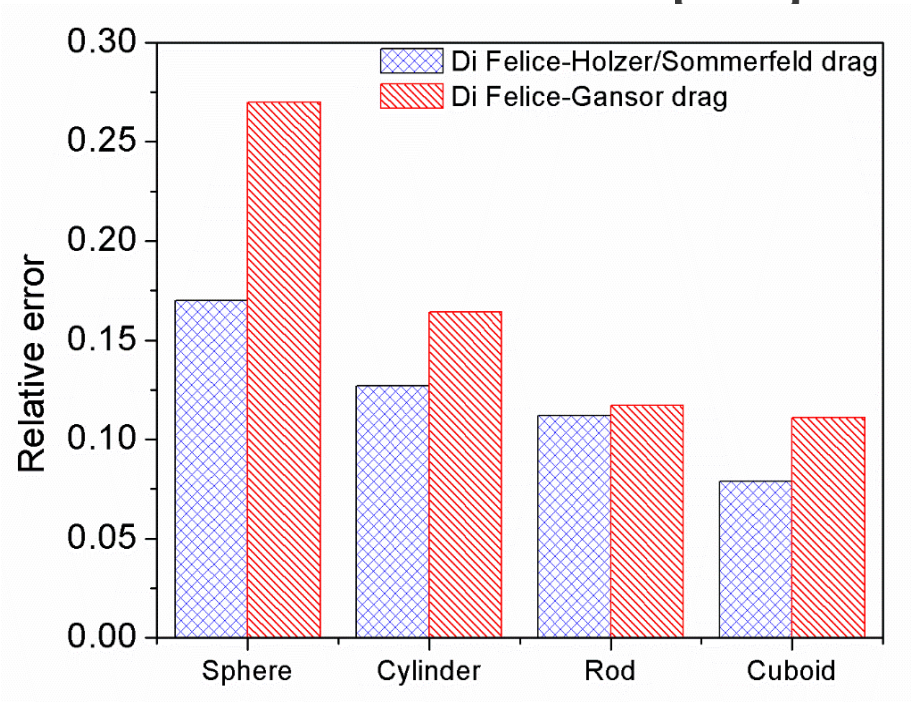
Fluidization of particles with different shapes

