Air-induced defect formation during powder compaction

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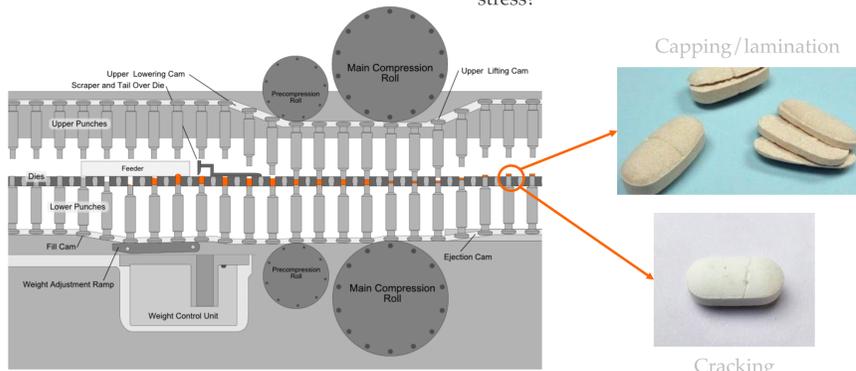
Project motivation and workflow

Use mechanics-based approach to predict defect formation to reduce waste material.

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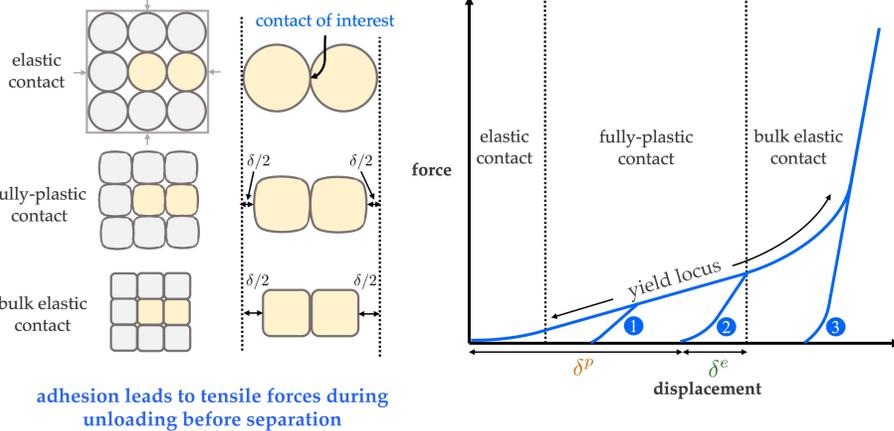

Capping/lamination

Cracking

DEM Contact Model — Develop elastic-plastic adhesive contact model valid for small to large deformations

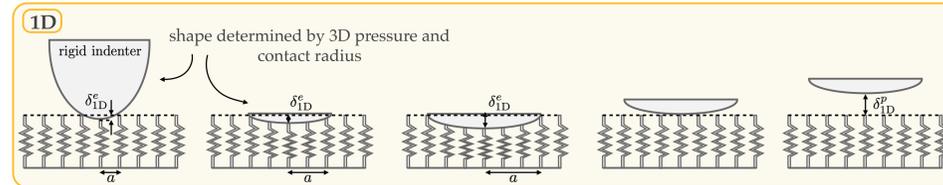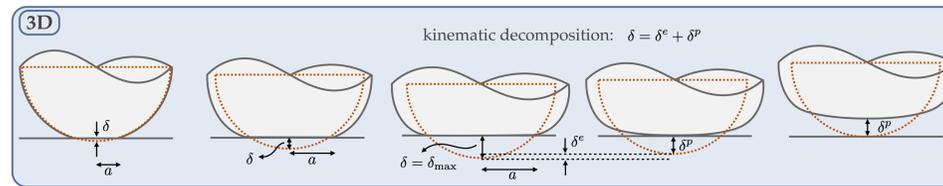**CFD-DEM** — Couple CFD-DEM for high fidelity numerical "experiments"

Two Phase Simulations — Full two-phase continuum simulations of powder compaction.

