Modelling Granular Fragmentation in Compacted Systems

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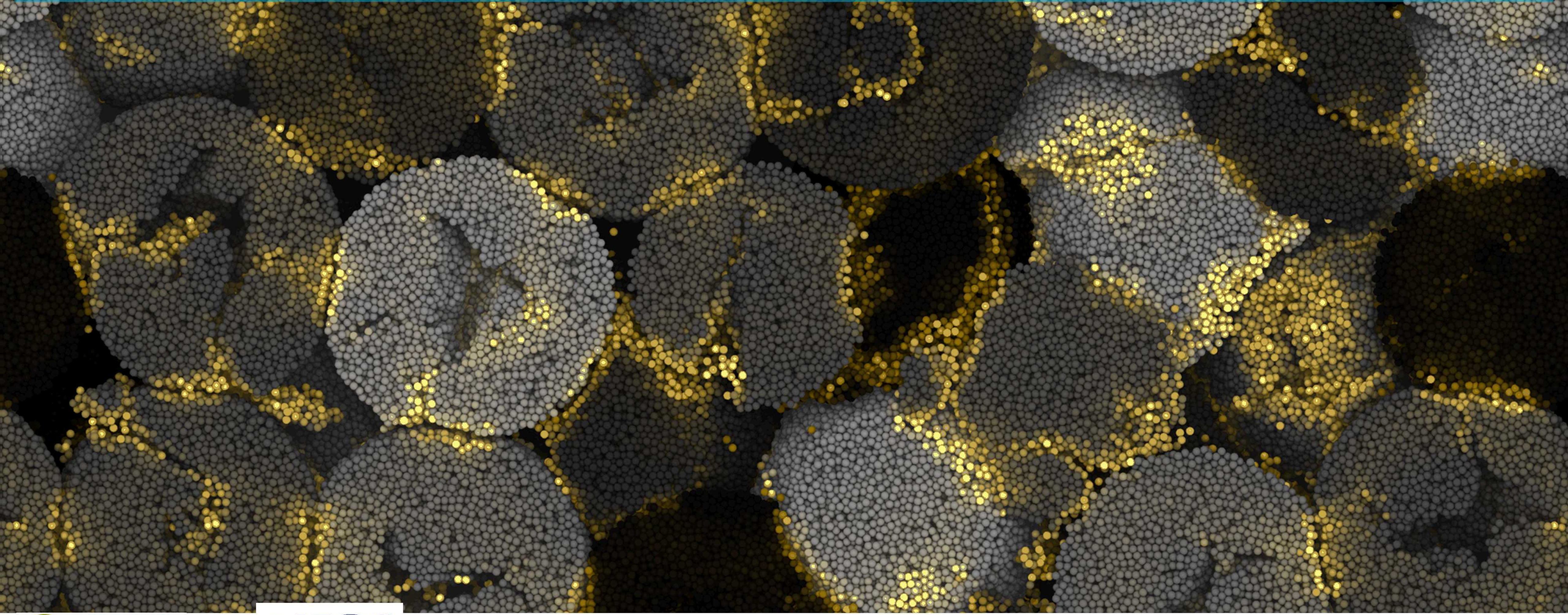

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Granular Compaction at High Pressure

Jamming in limit of zero pressure well understood but many granular flows are at high pressure:
- Geological motion of tectonic plates
- Ballistic impact of brittle materials
- Grinding of powders (comminution)

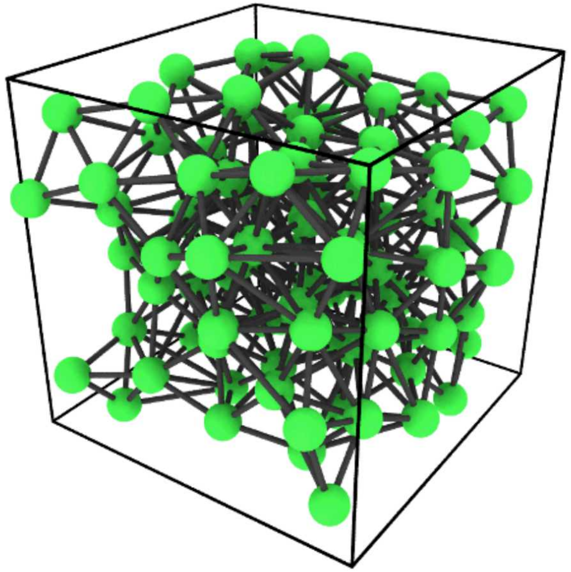
Increasing pressure densifies the system, different mechanisms for densification:
- Particle rearrangement
- Particle deformation
- Particle fracture

Many open questions for granular materials:
- Can we separate regimes of densification?
- What is the functional form of the yield surface?
- Can we connect a distribution of failure stresses to compaction curves?