Ug=1.6 m/s



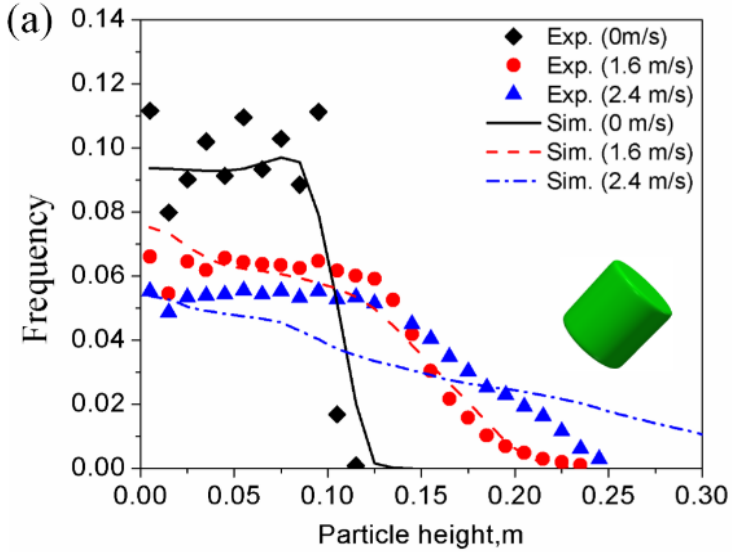
Validation-Pressure drop

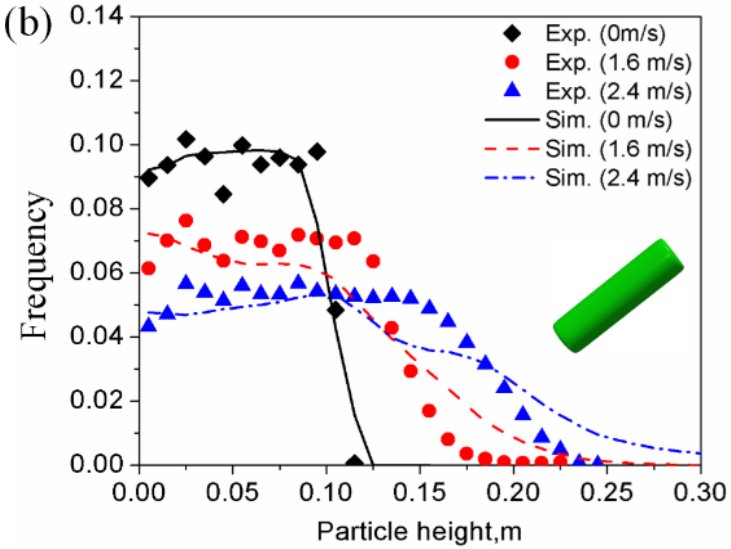


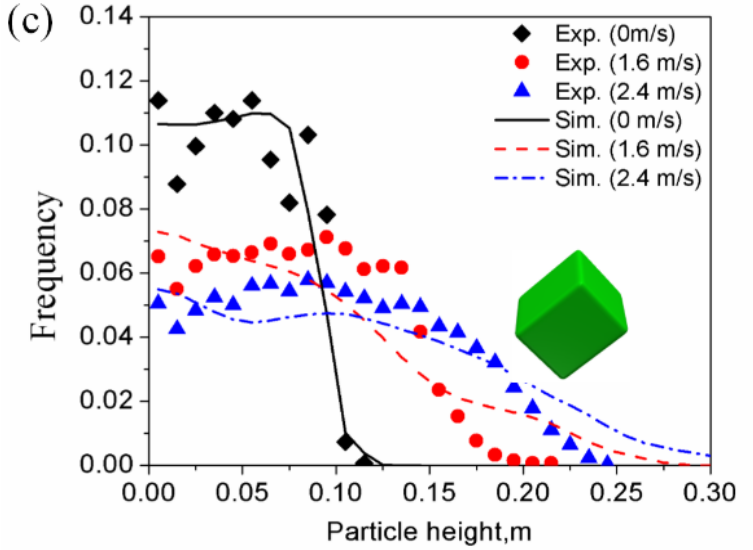


- Both drag models consider the effects of particle orientation and cell voidage
- Di Felice-Holzer/Sommerfeld drag correctly capture the pressure in both fixed bed and fluidized bed regimes for each shape particles.
- Unresolved SuperDEM-CFD can not capture the channeling flow. Particle-resolved DEM-CFD may be tested in the future.

