Air-induced defect formation during powder compaction

William Zunker, Sachith Dunatunga, and Ken Kamrin
Department of Mechanical Engineering
Massachusetts Institute of Technology

IFPRI AGM 2024

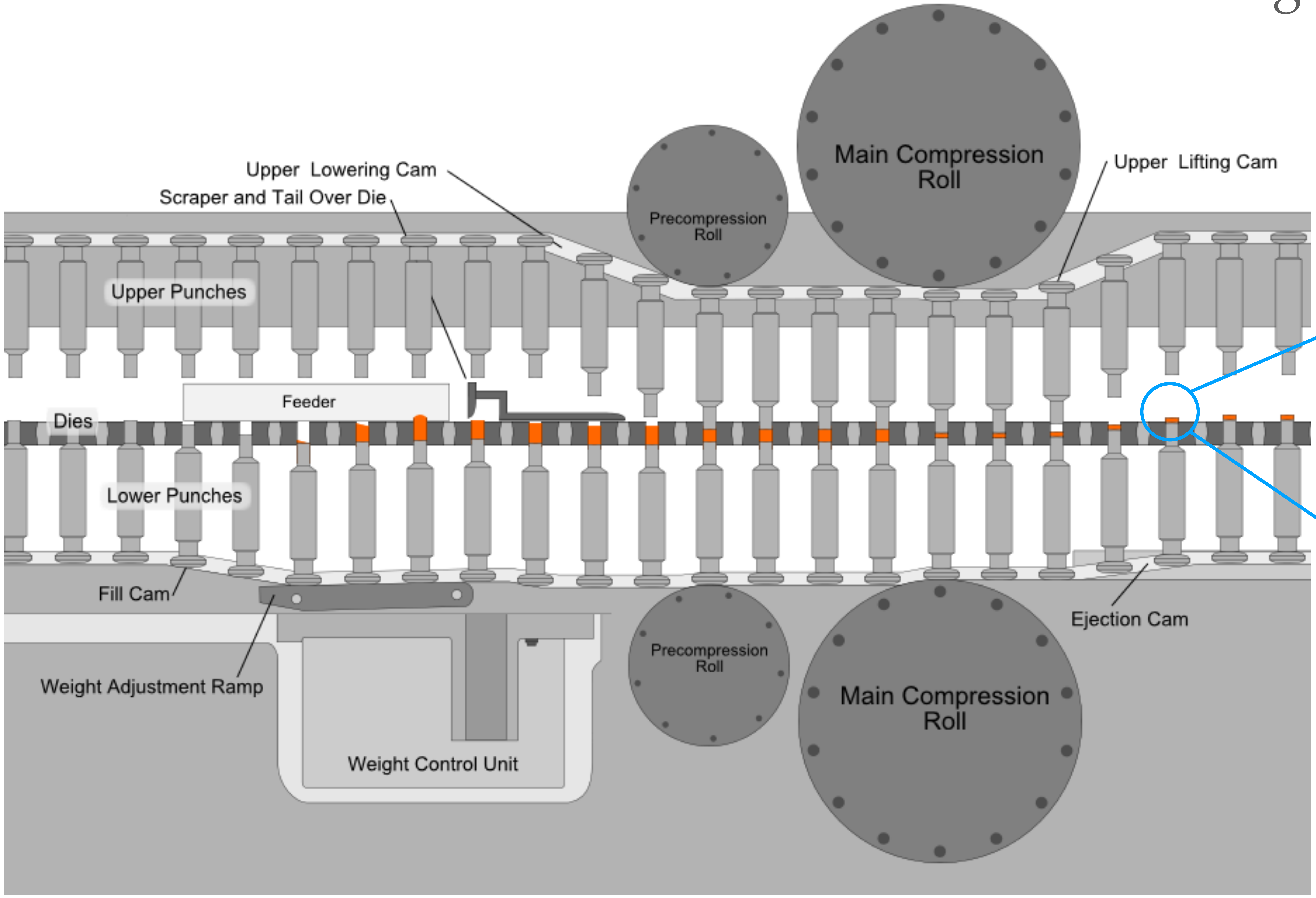
IFPRI
International Fine Particle Research Institute

MITMECHE

Project motivation

Use mechanics-based approach to predict defect formation in tableting.

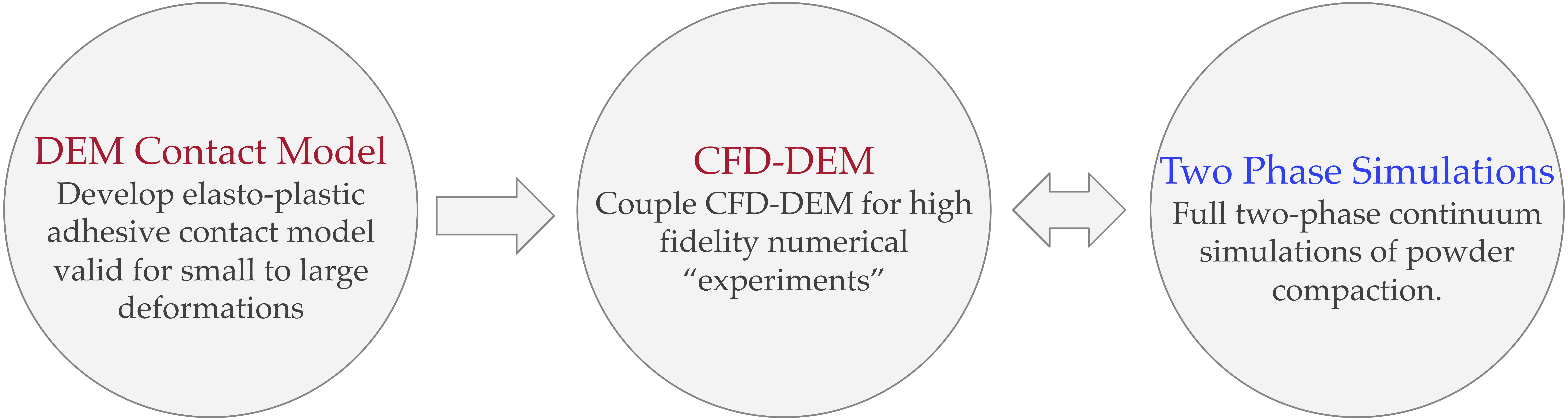
Question: What drives the fracturing process? Entrapped air? Inhomogeneous residual grain stress?



Capping / lamination

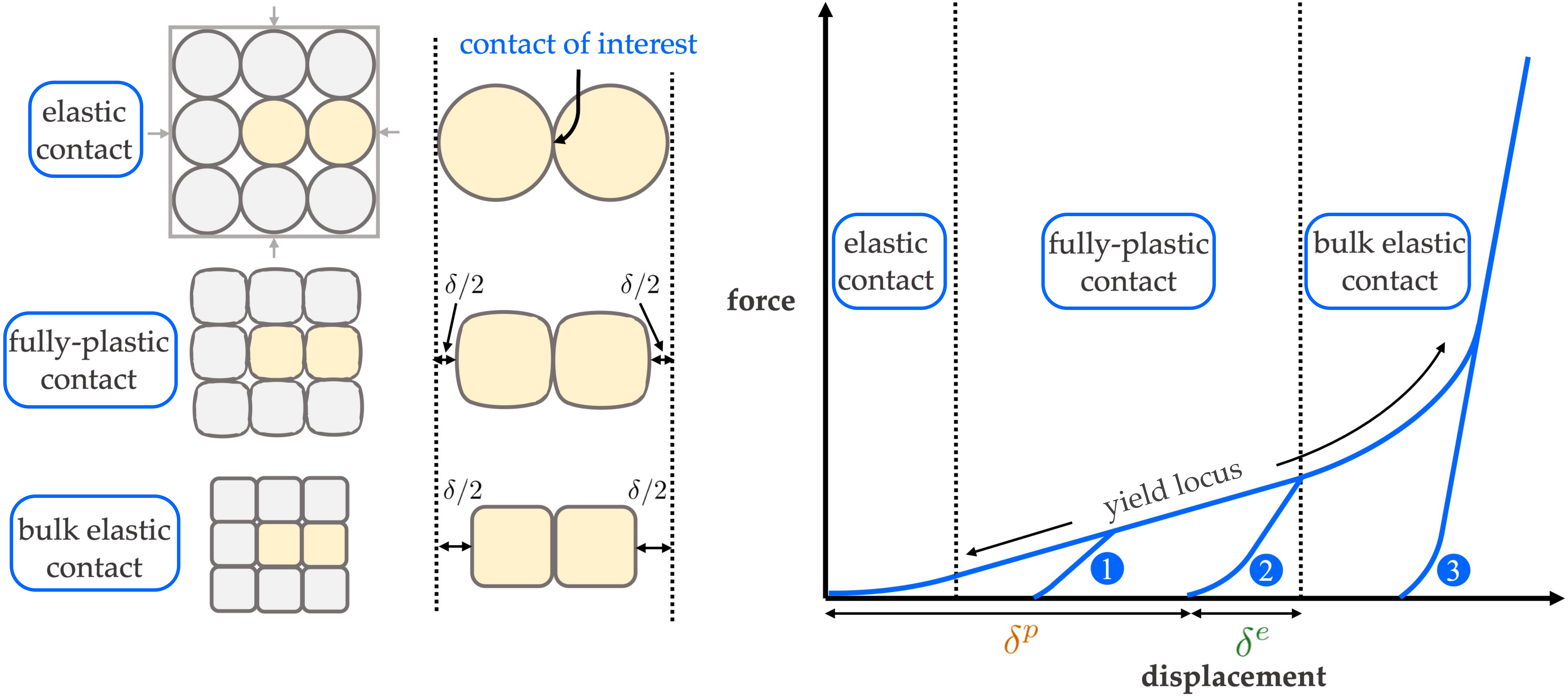
Cracking

Project workflow



Discrete / Continuum
Fully Continuum

Elastic-plastic particle behavior during powder compaction

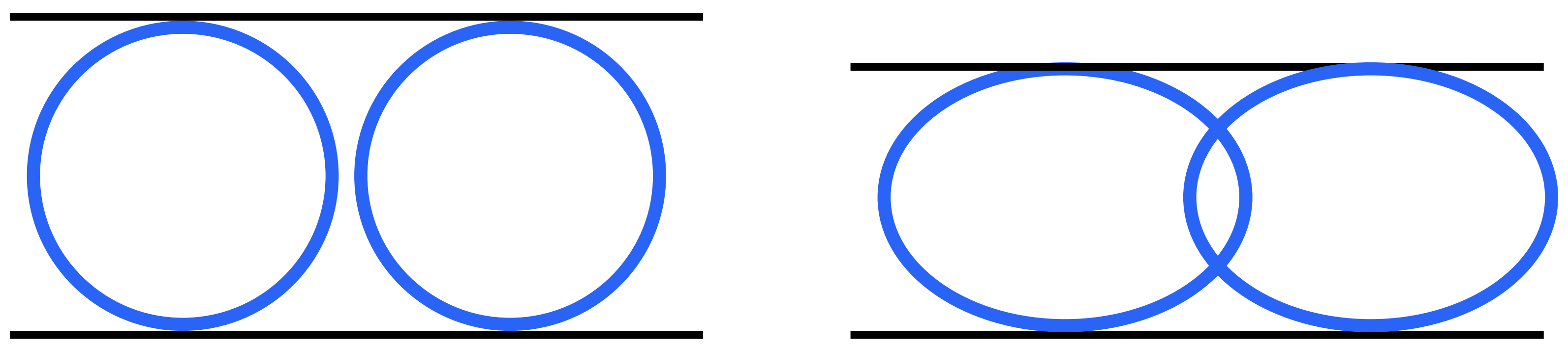


adhesion leads to tensile forces during unloading before separation

Previous contact models and their relevant features

Authors	Regimes	min(E/Y)	Unloading	Adhesion	Multi-neighbor dependent
Chang et al., 1987	E, FP	1000	no	no	no
Storåkers et al., 1997	FP	rig. plas.	no	no	no
Mesarovic and Johnson, 2000	FP	10000	yes	yes	no
Zhao et al., 2000	E, FP	1000	no	no	no
Jackson and Green, 2003 and 2005	E, FP	1000	no	no	no
Etsion et al., 2005	E, FP	300	yes	no	no
Harthong et al., 2009	E, FP, BE	1000	no	no	yes
Zait et al., 2010	E, FP	500	yes	no	no
Brake, 2012	E, FP	300	yes	no	no
Gonzalez et al., 2012 and 2018	E	n.a.	yes	no	yes
Olsson and Larsson, 2013	E, FP	1000	yes	yes	no
Frenning, 2013 and 2015	E, FP, BE	50	no	no	yes
Brodu et al., 2015	E	n.a.	yes	no	yes
Rathbone et al., 2015	E, FP	160	yes	no	no
Garner et al., 2018	E, FP, BE	100	yes	yes	yes
Gonzalez, 2019	E, FP	100	yes	yes	no
Edmans and Sinka, 2020	E, FP	1	yes	no	no
Giannis et al., 2021	E	n.a.	yes	no	yes
Giannis et al., 2021	E, FP, BE	n.r.	yes	yes	yes
Zhang et al., 2022	E, FP	79.4	no	no	no
Xu and Zhu, 2023	E, FP	400	no	no	no