Uniaxial compression of microcrystalline cellulose

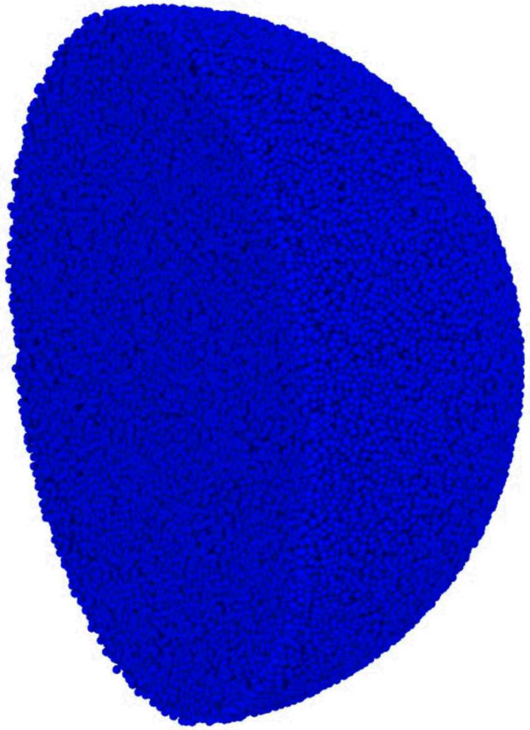
M. Cooper et al. SEM - Experimental and Applied Mechanics (2020)

Discrete Element Model



- Solid composed of repulsive point-particles representin local coarse grained regions (also testing models with rotational DoF)

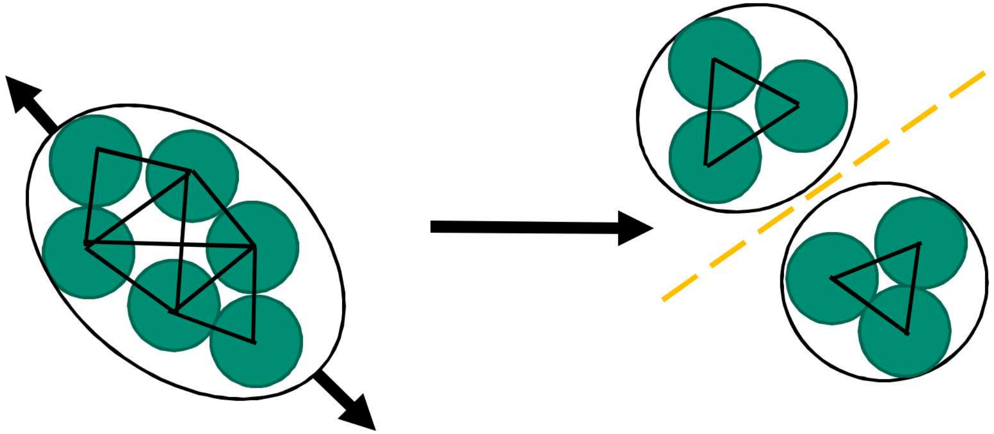
- Connect particles within a grain using a network of attractive bonds (Clemmer, Robbins 2020)



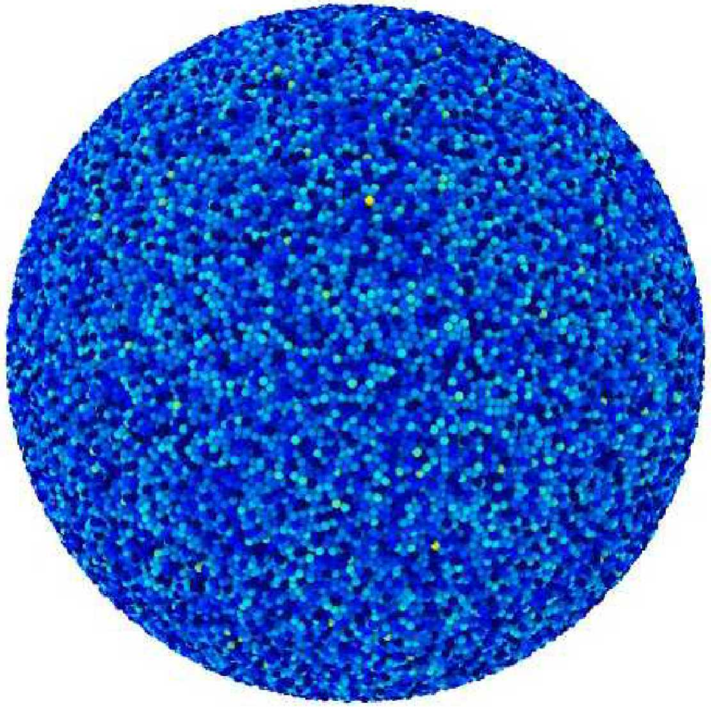
- Advantages of DEM:
  Lagrangian, grid-free method (no restrictions on geometry evolution)
  Full evaluation of stress field (not mean field)
  Complete tracking of individual grains