Validation-Particle height distribution

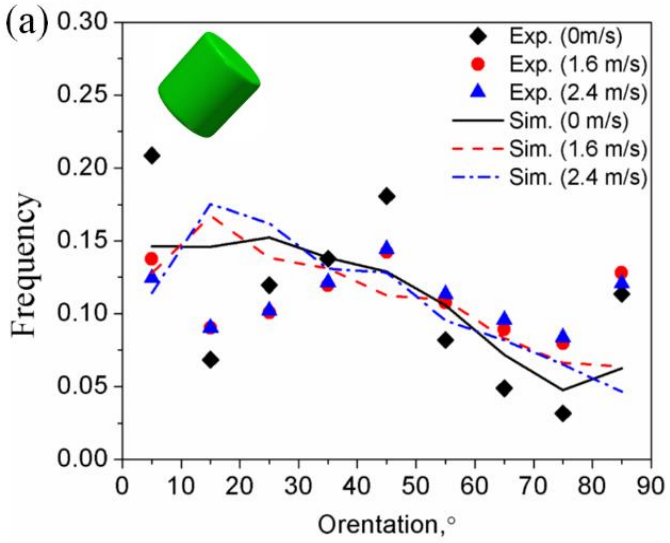


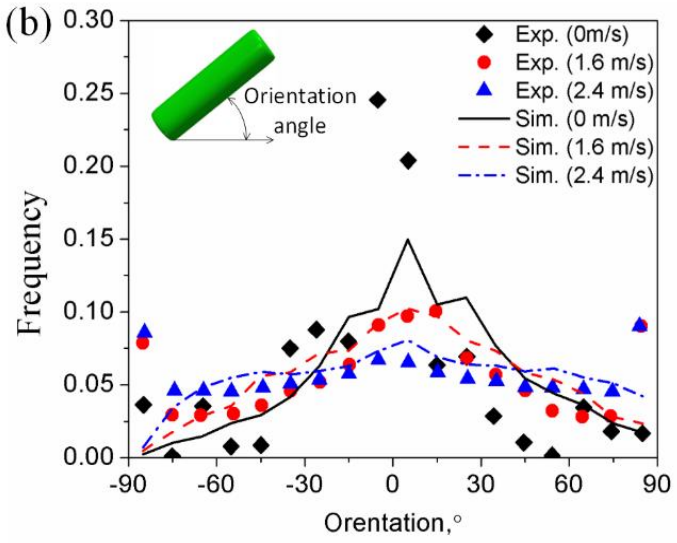


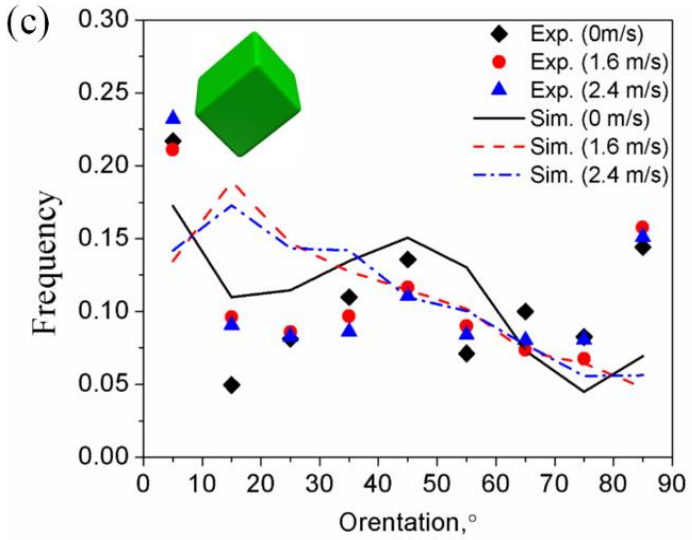


- SuperDEM-CFD correctly predict the particle height distribution at different gas velocities.
- Slight over predicted the expansion bed height as higher gas velocity.