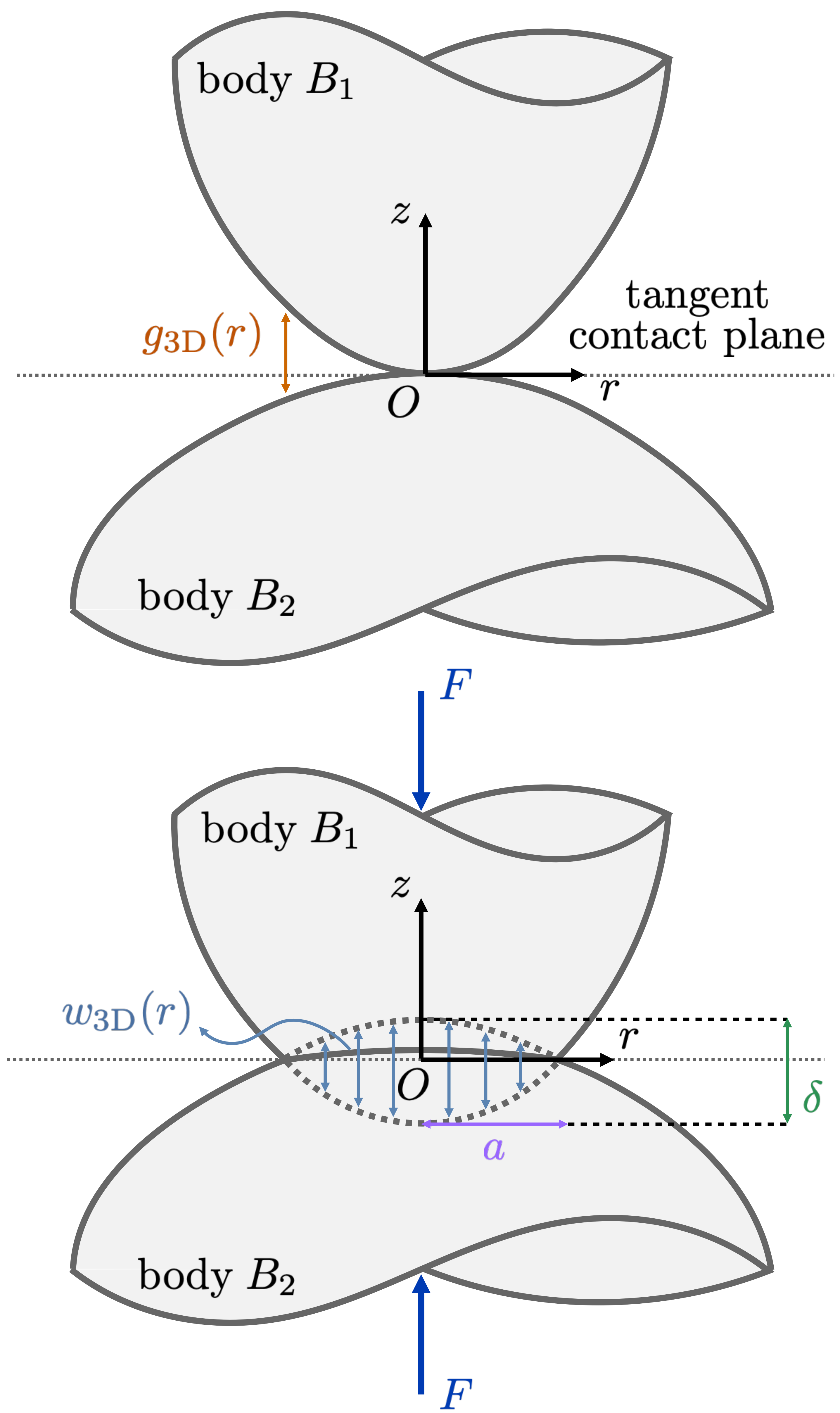
Multi-neighbor dependent effects



- **entirely empirically fitted**, no use of physical principles to determine contact law
- **requires refitting** for each new material being modeled.
- **no information beyond the force-displacement** is provided.

The method of dimensionality reduction (MDR): Popov and Heß

3D elastic axisymmetric contact



total force, contact radius, and displacement are the same between 3D problem and 1D counterpart

$$F = \int_{-a}^{a} q_{1D}(x)\,dx$$

$$= 2\pi \int_{0}^{a} p_{3D}(r) r\,dr$$

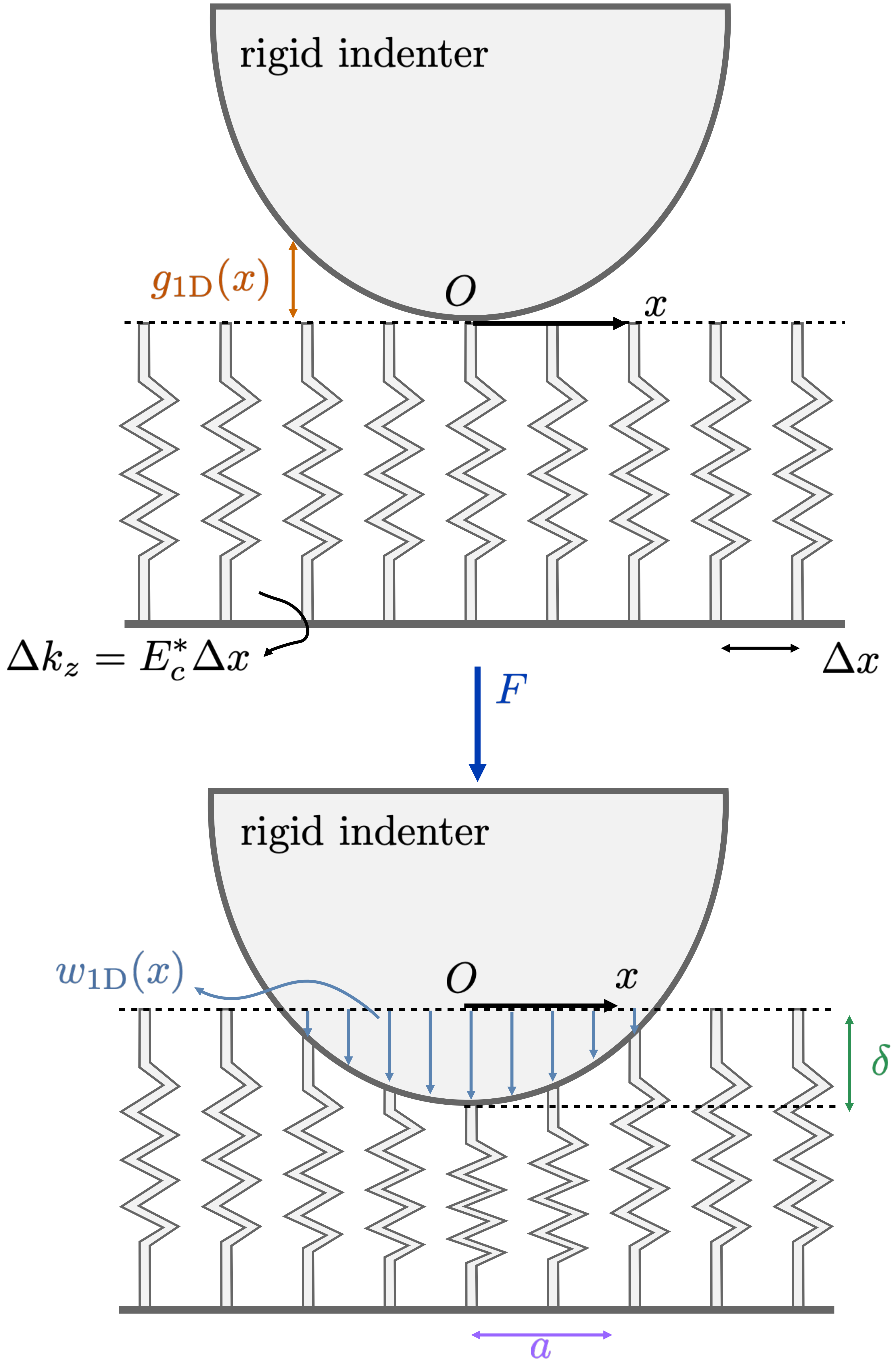
<u>**integral transforms**</u>

$g_{3D}(r)$ ⟷ **gap function** ⟷ $g_{1D}(x)$

$w_{3D}(r)$ ⟷ **normal disp.** ⟷ $w_{1D}(x)$

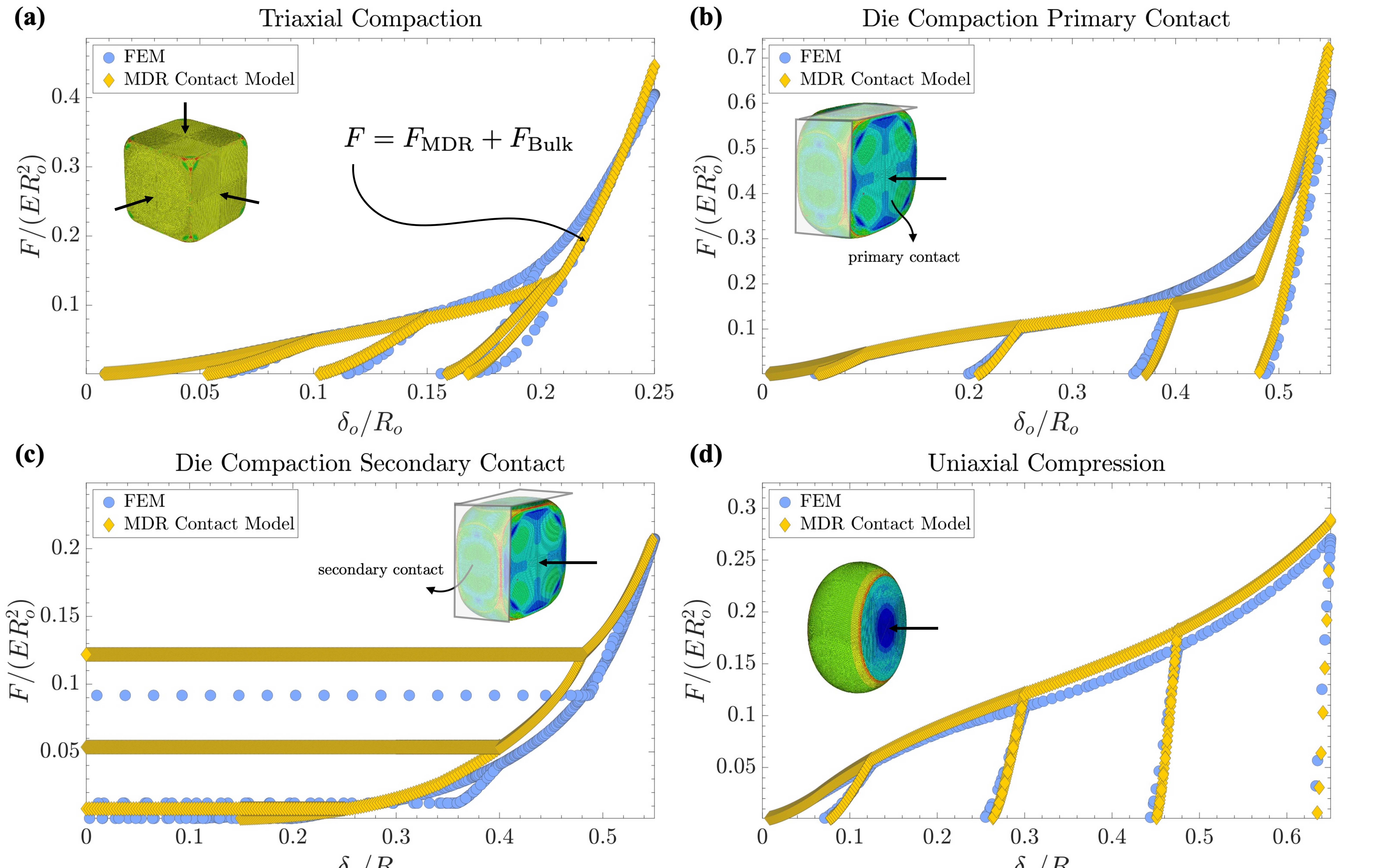
$p_{3D}(r)$ ⟷ **pressure** ⟷ $q_{1D}(x)$