Discrete/Continuum
Fully Continuum

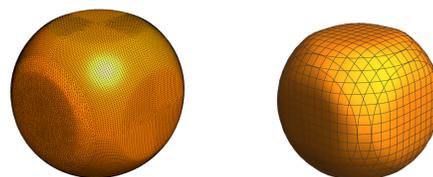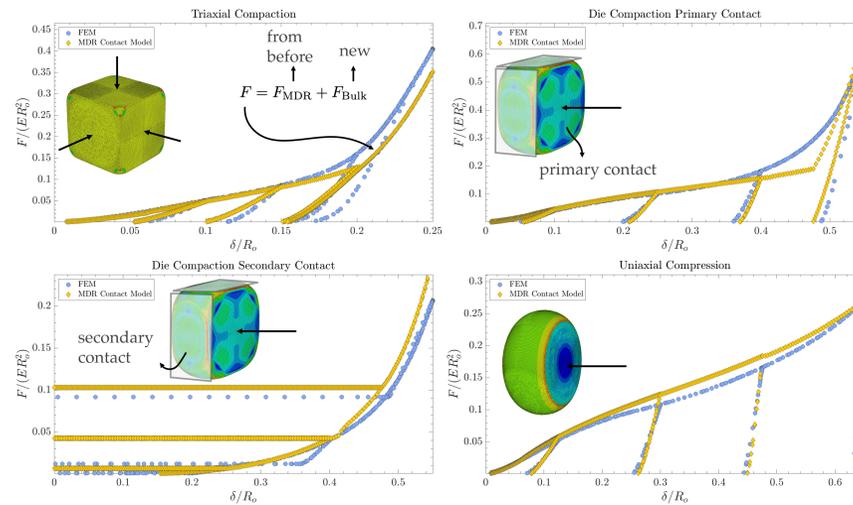## Elastic-plastic particle behavior during powder compaction

elastic contact
fully-plastic contact
bulk elastic contact

contact of interest

elastic contact | fully-plastic contact | bulk elastic contact

force

yield locus

δ^p δ^e

displacement

adhesion leads to tensile forces during unloading before separation

Previous contact models and their relevant features

Authors	Regimes	min(E/Y)	Unloading	Adhesion	Nonlocalized
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	yes	no
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	no
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	no
Giannis et al., 2021	E, FP, BE	n.r.	yes	yes	yes

nonlocalized effects

- **very close to rigid plastic**
- **empirically fitted**, reduced use of mechanics principles to determine contact law
- **requires refitting** for each new material being modeled.
- **no information beyond the force-displacement** is provided.

Single elastic-plastic contact – 3D and 1D MDR evolution

3D

kinematic decomposition: $\delta = \delta^e + \delta^p$

purely elastic | fully-plastic begins, yield criterion met | plastic deformation accumulates | unloading is an elastic process | blunted profile

δ a $\delta = \delta_{max}$ δ^c δ^p δ^p

1D

rigid indenter — shape determined by 3D pressure and contact radius

δ_{1D} δ_{1D}^e δ_{1D}^c δ_{1D}^p

sequence of elastic contacts

Some force-displacement comparison with finite element simulations

Triaxial Compaction

$F/(E R_o^2)$ vs δ/R_o

from before   new

$F = F_{MDR} + F_{Bulk}$

Die Compaction Primary Contact

primary contact

Die Compaction Secondary Contact

secondary contact

Uniaxial Compression

Finite Element   MDR contact model

Plastic contact deformation, contact areas, and volume are accurately tracked, allowing accurate reconstruction of the deformed particle from MDR model.

**Add JKR adhesion physics to obtain a plastic-cohesive contact model**

$F_{ij}/(E_i R_o^2)$ vs δ_{max}/R_o

FEM-MDR: $E/Y = 200$
MDR Contact Model
$E_i R_o/\Delta\gamma = 109890$
$Y R_o/\Delta\gamma = 125$
$a_c/r_{peak}|_{u_{max}(R_o - 8.5)} = 1.27$
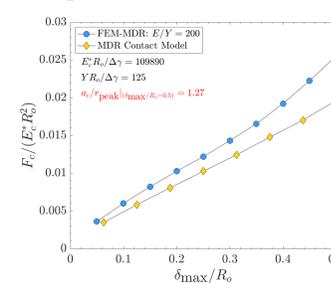
From single to many-interacting particles

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

rigid flat
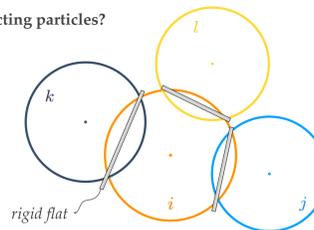
Large deformation DEM topological considerations

step 1: check if penalization is necessary

if $\delta_{ij} \leq 0$ or $\delta_{ik} \leq 0$ or $\delta_{jk} \leq 0$
$p_{ij} = 0$ $p_{ik} = 0$ $p_{jk} = 0$
break to **step 3**
end

step 2: calculate penalty for non-central particle contact

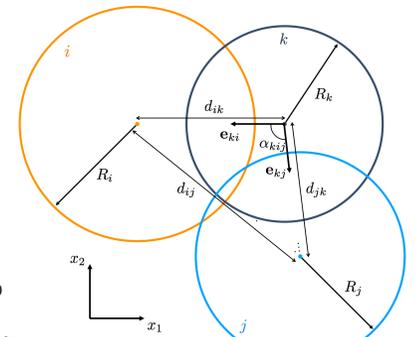$\max(d_{ij}, d_{ik}, d_{jk}) \to d_{ij}$