Bond Fracture

- To allow fracture, define critical stretch λ_C at which attractive bonds break (pairwise repulsion will remain)



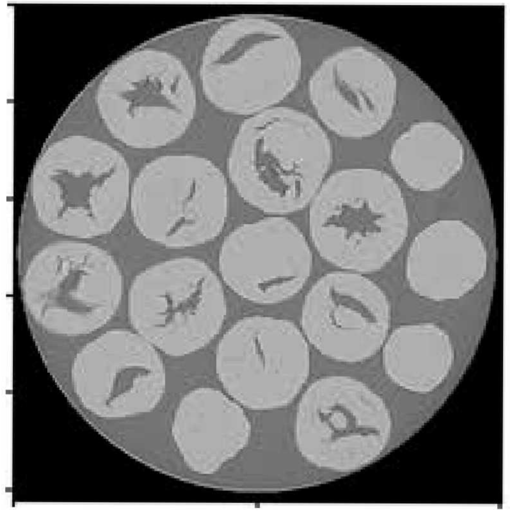
- Can control fracture toughness of material by tuning λ_C (useful for identifying where yield occurs)

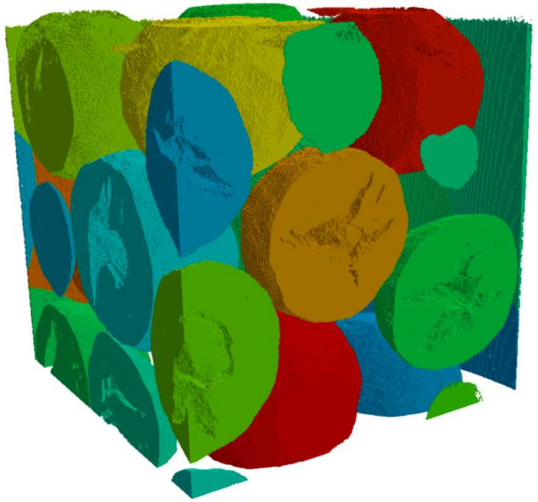


- Includes all mechanisms of densification:
  Rearrangement, deformation, fracture

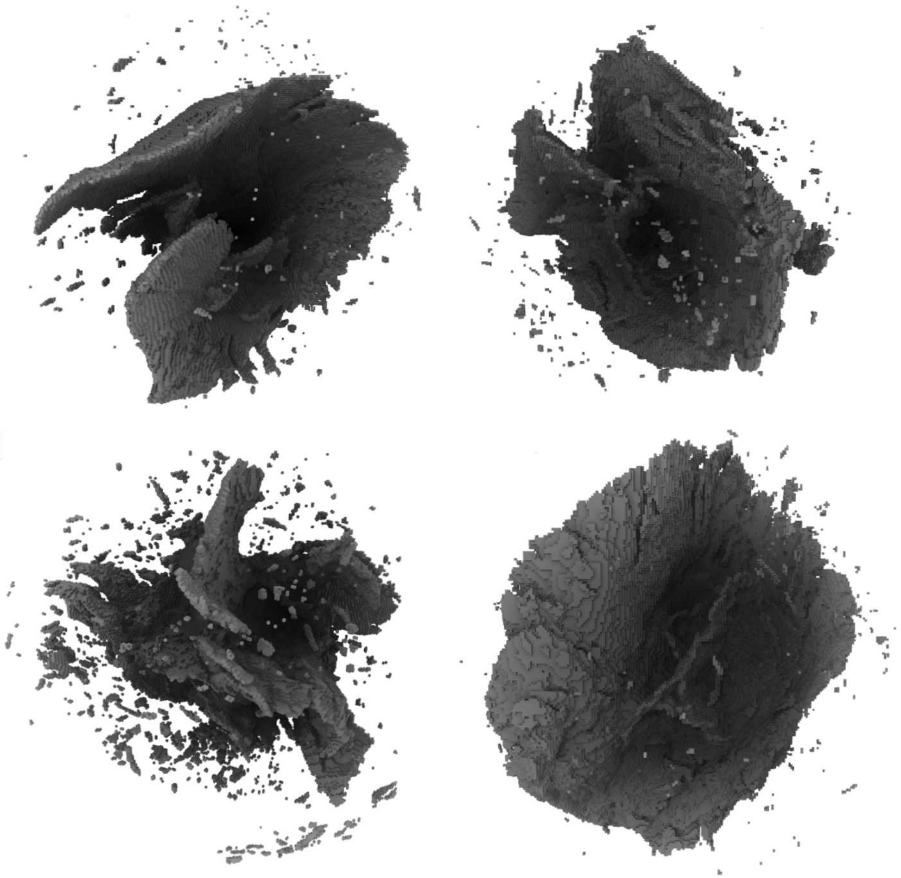
Micro CT Images of Microcrystalline Cellulose