Validation-Particle orientation distribution

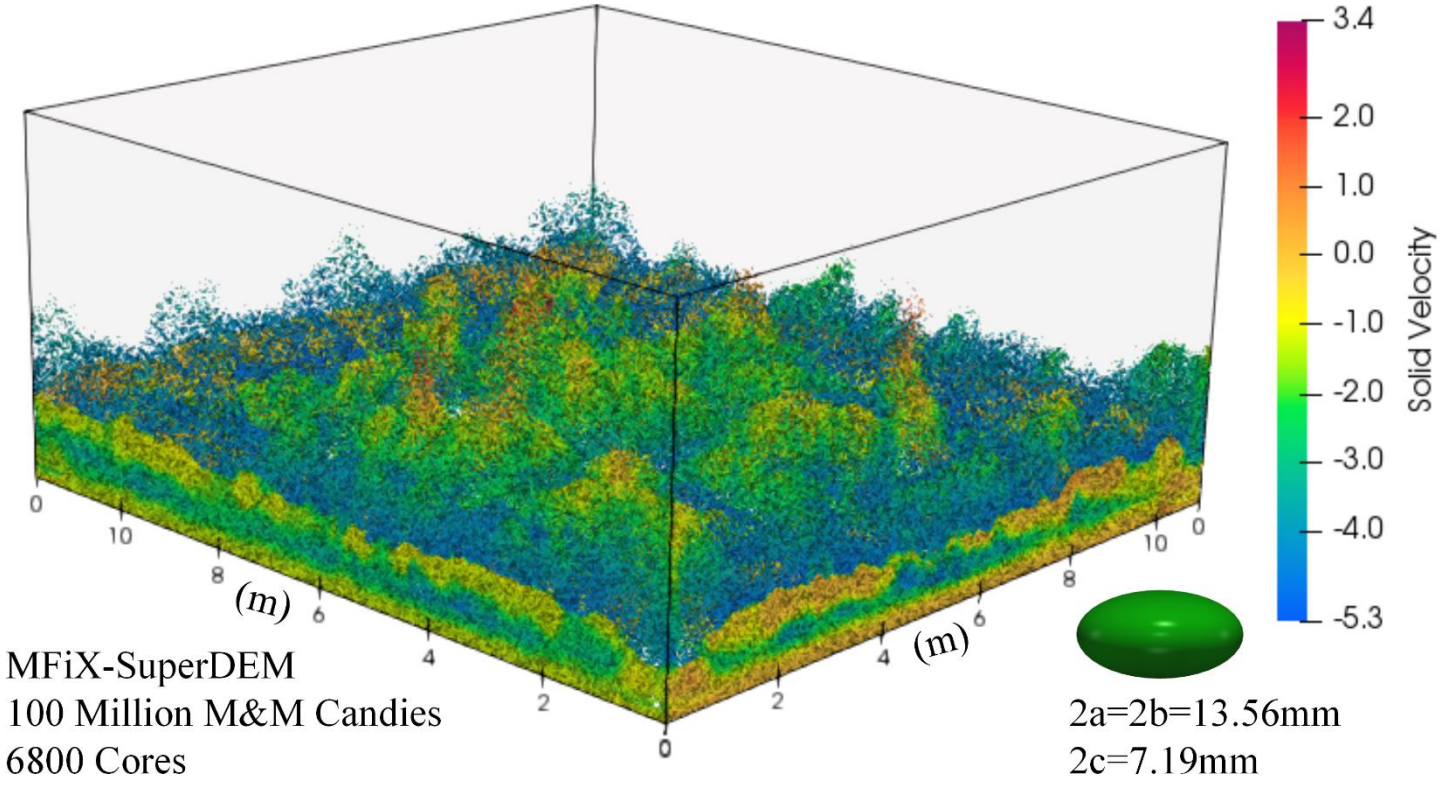


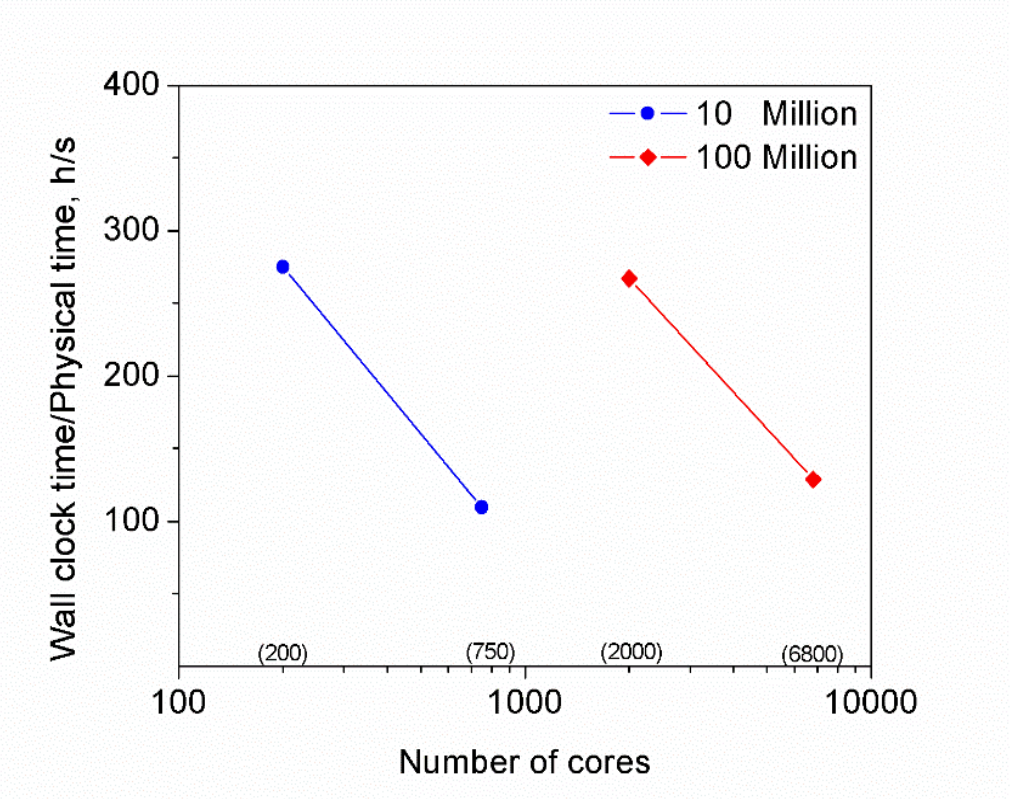




- For rod, with an increase of superficial gas velocity, the fraction of sanding up particles increase, and the fraction of laying down particles decreases
- The ideal cylinder and cuboid do not show a decrease of the fraction of laying down particles with the increasing of gas velocity.
- The SuperDEM-CFD correctly reproduced the behavior.

Massively Parallel SuperDEM Simulation





- The solver was paralleled using MPI.
- Simulation on NETL supercomputer Joule 2 (80K cores) , World Top 60, 2020
- Non-spherical particles fluidization simulation, 100 million (6800 cores)

Summary and Future Work

- **Summary**
  - Oriented bounding box (OBB) algorithm has been implemented and verified
  - Superquadric contact algorithm has been implemented and verified
  - Quaternion theory for object orientation (rotation between local and global) has been implemented and verified
  - VTP (xml) was modified to output tensor for superquadric particle visualization
  - Superquadric particle collision with wall (plane, STL)
  - Non-linear forces between superquadric particles
  - Parallelization (MPI)
  - 100 million non-spherical particles large scale simulation on 6800 cores
  - A new interpolation scheme (DPVM-Satellites) was developed.
  - Non-spherical drag models (Di Felice-Gansor and Di Felice Holzter/SommerFeld) considering particle orientation and cell voidage were implemented