1D Winkler foundation



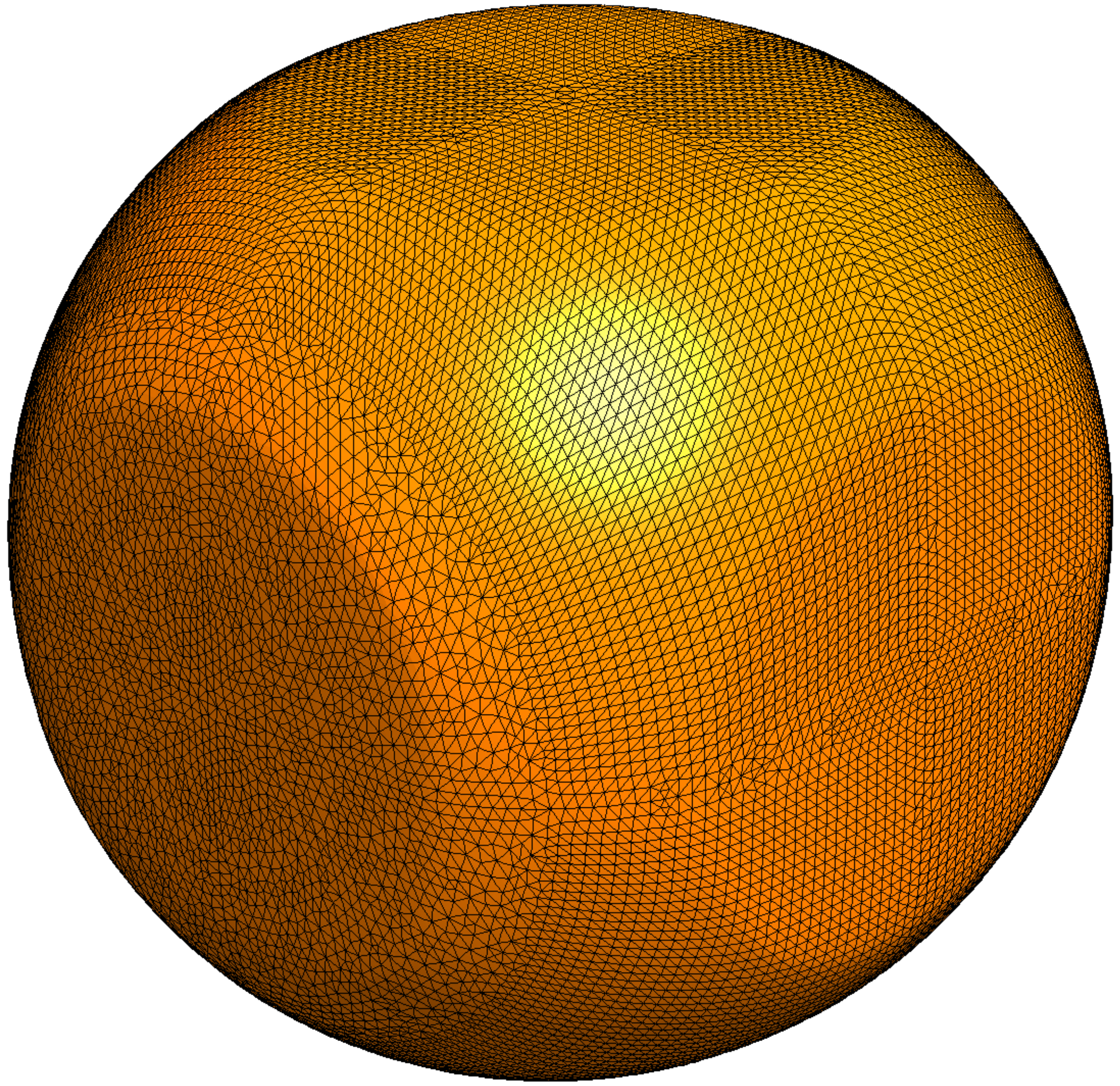
Single elastic-plastic contact—3D and 1D evolution

