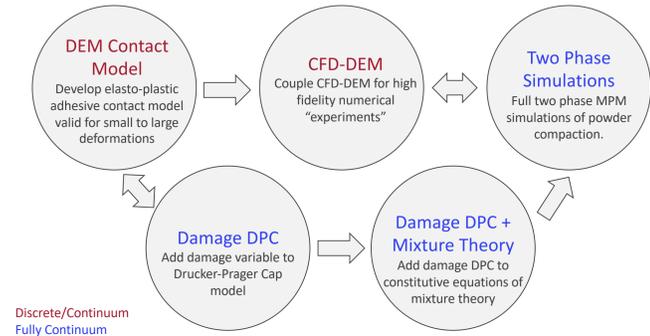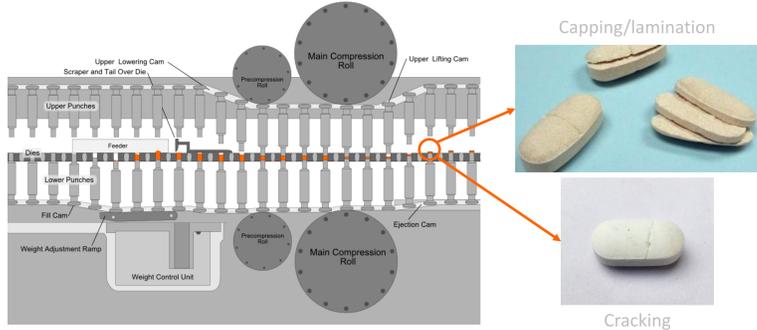# Air-induced defect formation during powder compaction

Towards continuum accuracy at low computational cost: a dimensionally reduced contact model for elastic-plastic bodies

William Zunker and **Ken Kamrin** || IFPRI Contacts Yi-Jiun (Nate) Lin (*Merck*), Weifeng Shi (*Nestle*), and Vincenzino Vivacqua (*Johnson Matthey*)

MIT — Kamrin Group — Continuum modeling from solids to fluids

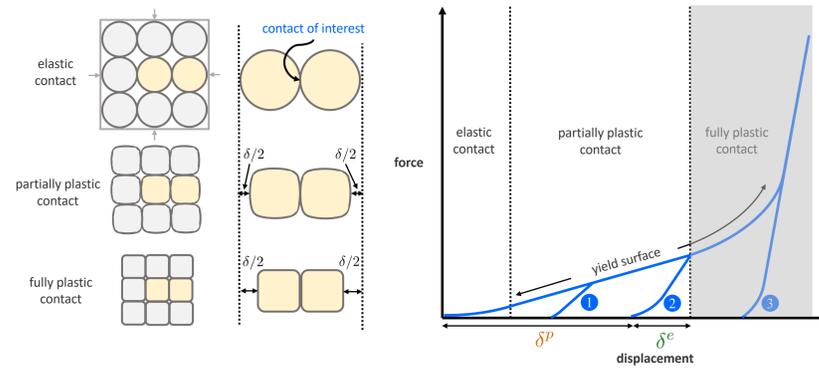IFPRI — International Fine Particle Research Institute

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Project Motivation and Workflow

Entrapped air causes defect formation upon ejection from die ⇒ Use mechanics-based approach to predict defect formation to reduce waste material
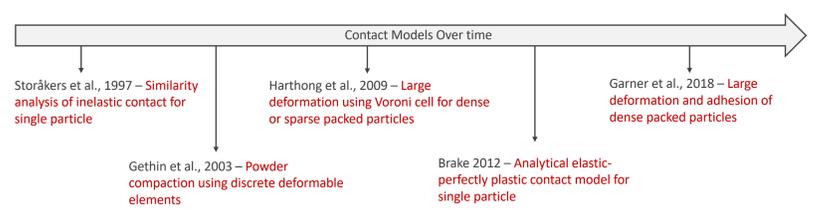