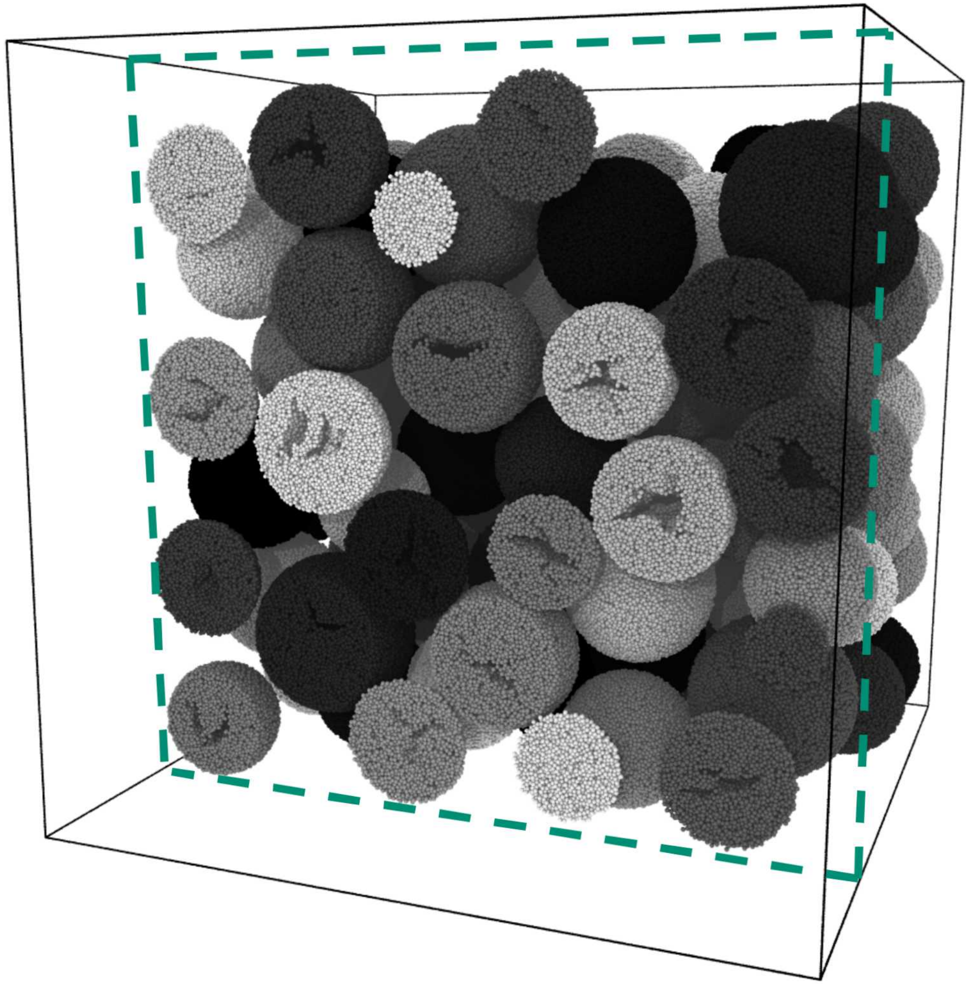
Process CT Images → Create library of internal voids → Apply to grains in DEM packings