MDR contact model **force**-displacement curves, all loadings

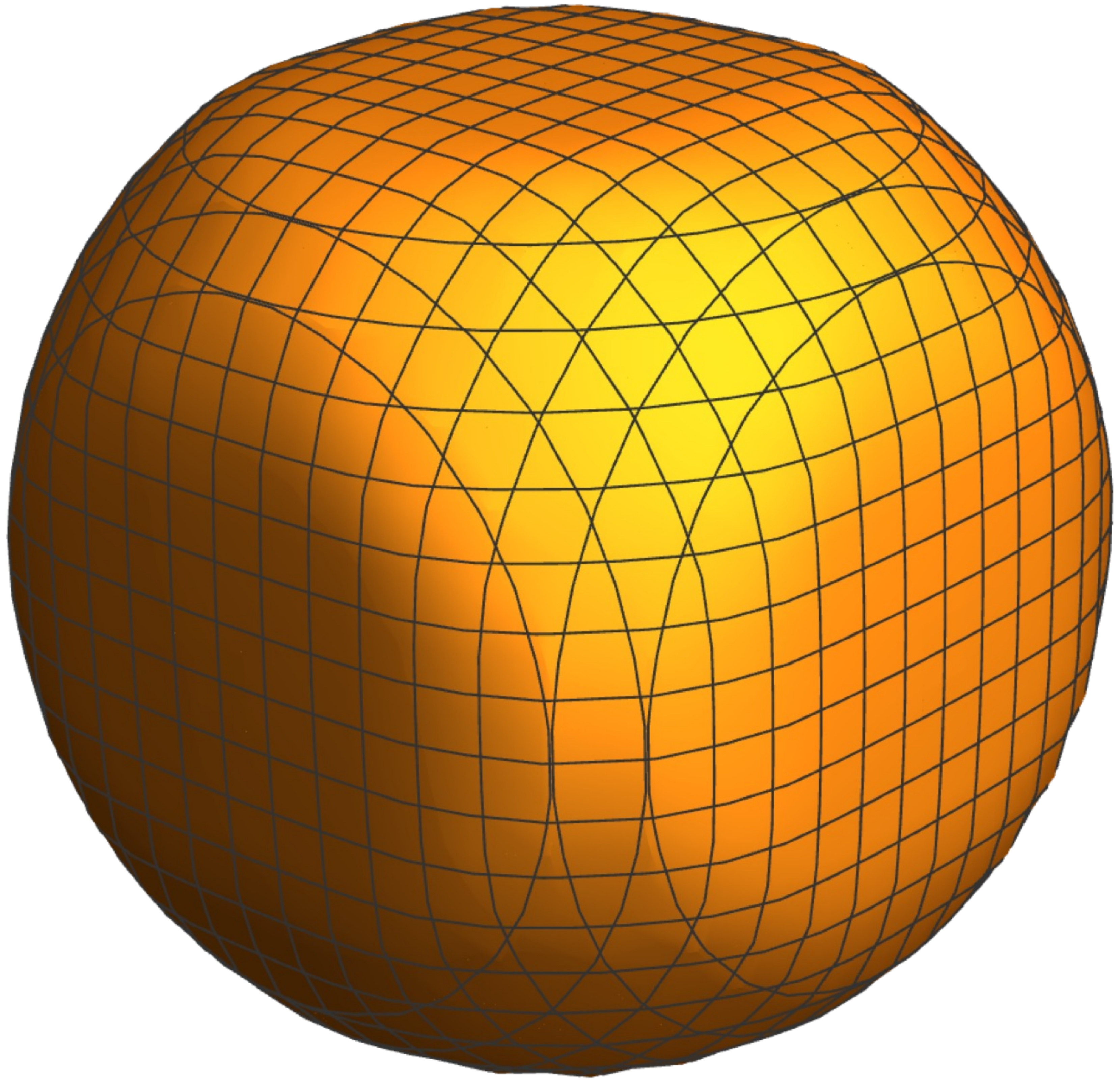


Deformed particle visualization

finite element



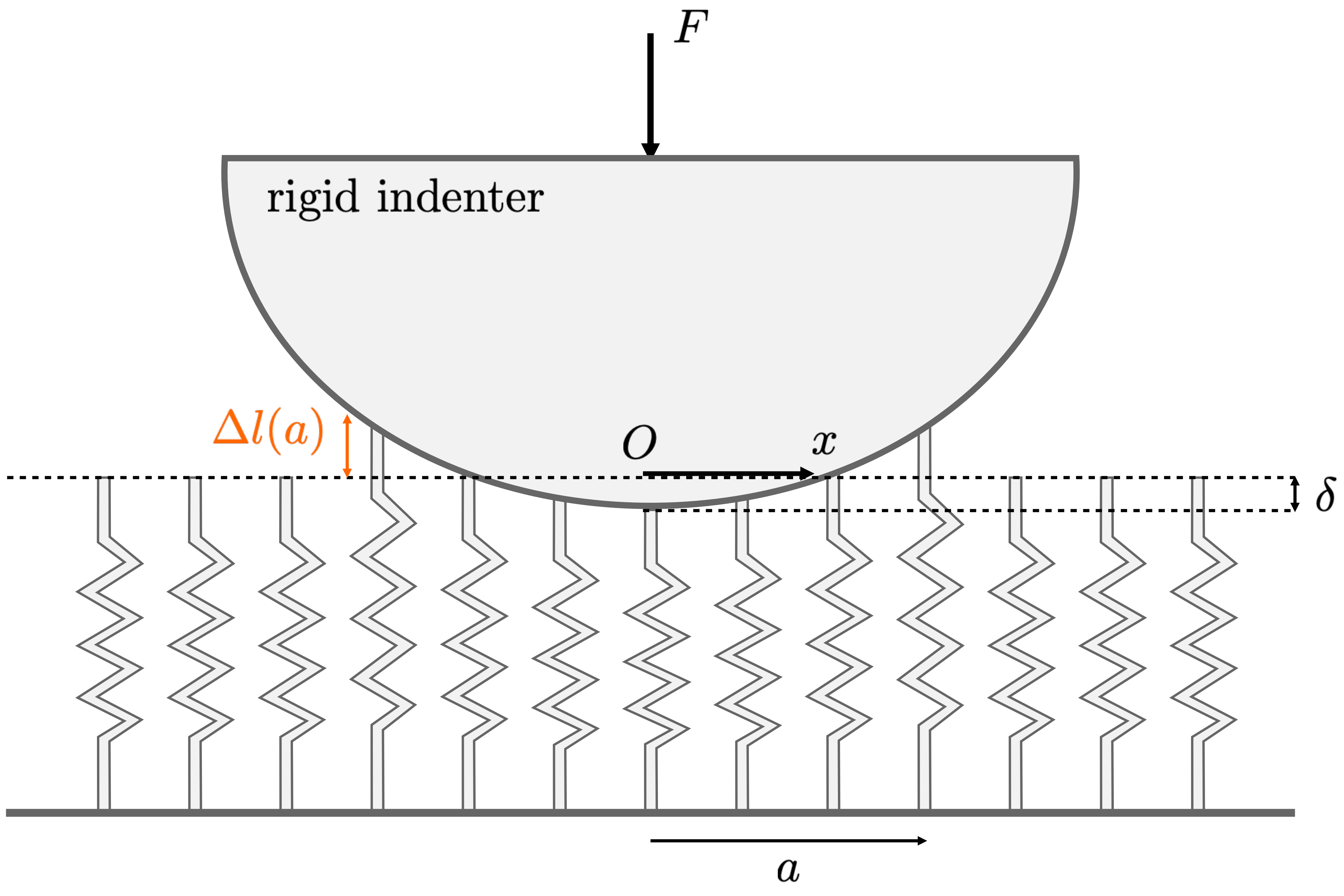
MDR contact model



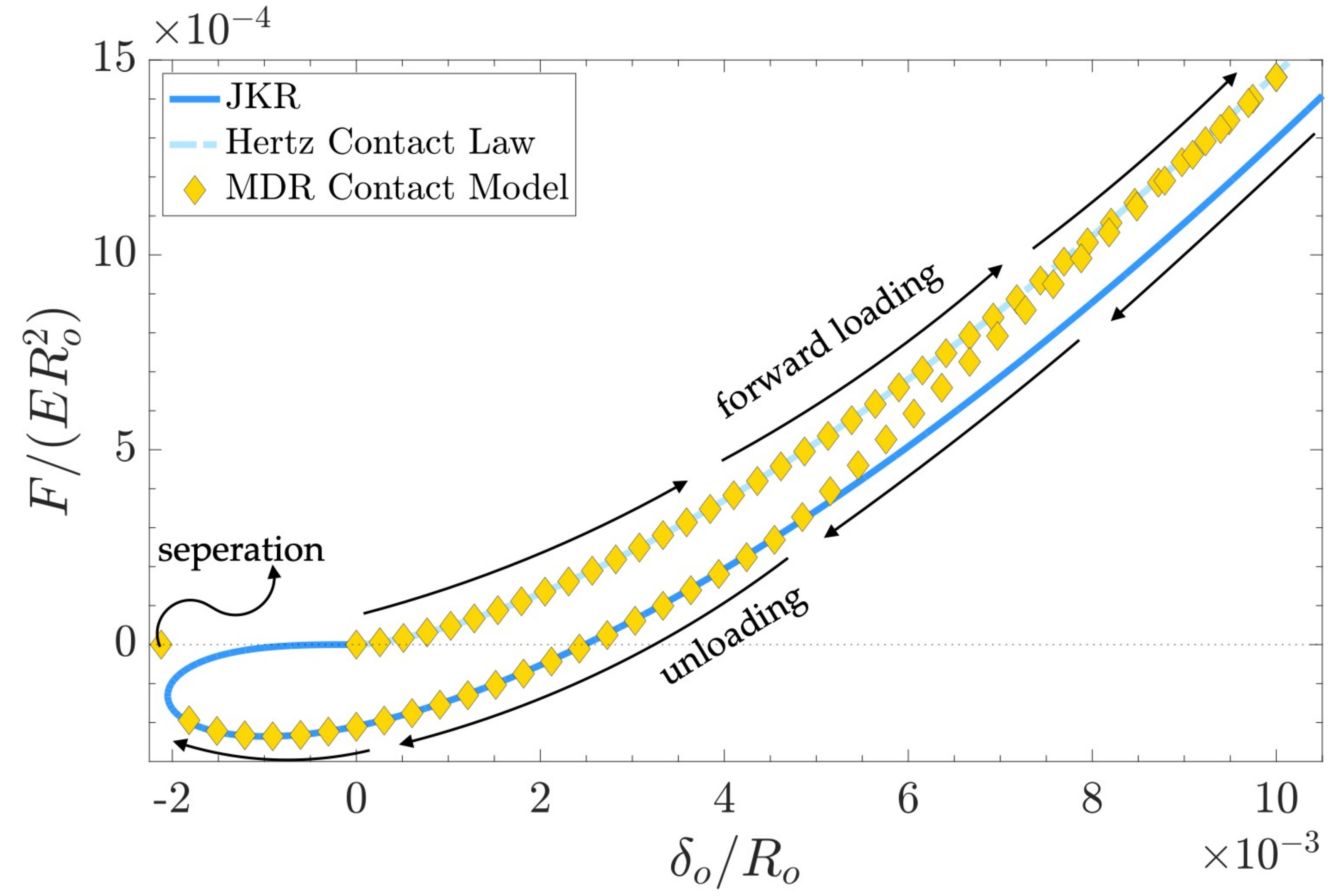
Plastic deformation, contact areas, and volume are accurately tracked, allowing for accurate reconstruction of the deformed particle

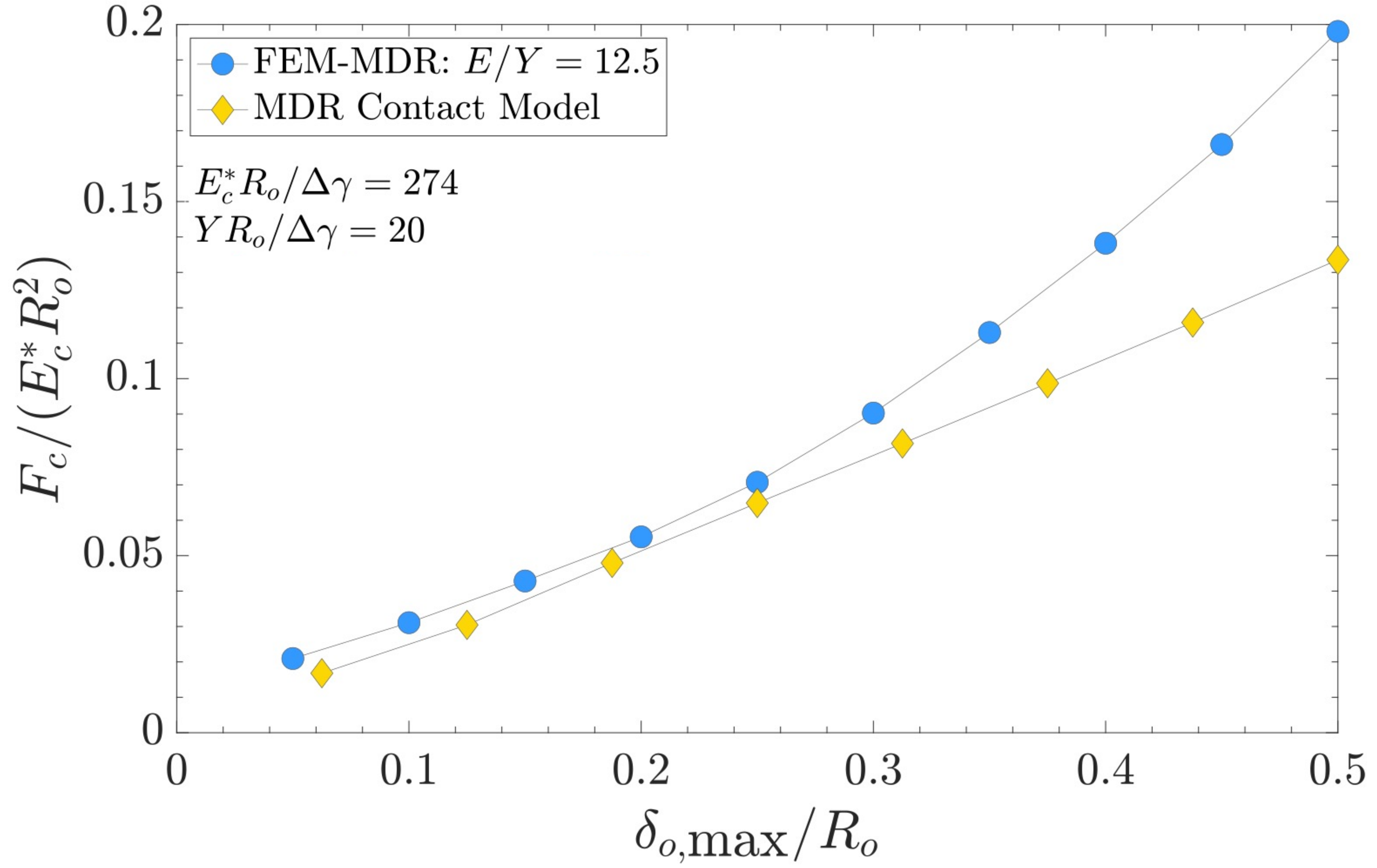
Johnson, Kendall, Roberts (JKR) theory of adhesion in the MDR

sticky springs with critical extensional length



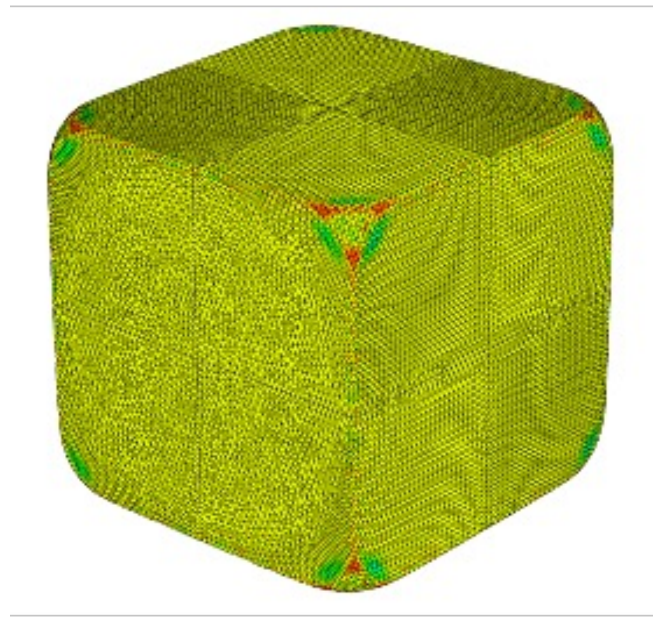
$$\Delta l(a) = \sqrt{\frac{2\pi a \Delta\gamma}{E_c^*}}$$



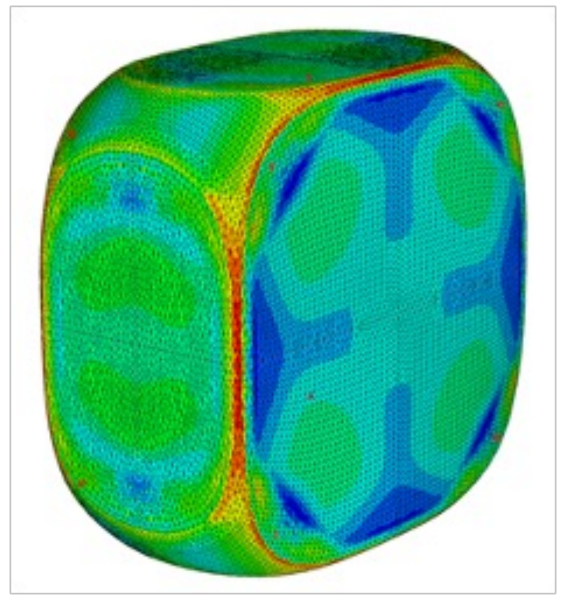


From single to many-interacting particles

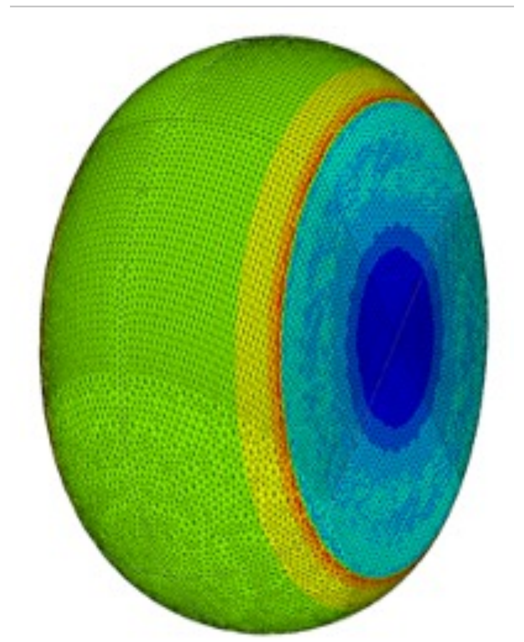
So far, we have only considered simple symmetric loading of single particles and rigid flats:



triaxial compaction



die compaction

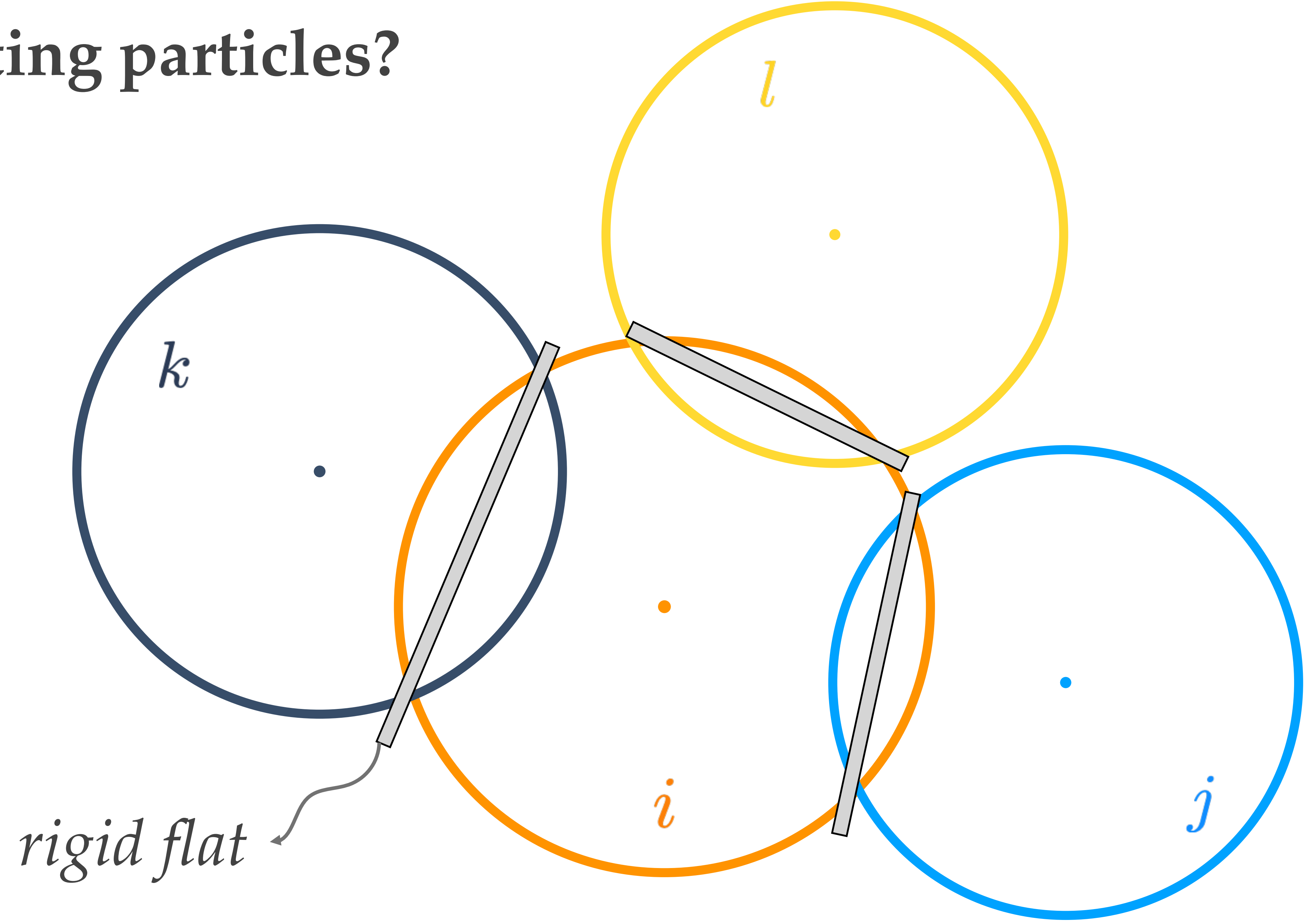


uniaxial compression

How do we handle many interacting particles?

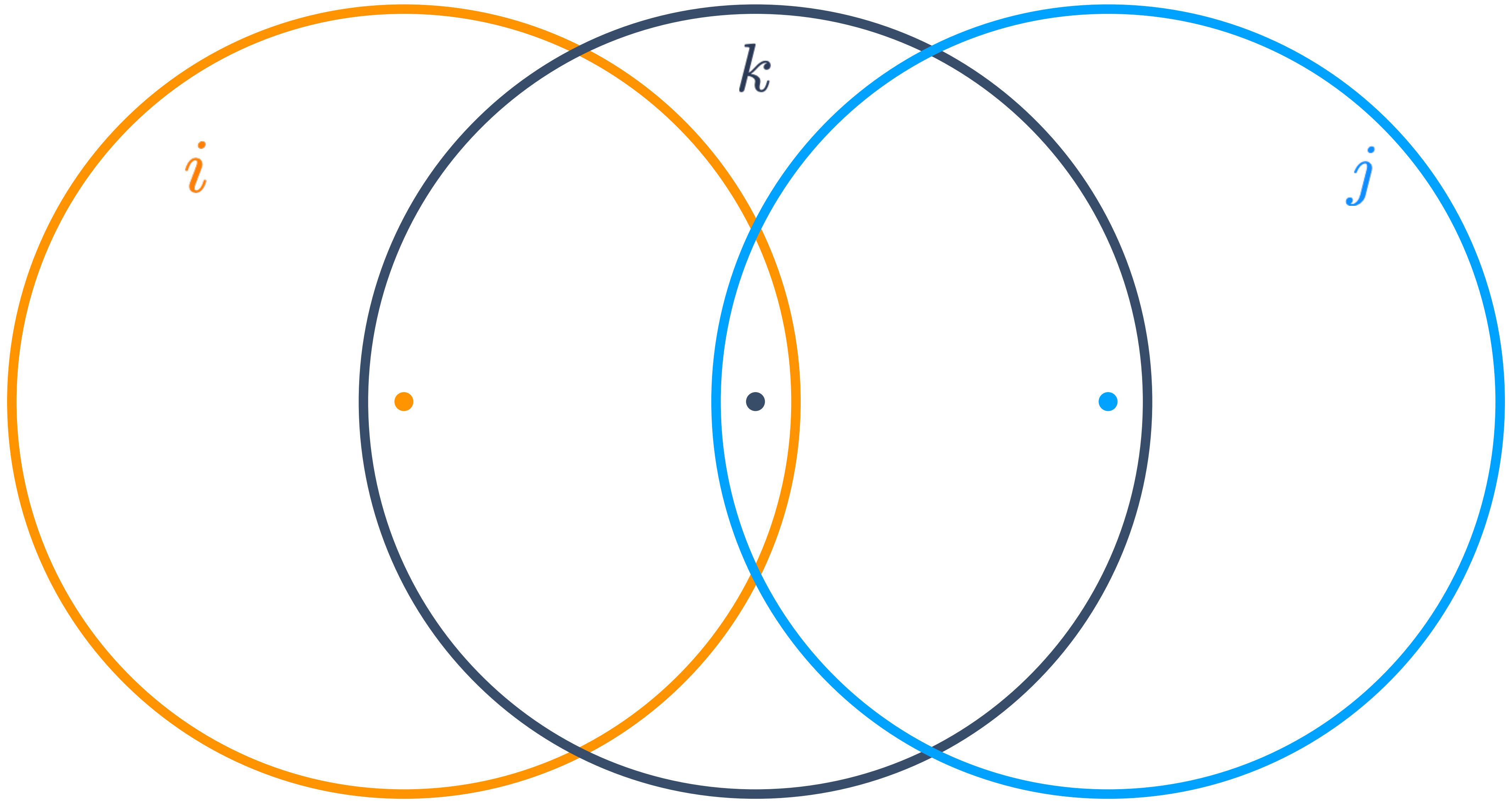
Objective: extend idea of isolated particles surrounded by rigid flats to many-interacting particle case

Solution:
1. Place rigid flats at overlap midpoints between particles
2. Calculate force on either side assuming interaction with rigid flat
3. Average force on each side to determine final force



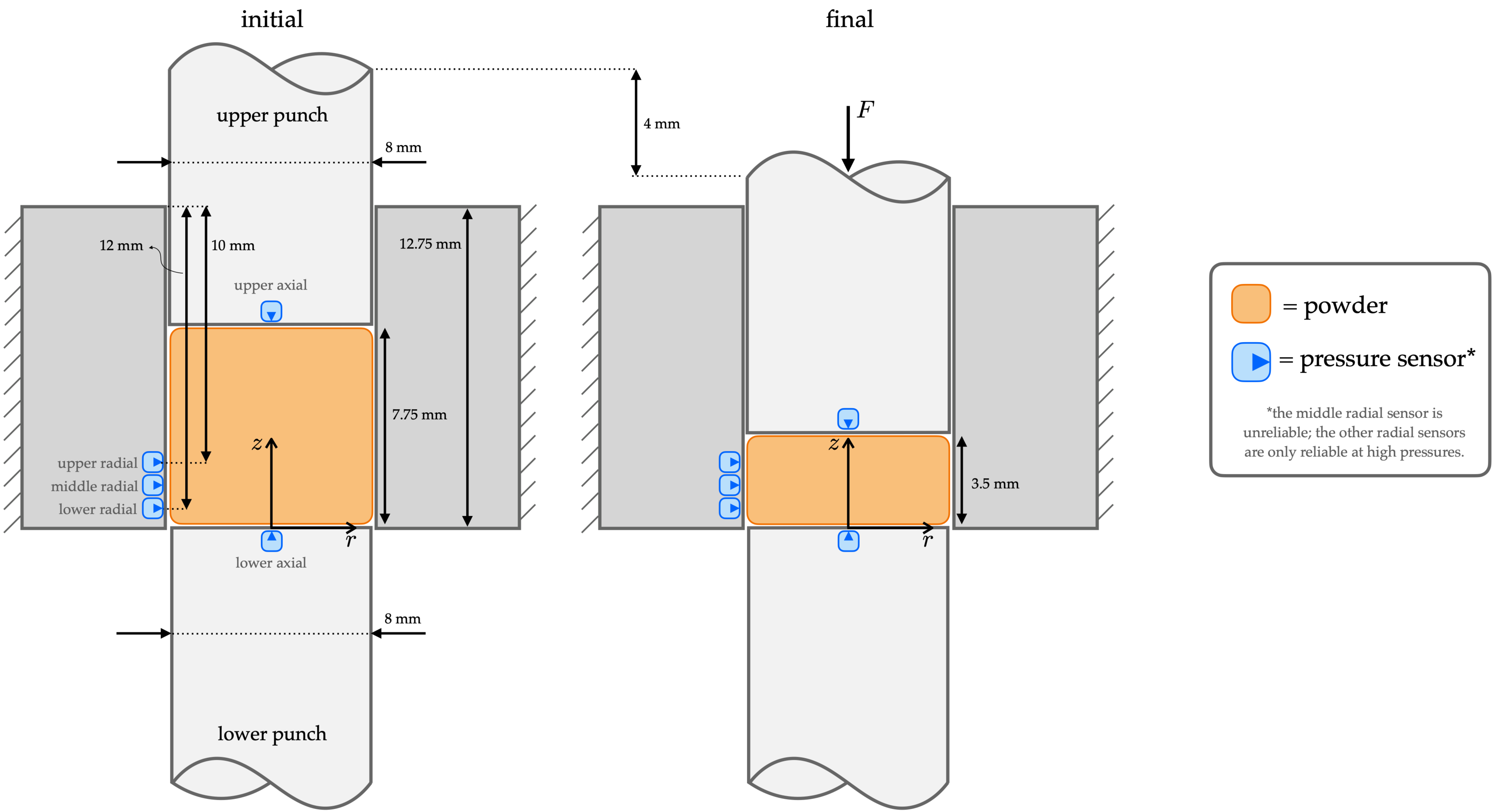
Peculiarities of large deformation DEM: Example 1

Should particle i be able to contact particle j?



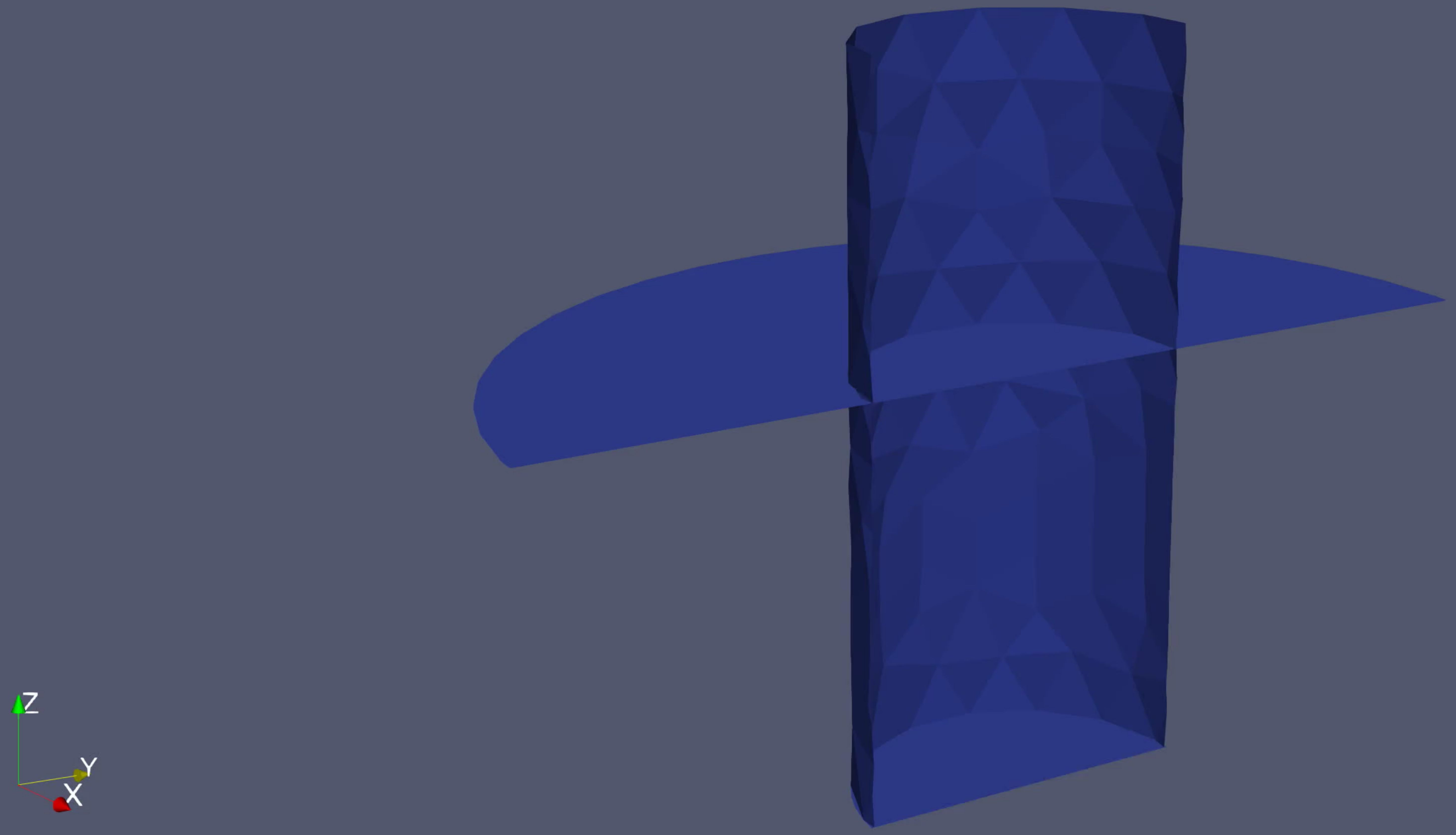
The answer is **no**, but standard DEM does not recognize this.

