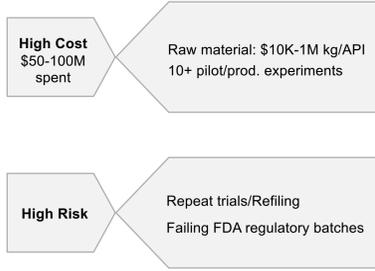
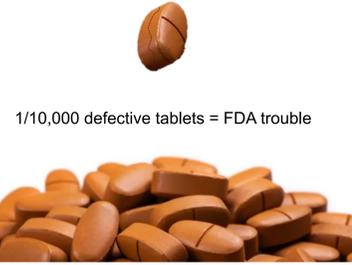


Project Motivation

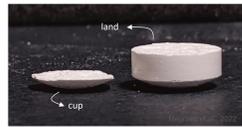
Drug manufacturing development process



10k-1M tablets per hour

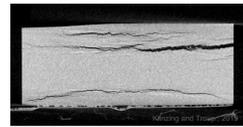


Capping



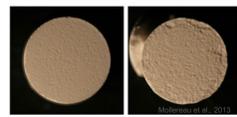
- Primarily observed in bi-convex tablets.
- Combined effects: Mode II shear stress and entrapped air.

Lamination



- Type I: Multiple fracture caused by air entrapment.
- Type II: Shear stresses combined with radial expansion during ejection.

Sticking/Picking



- Caused by adhesion to punch face being on a similar order to that of the interparticle adhesion.

Approach

Discrete element method



- computational efficiency between continuum & MPFEM
- particle-level details
- pore-level resolution gas phase coupling possible

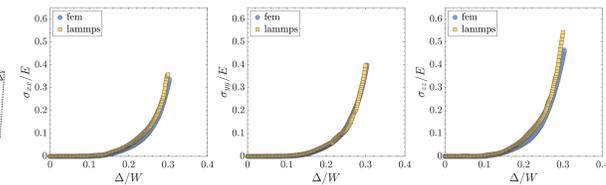
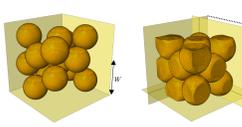
Method of dimensionality reduction (MDR) contact model



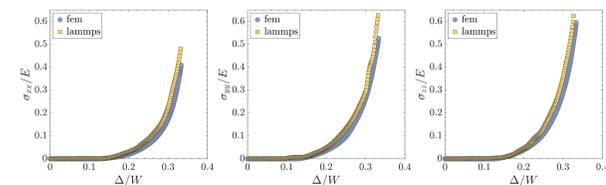
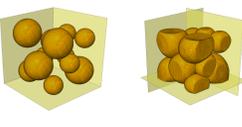
- Analytical mechanics-based formulation
- Physical model inputs: $E, \nu, Y, \Delta\gamma$
- Models elasto-plastic behavior into high confinement and during unloading
- Includes JKR type (fracture) adhesion
- Formally implemented into main LAMMPS repository: [LAMMPS](#)

MPFEM

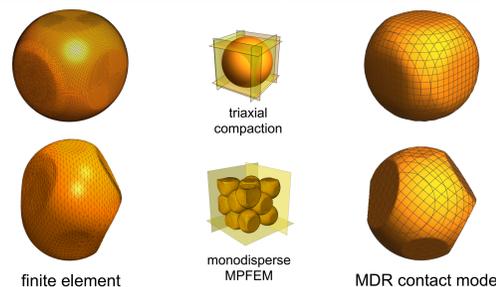
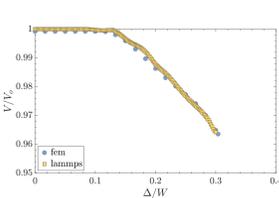
monodisperse



tridisperse



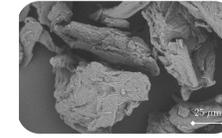
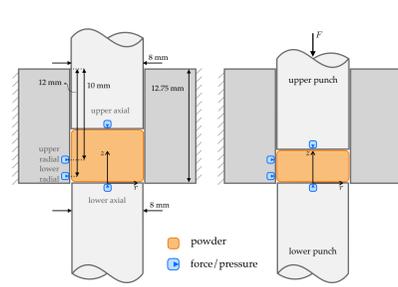
Deformed Particle Reconstruction



