Air-induced defect formation during powder compaction

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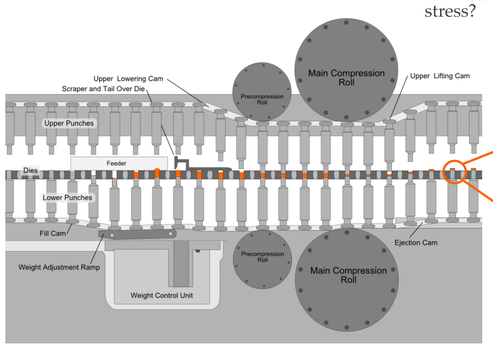
Project motivation and workflow

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

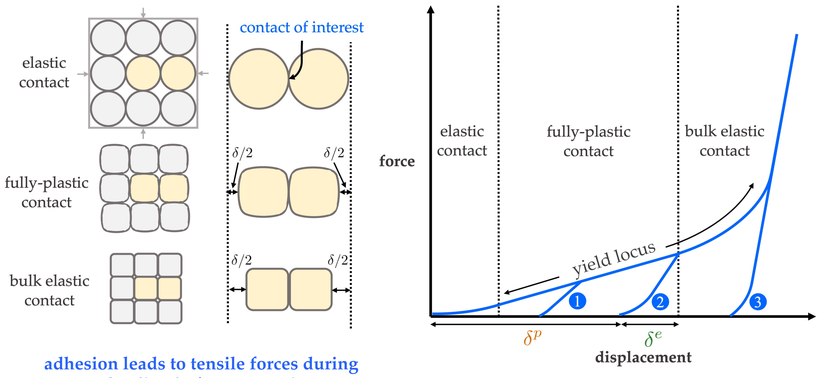
DEM Contact Model
Develop elastic-plastic adhesive contact model valid for small to large deformations

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

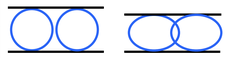


adhesion leads to tensile forces during unloading before separation

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	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

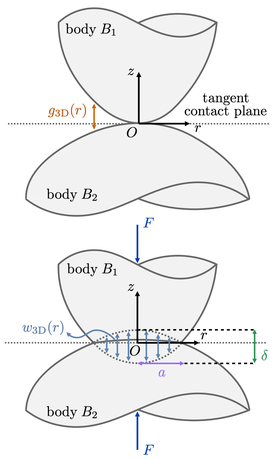
nonlocalized effects



- **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.

Project motivation and workflow

3D elastic axisym. contact



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

$$F = \int_{-a}^{a} q_{1D}(x)\,dx = 2\pi \int_0^a p_{3D}(r) r\,dr$$

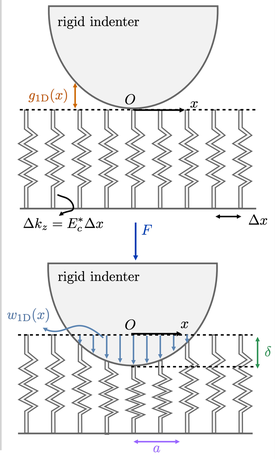
integral transforms

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

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

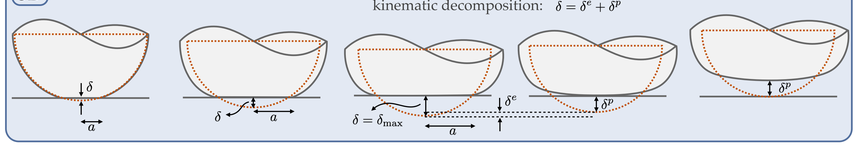
$p_{3D}(r)$ ⟷ (pressure) ⟷ $q_{1D}(x)$

1D Winkler foundation



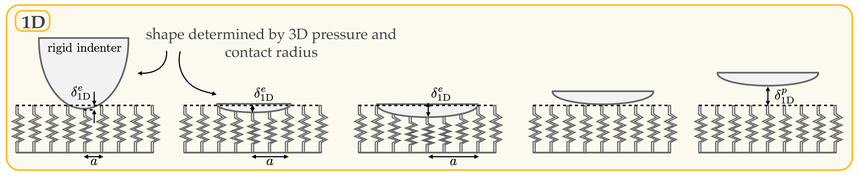
Single elastic-plastic contact – 3D and 1D evolution