Compaction simulator set-up



LIGGGHTS Avicel tableting simulation (NO AIR)

1195 polydisperse particles



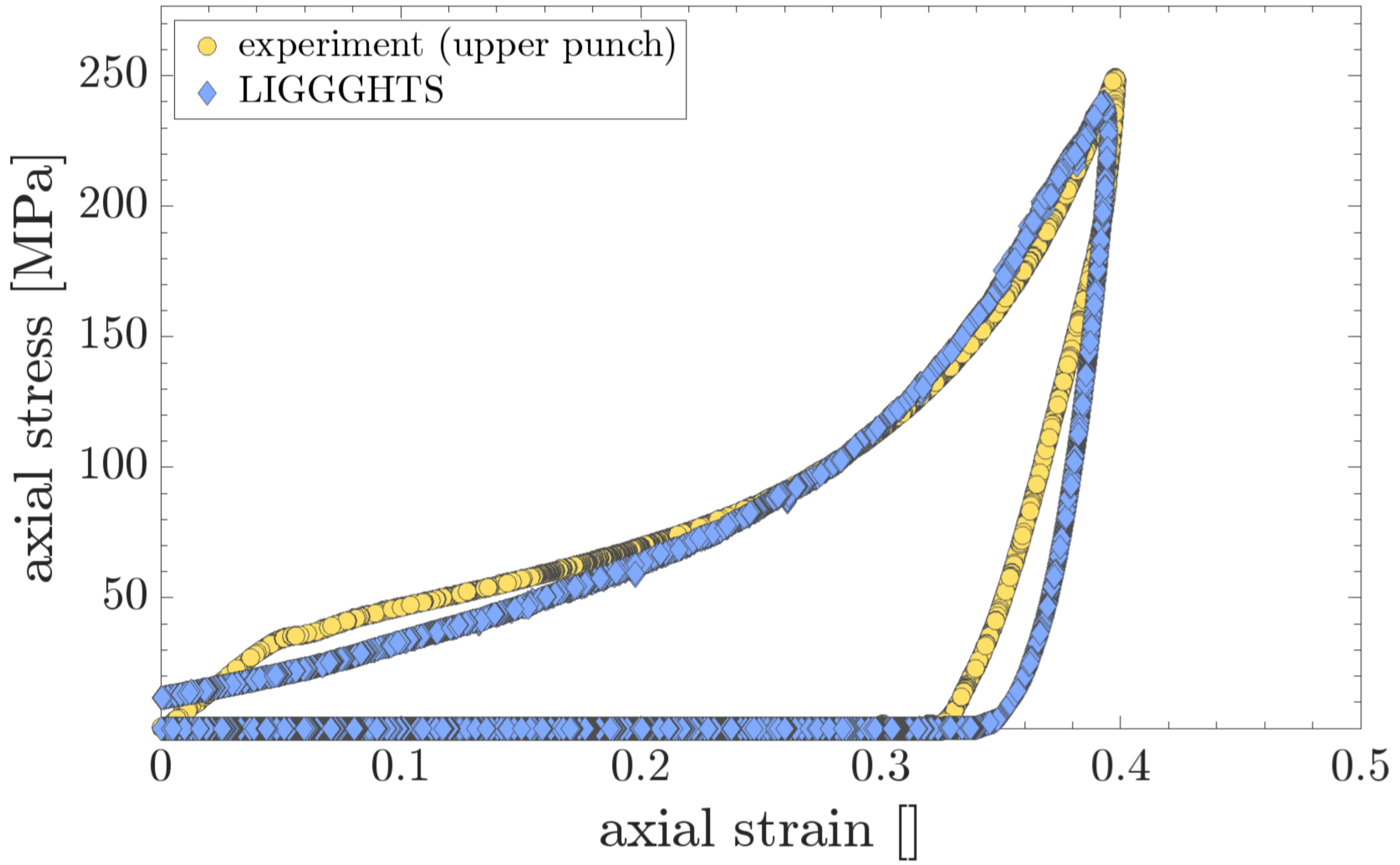
LIGGGHTS Avicel tableting simulation (NO AIR)

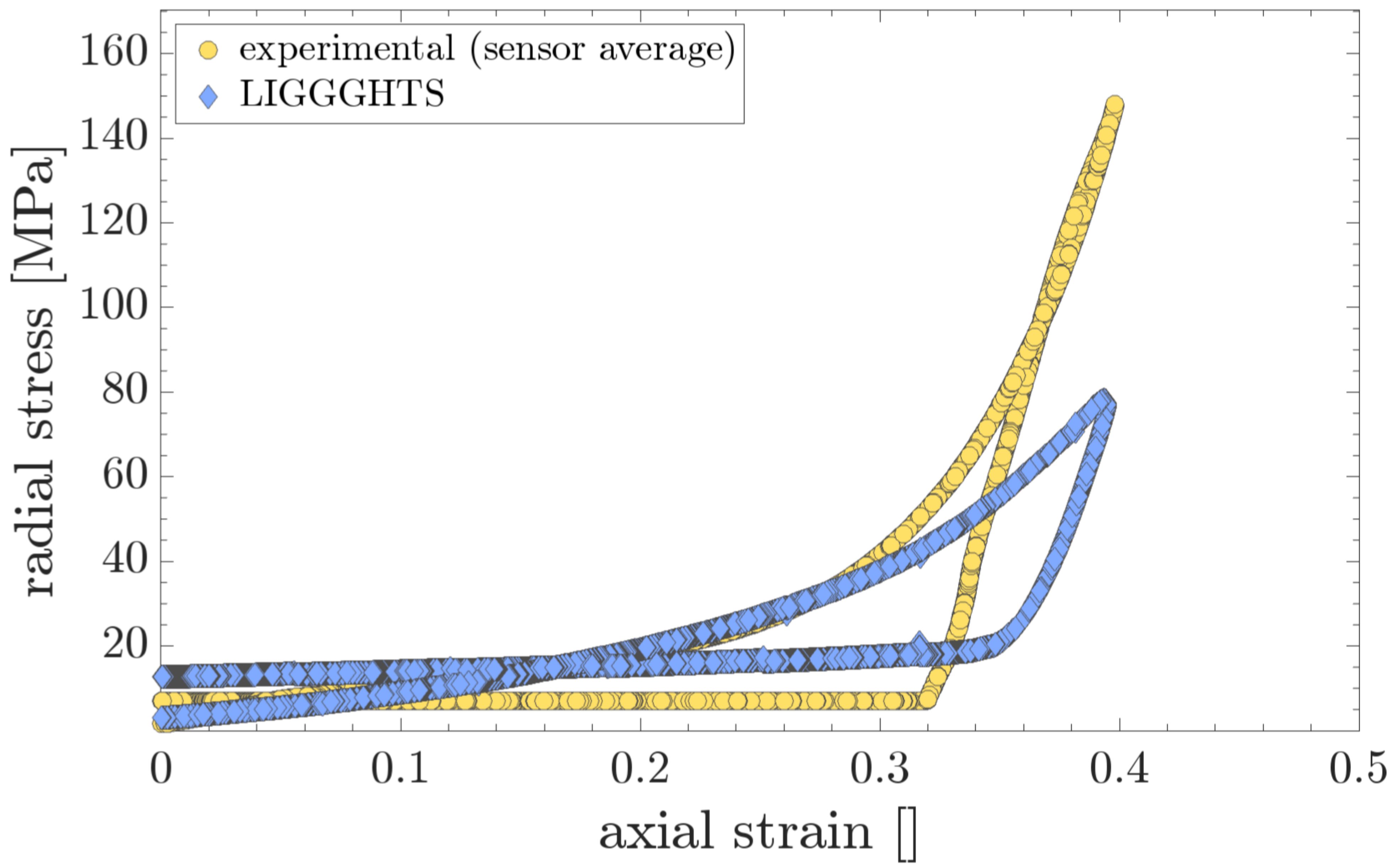
1195 polydisperse particles

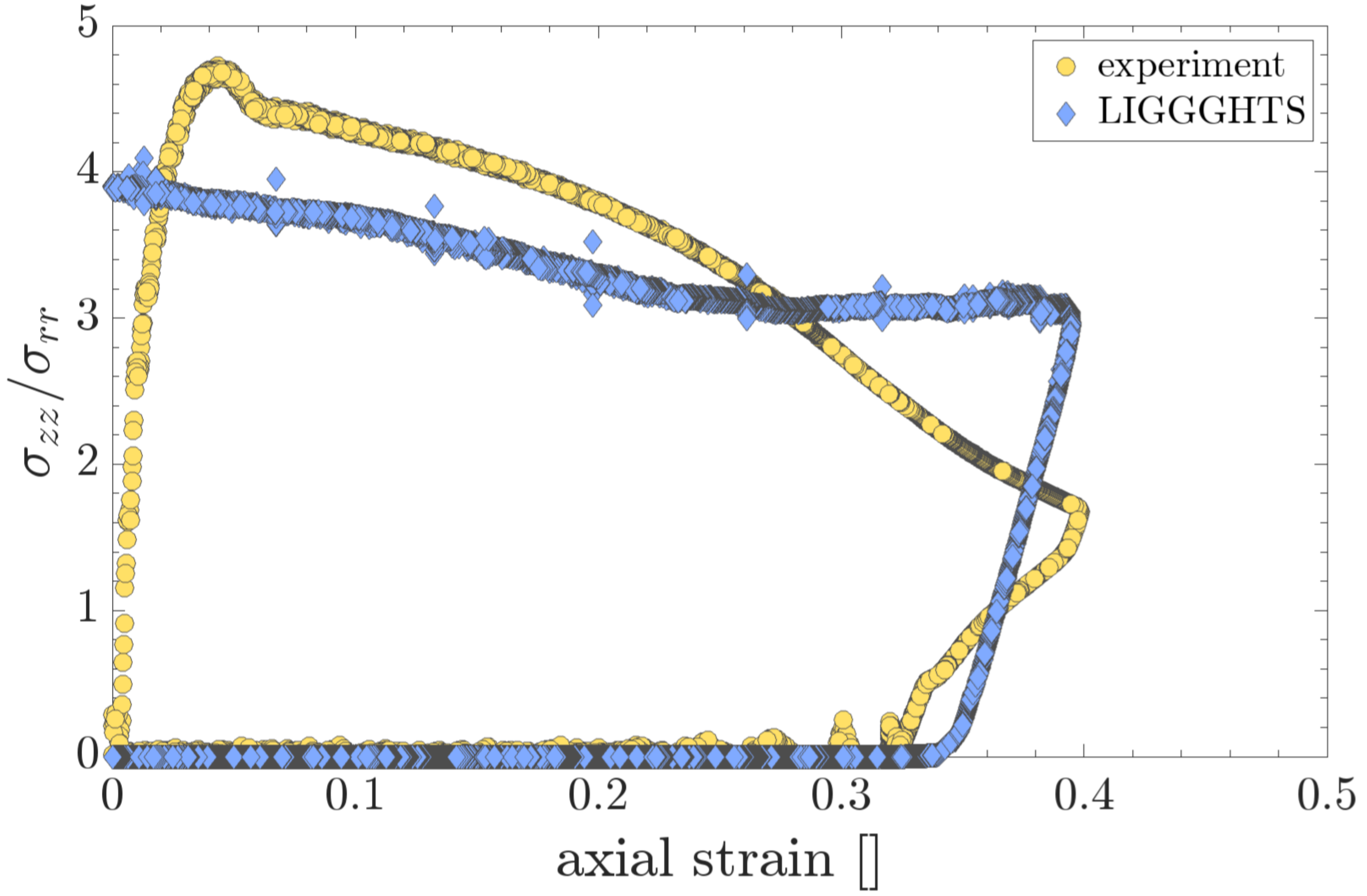
material properties

$E = 10$ [GPa]*	CoR = 0.5 [ ]
$\nu = 0.3$ [ ]*	CoF = 0.7 [ ]
$Y = 17$ [MPa]	CoRF = 0.55 [ ]
$\Delta\gamma = 3000$ [J/m^2]*	
$R_o = 320 \pm 64$ [μm]	