Pharmaceutical Tableting: Experiment

Avicel PH102

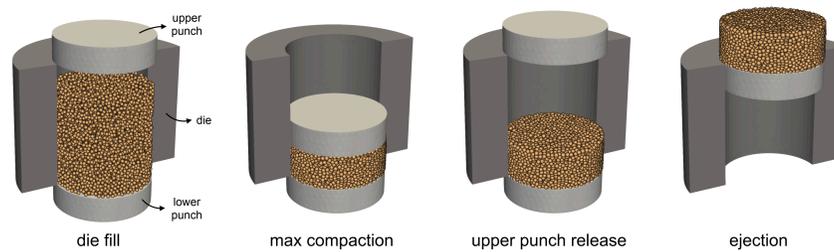
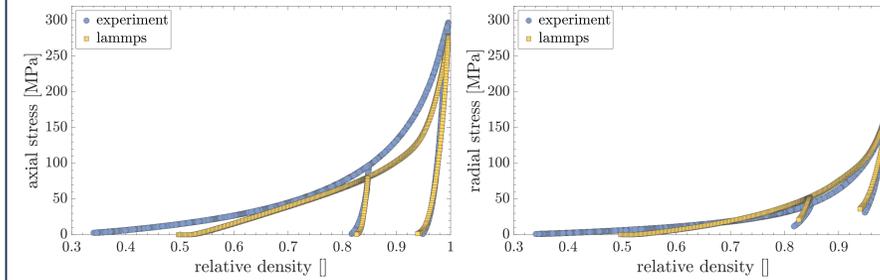
Experimental Compaction Simulator



Calibrated DEM Parameters

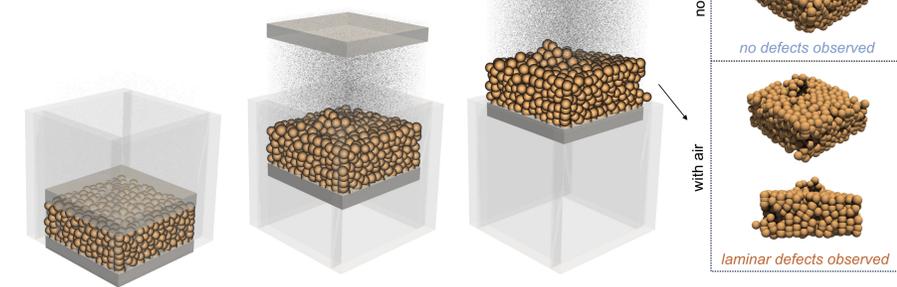
Normal (MDR)	Tangential (LH)
$E = 8 \text{ GPa}$	$k_t = \frac{2}{3} ER_{\text{mean}} \text{ N/m}$
$\nu = 0.3$	$x_{r,p} = 1.0$
$Y = 77 \text{ MPa}$	$\mu_s = 0.3$
$\Delta\gamma = 900 \text{ J/m}^2$	$\mu_{\text{wall}} = 0.1$
$\psi_b = 0.125$	
$\eta_n = 1e-4 \rho_{\text{mean}}^2 \nu_p \text{ kg/s}$	
Rolling (SDS)	Particle
$k_{\text{roll}} = \frac{1}{2} r_{\text{roll}}^2 ER_{\text{mean}} \text{ N/m}$	$R_{\text{min}} = 139 \mu\text{m}$
$\gamma_{\text{roll}} = \eta_n$	$R_{\text{max}} = 160 \mu\text{m}$
$\mu_{\text{roll}} = 1.0$	$\rho = 1560 \text{ kg/m}^3$