Capping/lamination

Cracking

- **DEM Contact Model** — Develop elasto-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 MPM simulations of powder compaction.
- **Damage DPC** — Add damage variable to Drucker-Prager Cap model
- **Damage DPC + Mixture Theory** — Add damage DPC to constitutive equations of mixture theory

Discrete/Continuum
Fully Continuum

Contact Model: Building a Strong Foundation

Contact model underlies all numerical "experiments" used to validate continuum models ⇒ Critical to model the complex force-displacement curve accurately
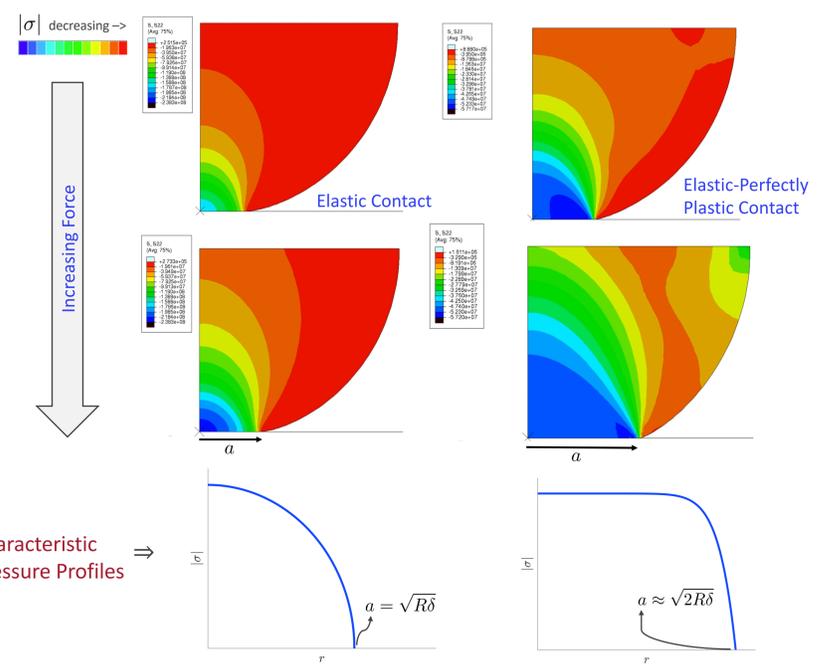

elastic contact

partially plastic contact

fully plastic contact

contact of interest

$\delta/2$ $\delta/2$

force — elastic contact — partially plastic contact — fully plastic contact — yield surface

δ^p δ^e displacement

Prior Inelastic Contact Models

Contact Models Over time

- Storåkers et al., 1997 – Similarity analysis of inelastic contact for single particle
- Harthong et al., 2009 – Large deformation using Voroni cell for dense or sparse packed particles
- Garner et al., 2018 – Large deformation and adhesion of dense packed particles
- Gethin et al., 2003 – Powder compaction using discrete deformable elements
- Brake 2012 – Analytical elastic-perfectly plastic contact model for single particle