  - A new general scheme to calculate the projection area of non-spherical particle perpendicular to the flow was developed.
  - 100 million non-spherical particles fluidization simulation on 6800 cores

- **Future work**
  - Heat transfer, mass transfer, chemical reaction
  - Coupling with other sub-models
  - Multi-superquadric particles to model moving internals, such as baffle, moving wall, etc.
  - Advanced superquadric contact algorithm

Reference

1. Gao, X*., Yu, J., Lu, L., Li, C., Rogers, W. Development and validation of SuperDEM-CFD coupled model for simulating non-spherical particles hydrodynamics in fluidized beds. Chemical Engineering Journal, accepted for publication, 2020.

2. Gao, X*., Yu, J., Portal, R., Dietiker, J.F., Shahnam, M., Rogers, W. Development and validation of SuperDEM for non-spherical particulate systems using a superquadric particle method. Particuology, In revision, 2020.

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4. Gao, X., Yu, J., Portal, R., Rogers, W.A. Superquadric particle method for non-spherical DEM simulation in open source MFiX: development, implementation and verification. AIChE 2019 Annual Meeting, Pittsburgh, Orlando, Nov 2019.

5. Gao, X., Yu, J., Lu, L., Li, C., Rogers, W. Superdem-CFD: Open Source Parallel Solver for Non-Spherical Particle-Fluid Fluidization Systems. AIChE 2020 Annual Meeting, San Francisco, Nov 2020.

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