3D



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

1D



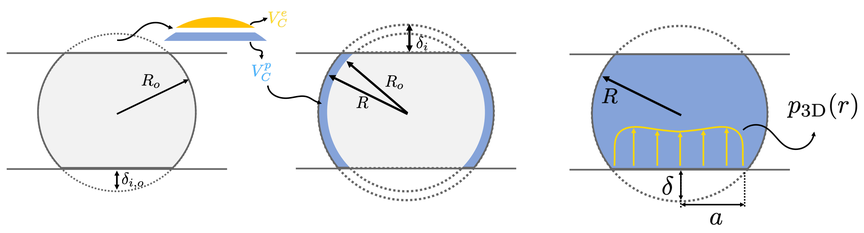
sequence of elastic contacts

Fundamental solution pathway

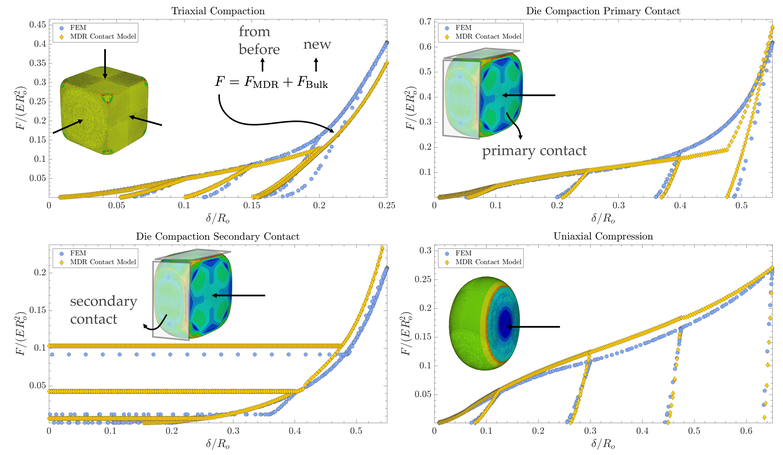
Idea: Determine corresponding 1D indenter shape at each instant: $g_{1D} = \hat{g}_{1D}(\delta^p \text{ or } \delta_{max})$

Pathway: Use reverse contact solution methodology supplied by the MDR: $\{p_{3D}(r), a\} \rightarrow g_{1D}(x)$

- **exploit three simple properties of elastic-plastic spherical contact**
  1. pressure is approximately uniform in fully plastic regime
  2. area is purely geometric in fully plastic regime
  3. plastic deformation is incompressible



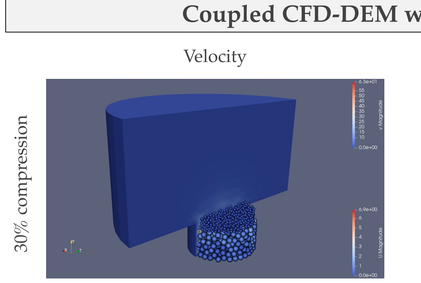
Some force-displacement comparison with finite element simulations



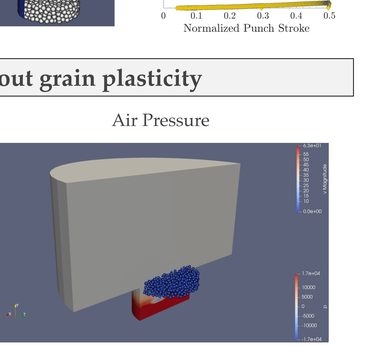
Adhesion – an easy addition in the MDR framework

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

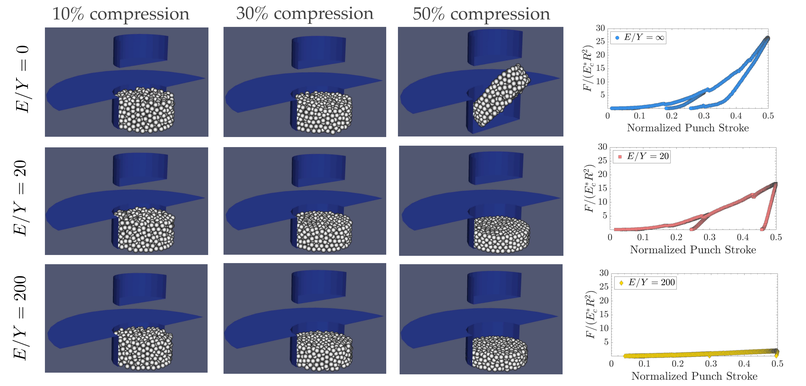
sticky springs with critical extensional length



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



Pure DEM tablet compaction in LIGGGHTS with MDR contact model



Coupled CFD-DEM without grain plasticity