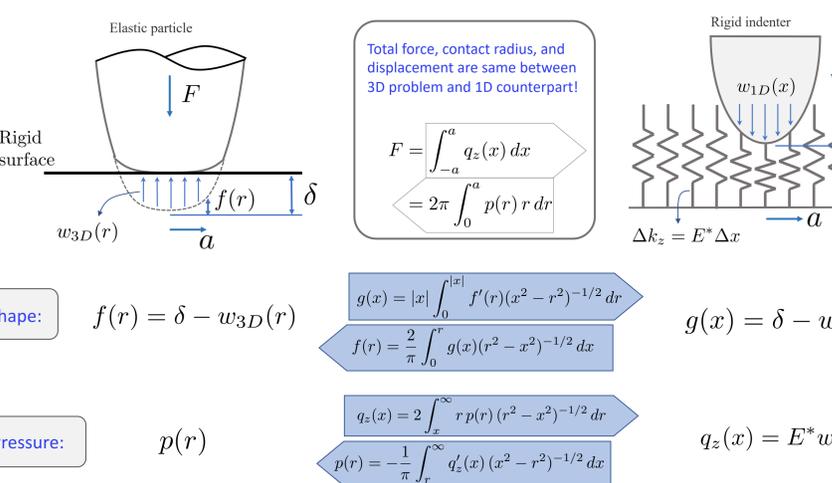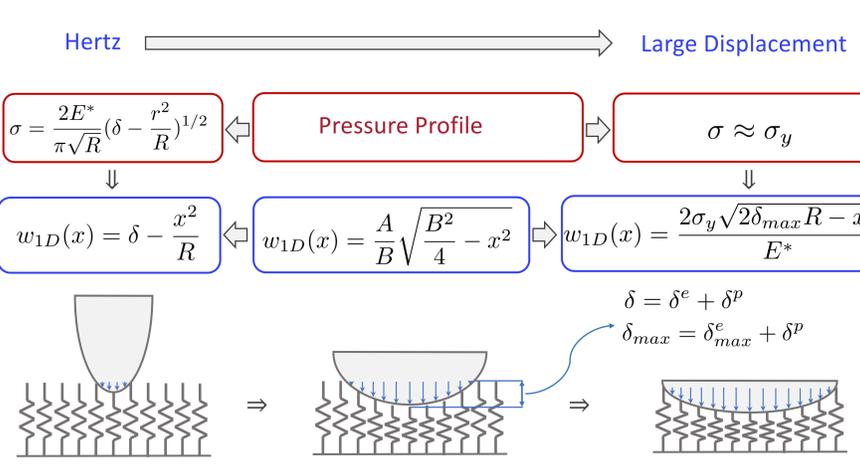| Continuum Models	Reduced-Continuum Models	"Classical" Contact Model
Full field solutions • Stresses/Total force • Strains • Displacements — High resolution at high computational cost	Partial field solutions • Stresses/Total force at contact • Surface displacements at contact — Moderate resolution at moderate/low computational cost	Single valued solutions • Total force at contact • Displacements at point of first contact — Low resolution and limited robustness at low computational cost

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Finite Element Contact Simulations

$|\sigma|$ decreasing →

Increasing Force

Elastic Contact

Elastic-Perfectly Plastic Contact

a

Characteristic Pressure Profiles ⇒

$a = \sqrt{R\delta}$

$a \approx \sqrt{2R\delta}$

Demands of Model

Force-Displacement ✓	Stress-Profile ✓	Plastic Displacement ✓
• Hertz in elastic limit • Linear force displacement in partially plastic contact • Accurate unloading curves	• Pointwise contact stress profile • Hertz profile in elastic limit • Flattened profile in partially plastic limit	• Pointwise plastic surface displacement • Predict reasonable blunted shape upon unloading.