k = central particle

$\alpha_{kij} = \arccos(\mathbf{e}_{ki} \cdot \mathbf{e}_{kj})$

$p_{ij} = \dfrac{1}{1 + \exp\left(-50\left(\frac{\alpha_{kij}}{\pi} - \frac{1}{2}\right)\right)}$ $p_{ik} = 0$ $p_{jk} = 0$
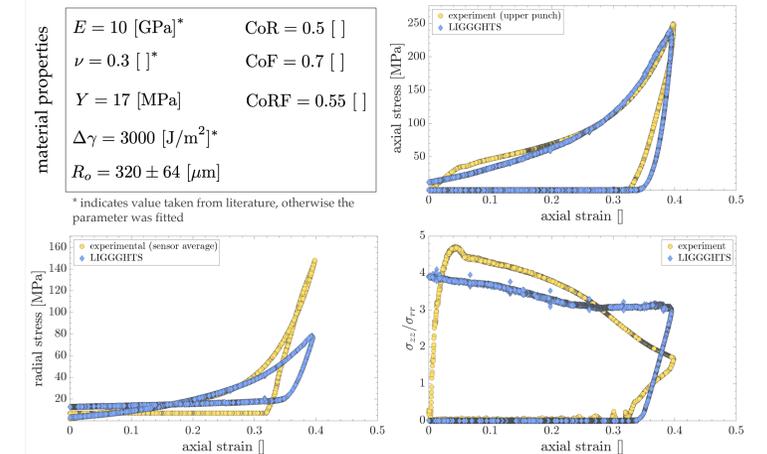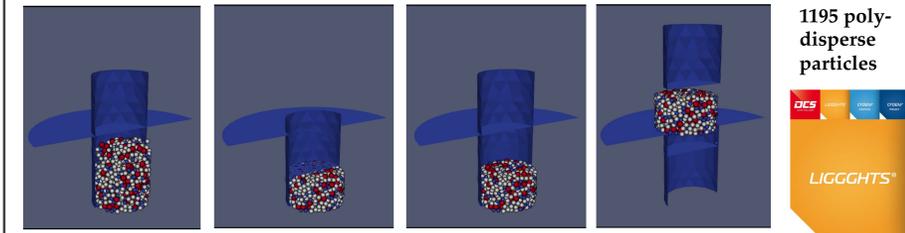
repeat for all neighbor triplets superimposing all penalties

step 3: calculate contact weights given penalties

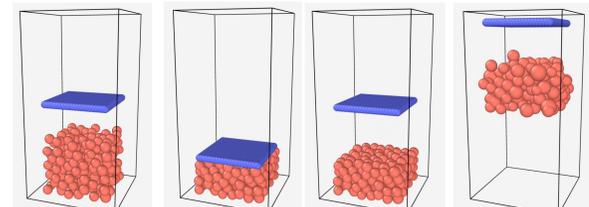$w_{ij} = \max(1 - p_{ij}, 0)$ $w_{ik} = \max(1 - p_{ik}, 0)$ $w_{jk} = \max(1 - p_{jk}, 0)$

DEM tablet compaction in LIGGGHTS with MDR contact model

1195 poly-disperse particles

LIGGGHTS®

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

axial stress vs axial strain — experiment (upper punch) / LIGGGHTS

radial stress [MPa] vs axial strain — experimental (sensor average) / LIGGGHTS

σ_{zz}/σ_{rr} vs axial strain — experiment / LIGGGHTS

Adding in air: Coupled MPCD-MDR Model
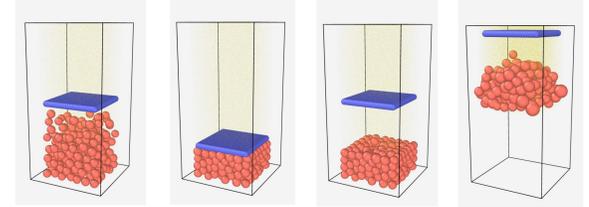
LAMMPS

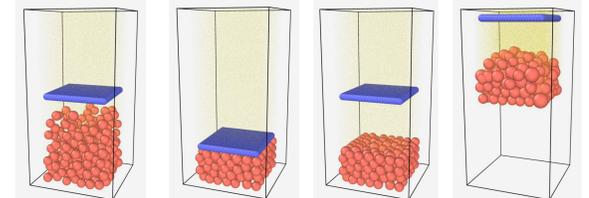**Compaction without air present**

230 DEM particles
0.14 sec real time simulation
0.024 second compression

Compaction with air present

230 DEM particles
450,000 MPCD particles
0.14 sec real time simulation
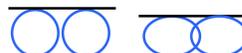0.024 second compression

Slower compaction with air present

230 DEM particles
450,000 MPCD particles
0.338 sec real time simulation
0.12 second compression