* indicates value taken from literature, otherwise the parameter was fitted





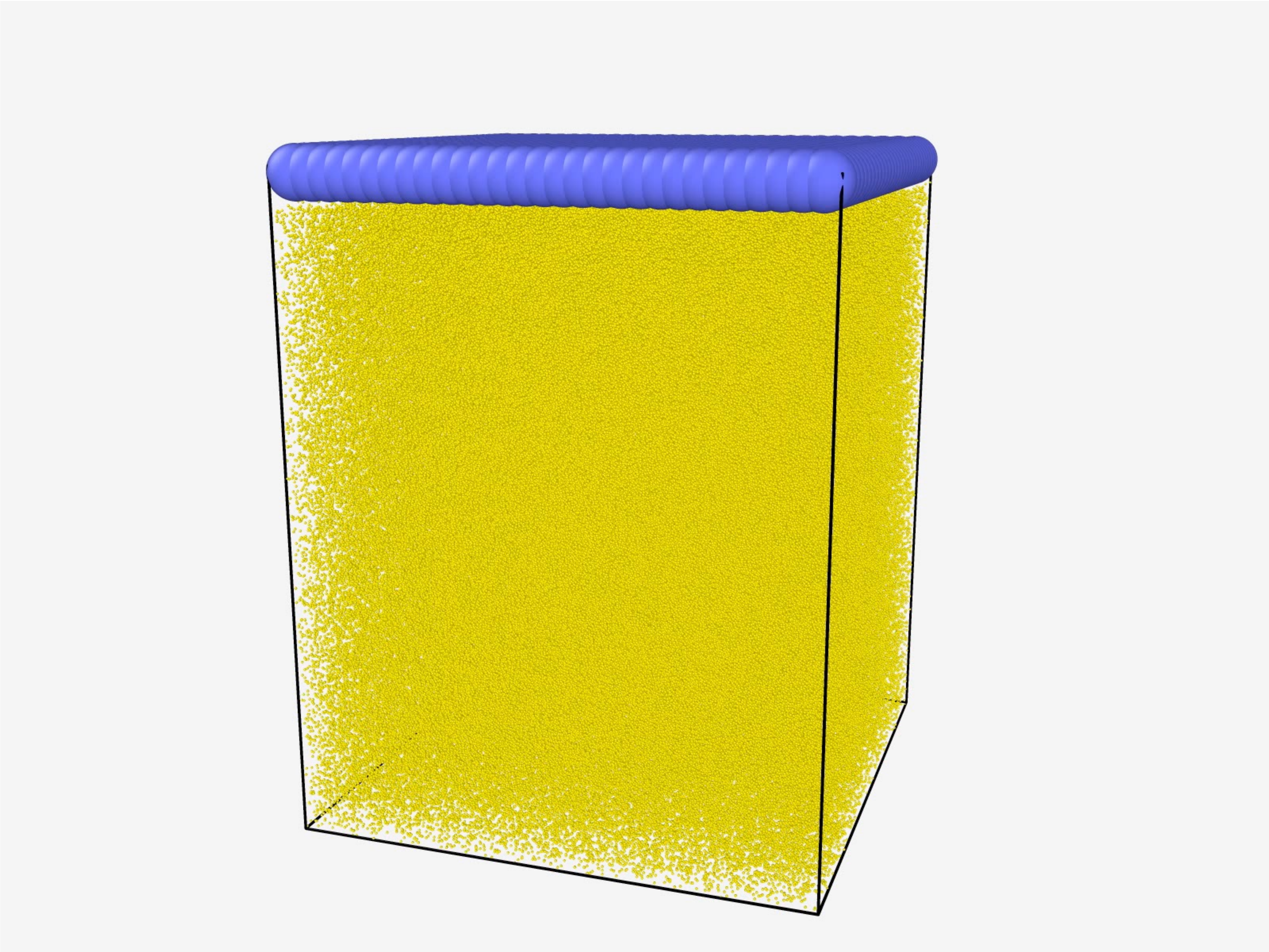


Adding in air

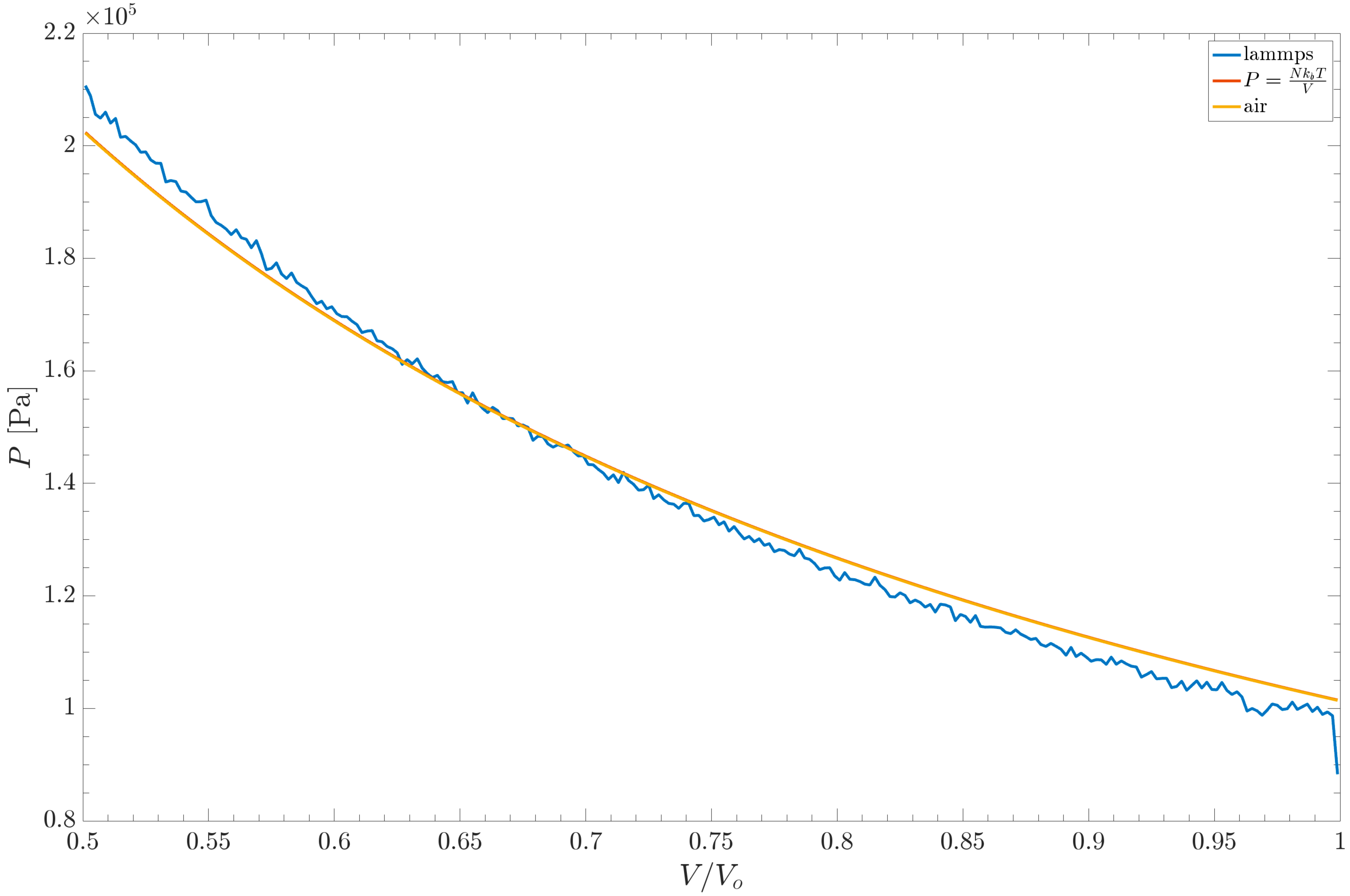
Multi-particle collision dynamics (MPCD or SRD)

Fluid is represented by mesoscale particles with no pairwise particle/particle interactions.

- Streaming – propagates momentum
- Collision – swaps momentum
- Reproduces fluid compressibility and momentum