- Convert 3D axisymmetric problem to a semi-equivalent 1D Winkler foundation penetrated by a generic elliptical displacement profile using the *Method of Dimensionality Reduction*.
- Elastic and elastic-plastic contact are linearly interpolated between.
- Keep $\delta^p \equiv w^p(r=0)$ as a *state variable* on the contact that changes 3D particle and 1D rigid indenter shapes (i.e. we can use δ^p to reconstruct an estimate of $w^p(r)$).
- Determine the force under the corresponding pressure distribution $F = F(\delta, \delta^p)$.
- Enforce yield condition $\sigma(r=0) \approx 2Y$ to update δ^p.
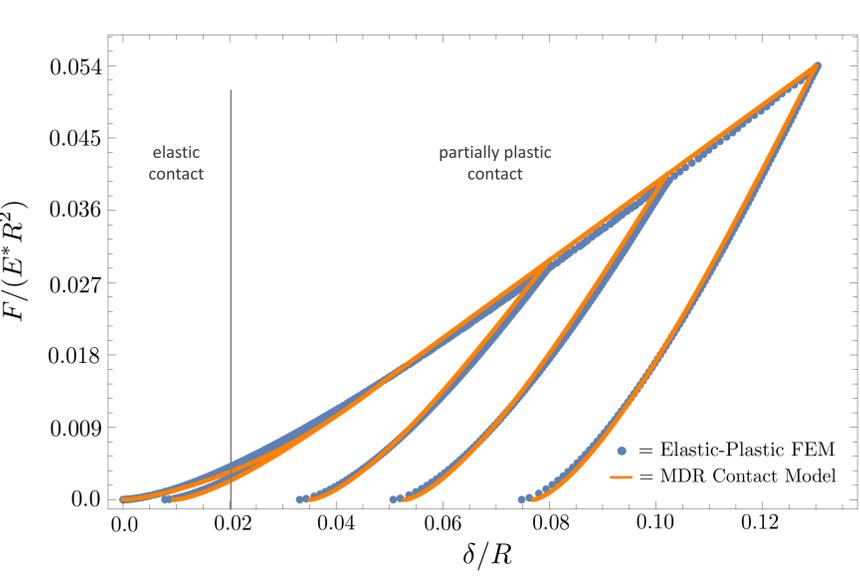

R r δ $w^p(r)$

Method of Dimensionality Reduction (MDR) (Popov and Heß)

Elastic particle

Rigid indenter

Total force, contact radius, and displacement are same between 3D problem and 1D counterpart!

$$F = \int_{-a}^{a} q_z(x)\,dx = 2\pi \int_0^a p(r)\,r\,dr$$

Rigid surface

$w_{3D}(r)$ $f(r)$ δ a

$w_{1D}(x)$ δ $\Delta k_z = E^* \Delta x$ a Δx

Shape:
$$f(r) = \delta - w_{3D}(r)$$
$$g(x) = |x|\int_0^{|x|} f'(r)(x^2 - r^2)^{-1/2}\,dr$$
$$f(r) = \frac{2}{\pi}\int_0^r g(x)(r^2 - x^2)^{-1/2}\,dx$$
$$g(x) = \delta - w_{1D}(x)$$

Pressure:
$$p(r)$$
$$q_z(x) = 2\int_x^\infty r\,p(r)\,(r^2 - x^2)^{-1/2}\,dr$$
$$p(r) = -\frac{1}{\pi}\int_r^\infty q_z'(x)(x^2 - r^2)^{-1/2}\,dx$$
$$q_z(x) = E^* w_{1D}(x)$$

Evolution of Displacement Profile

Hertz → Large Displacement

$$\sigma = \frac{2E^*}{\pi\sqrt{R}}\left(\delta - \frac{r^2}{R}\right)^{1/2}$$

Pressure Profile

$$\sigma \approx \sigma_y$$

$$w_{1D}(x) = \delta - \frac{x^2}{R}$$
$$w_{1D}(x) = \frac{A}{B}\sqrt{\frac{B^2}{4} - x^2}$$
$$w_{1D}(x) = \frac{2\sigma_y\sqrt{2\delta_{max}R - x^2}}{E^*}$$

$$\delta = \delta^e + \delta^p$$
$$\delta_{max} = \delta_{max}^e + \delta^p$$

Force-Displacement Curve

$F/(E^* R^2)$ vs δ/R

elastic contact

partially plastic contact

- = Elastic-Plastic FEM
- = MDR Contact Model

Next Steps

Extend normal contact model to fully plastic regime ⇒ Implement contact model in LIGGGHTS and run CFD-DEM compaction simulations. ⇒ Develop continuum models

Include cohesion, tangential contact model, and rolling resistance.

Cohesion easy to add with MDR approach!

Velocity in Grains (m/s)

Full Volume Fraction