Pharmaceutical Tableting: Simulation

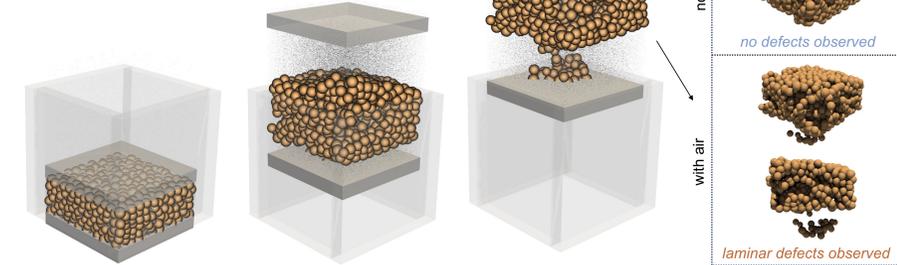


Air-Induced Defects: Lamination

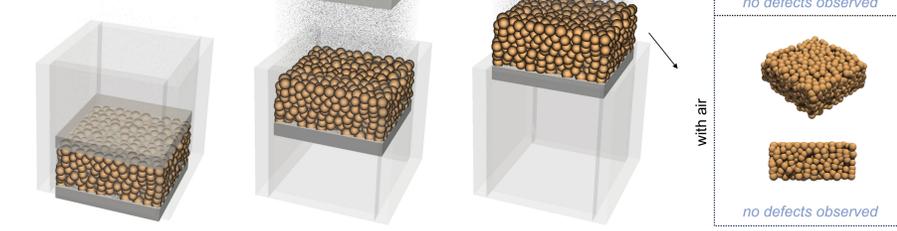
Reference



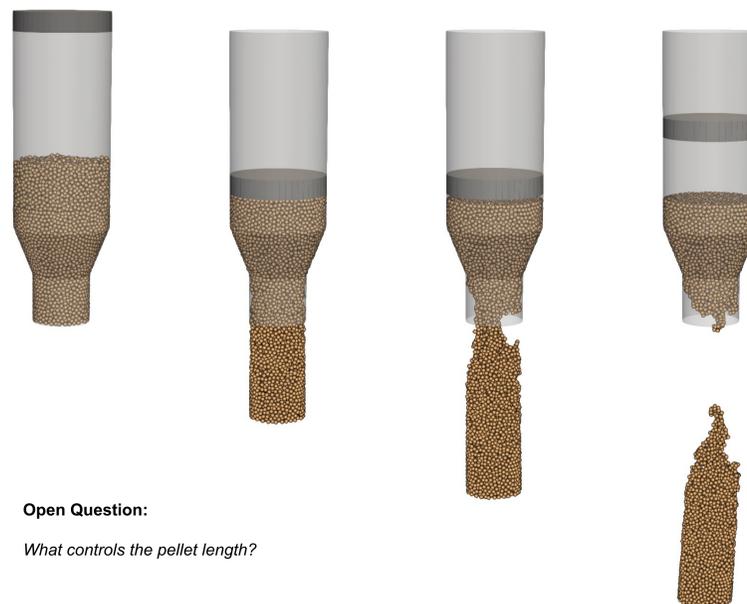
10x increased air viscosity



10x increased air viscosity and reduce maximum relative density from (0.98 to 0.9)



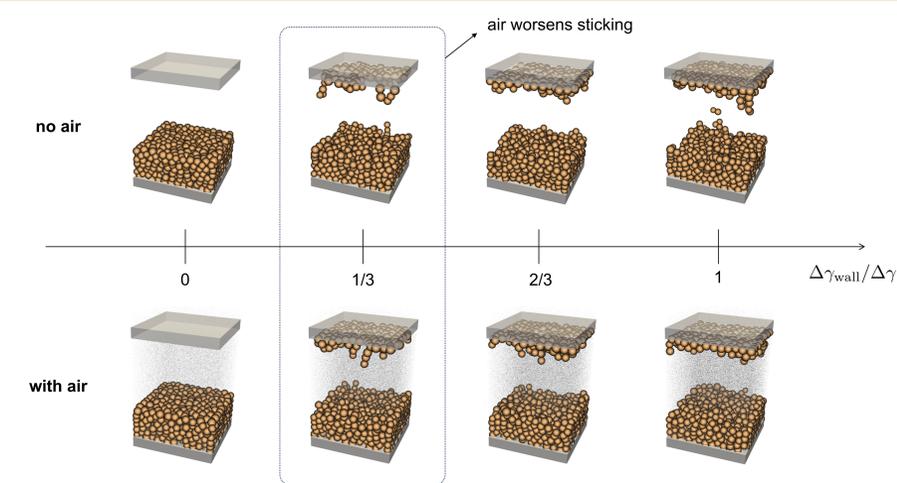
Beyond Tableting: Pieter's Pelleting Process



Open Question:

What controls the pellet length?

Sticking Study



Publications

- Zunker, W., & Kamrin, K. (2024). A mechanically-derived contact model for adhesive elastic-perfectly plastic particles, Part I: Utilizing the method of dimensionality reduction. *Journal of the Mechanics and Physics of Solids*, 183, 105492.
- Zunker, W., & Kamrin, K. (2024). A mechanically-derived contact model for adhesive elastic-perfectly plastic particles, Part II: Contact under high compaction—modeling a bulk elastic response. *Journal of the Mechanics and Physics of Solids*, 183, 105493.
- Zunker, W., Dunatunga, S., Thakur, S., Tang, P., & Kamrin, K. (2025). Experimentally validated DEM for large deformation powder compaction: Mechanically-derived contact model and screening of non-physical contacts. *Powder Technology*, 459, 120972.