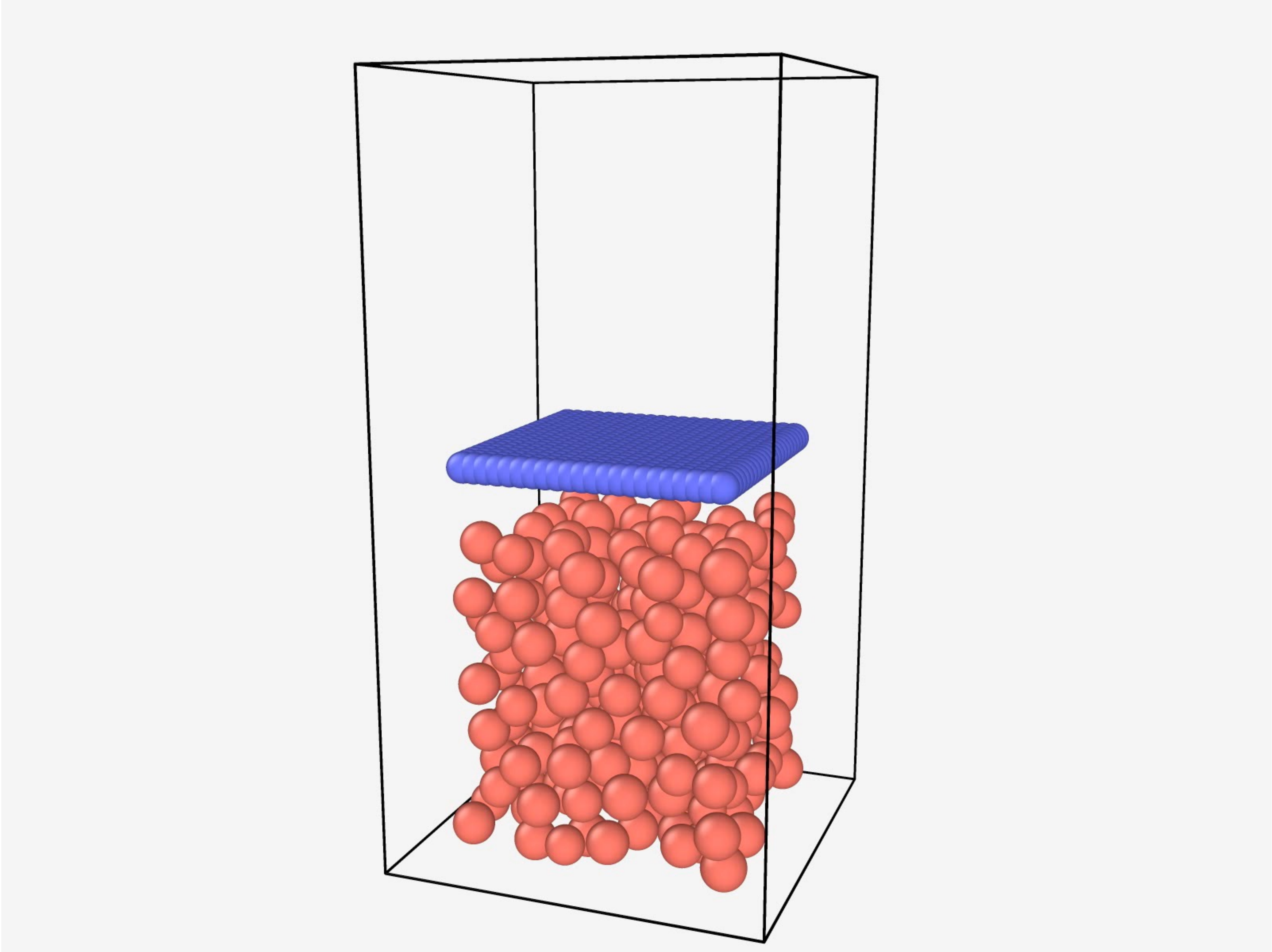


500,000 mpcd particles



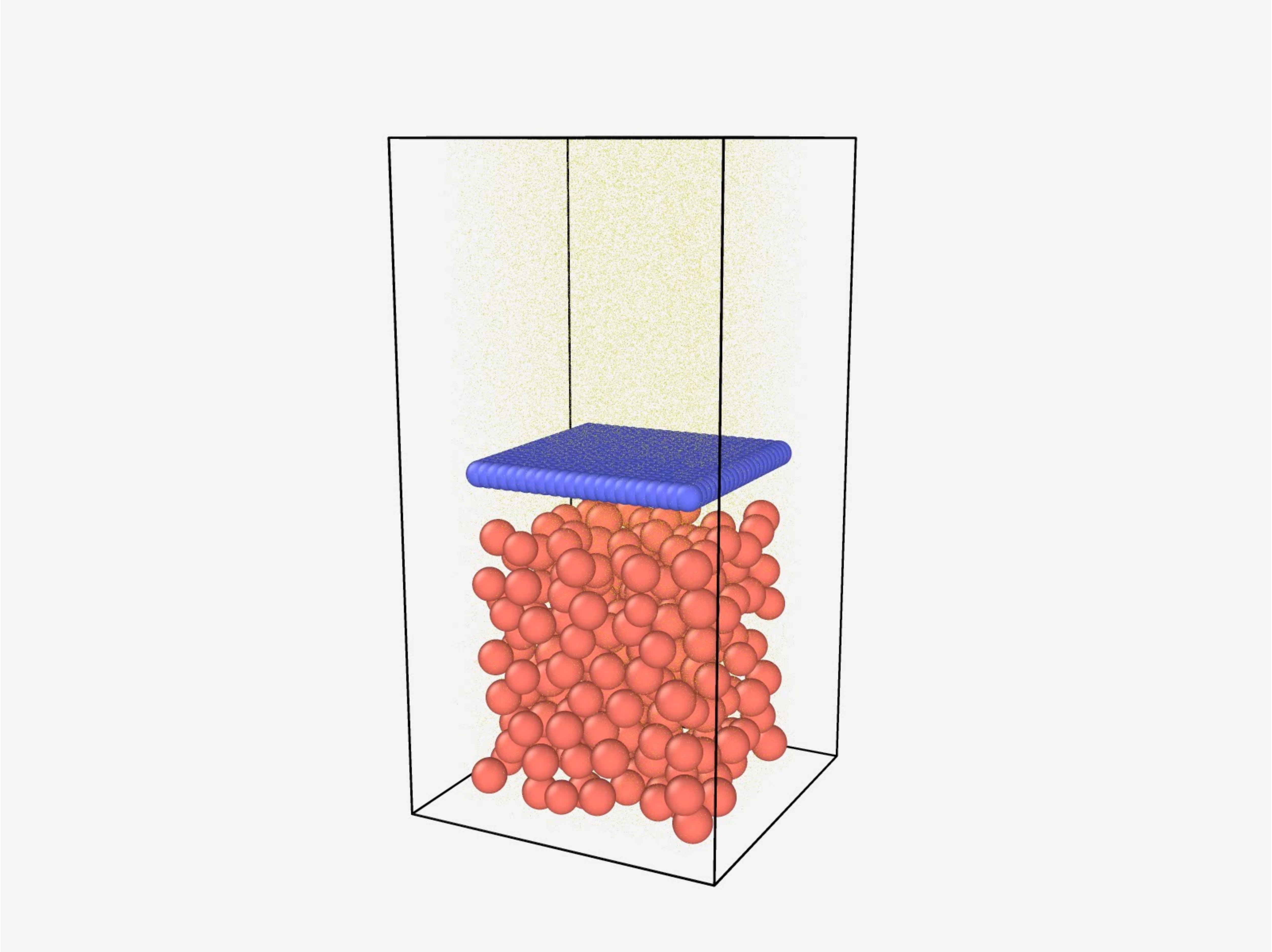
Tabeting in presence of air

Compaction without air present



230 DEM particles
0.14 sec real time simulation, 0.024 second compression
18 min runtime in serial

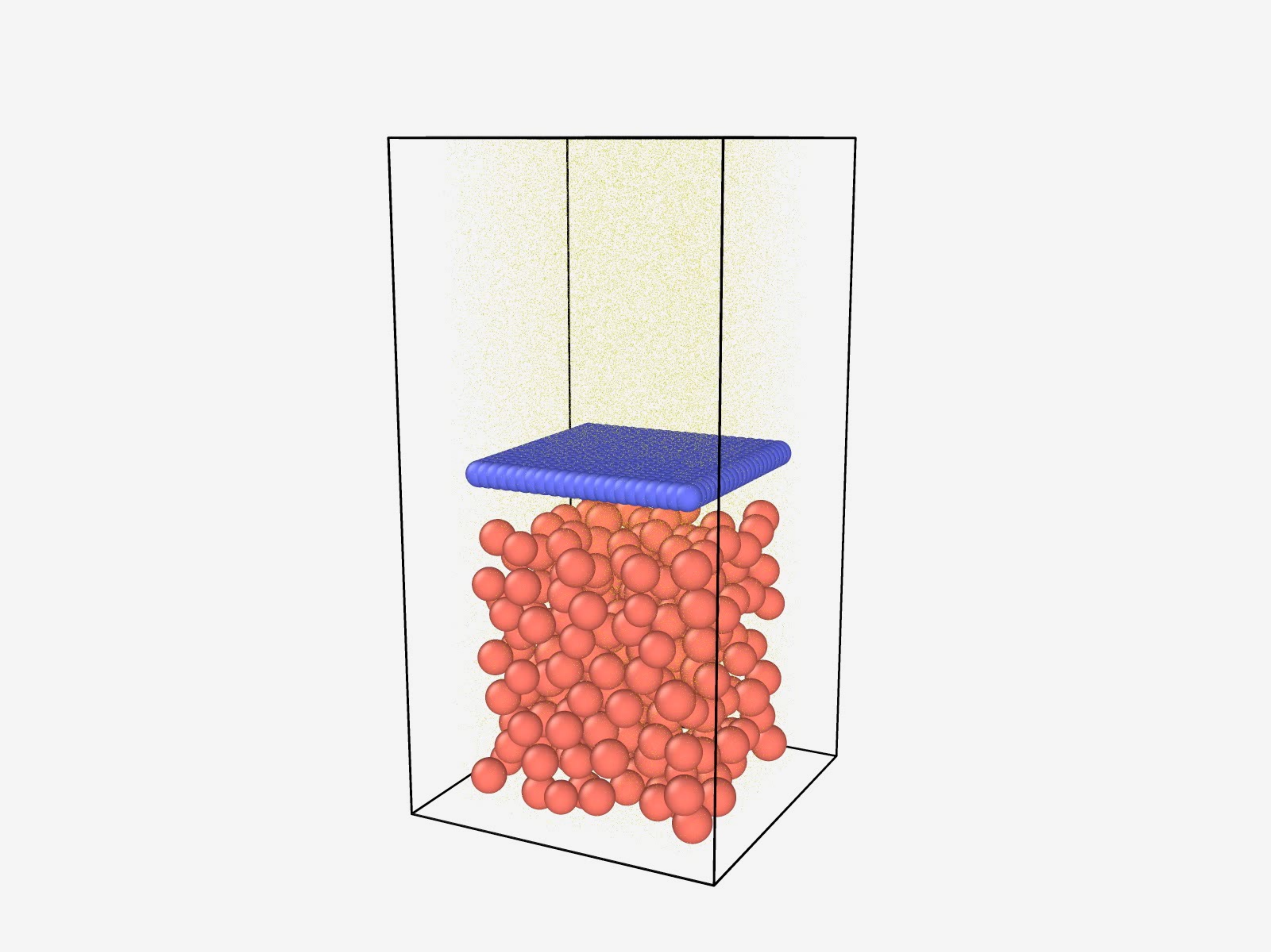
Compaction with air present



230 DEM particles, 450,000 MPCD particles
0.14 sec real time simulation, 0.024 second compression
30 hrs runtime in serial

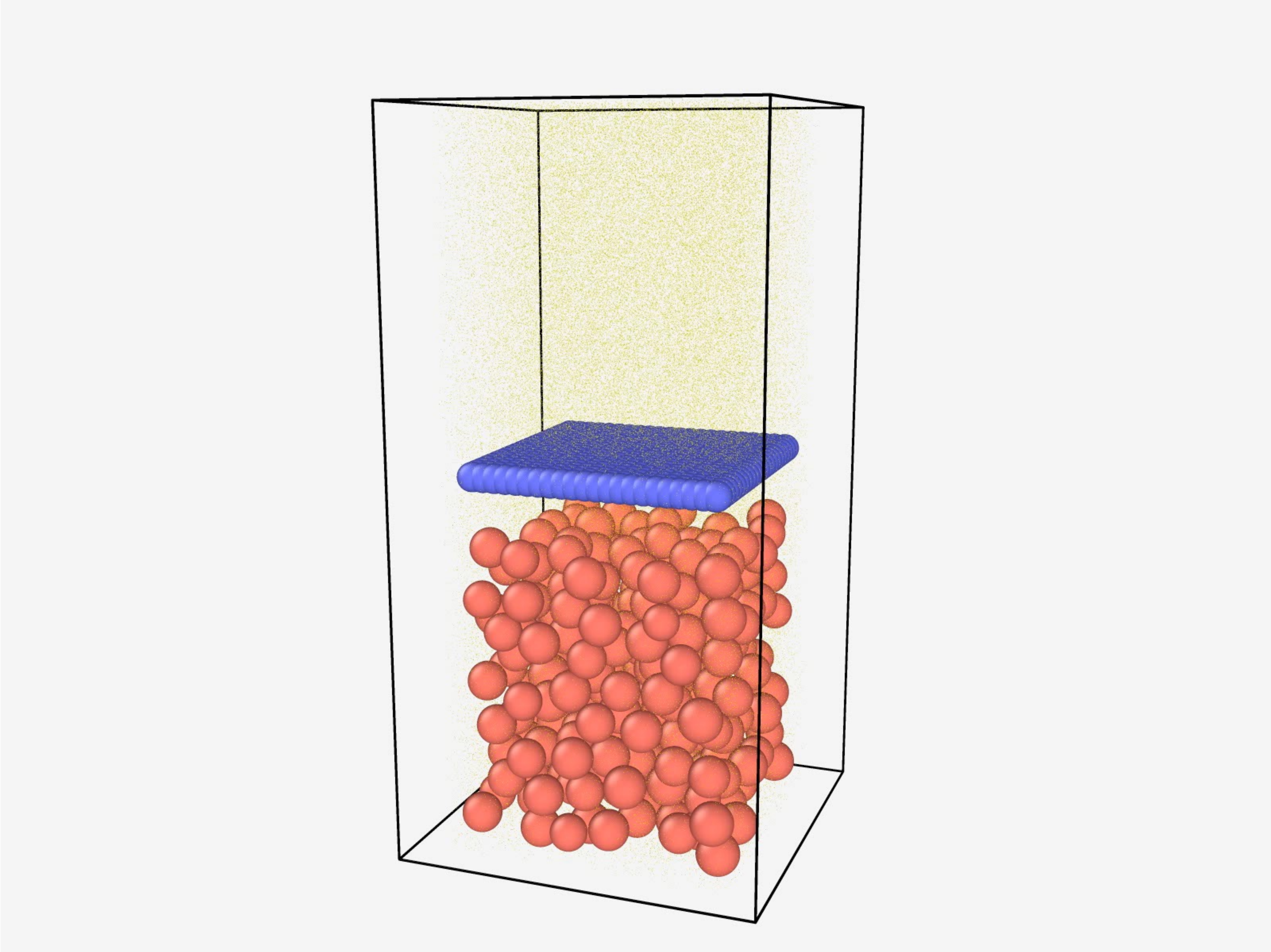
Rate effects

"Fast" compaction with air present



230 DEM particles, 450,000 MPCD particles
0.14 sec real time simulation, 0.024 second compression
30 hrs runtime in serial

"Slow" compaction with air present



230 DEM particles, 450,000 MPCD particles
0.338 sec real time simulation, 0.12 second compression
68 hrs runtime in serial