M. Cooper et al. (2020)





Simulation Protocol

Run simulations using LAMMPS (Plimpton 1995)

- Provides parallelization and suite of numerical tools
- Currently lacks ability to model bonded DEMs

Initialize packing of 100 spheres of ~30k particles

- Apply internal porosity

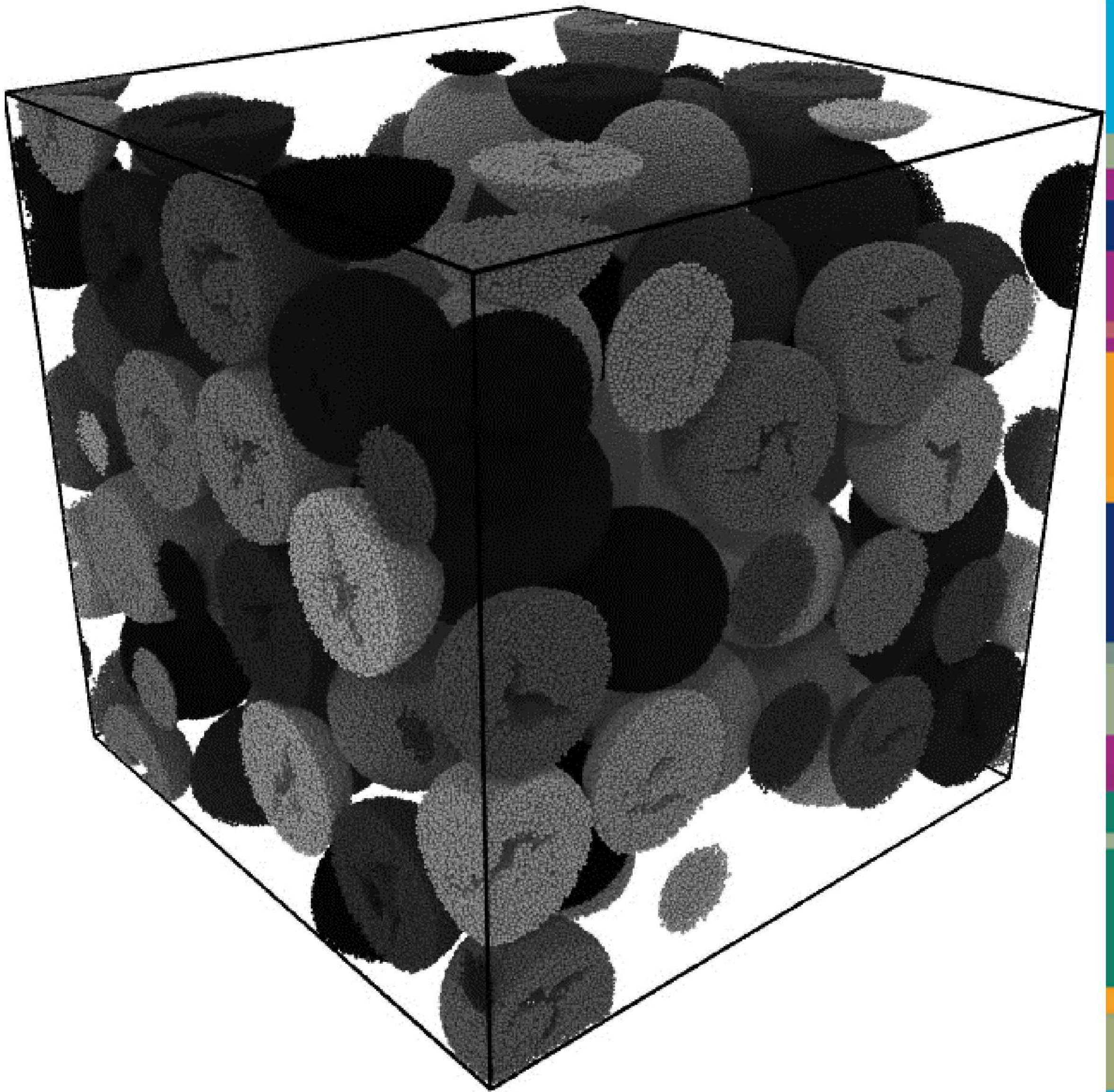
Periodic boundary conditions

Constant volumetric strain rate

- Affinely remap particle positions

Track grain history, bond breakage, system stress

At low pressures, see granular rearrangement
At higher pressures, see deformation/fracture of grains



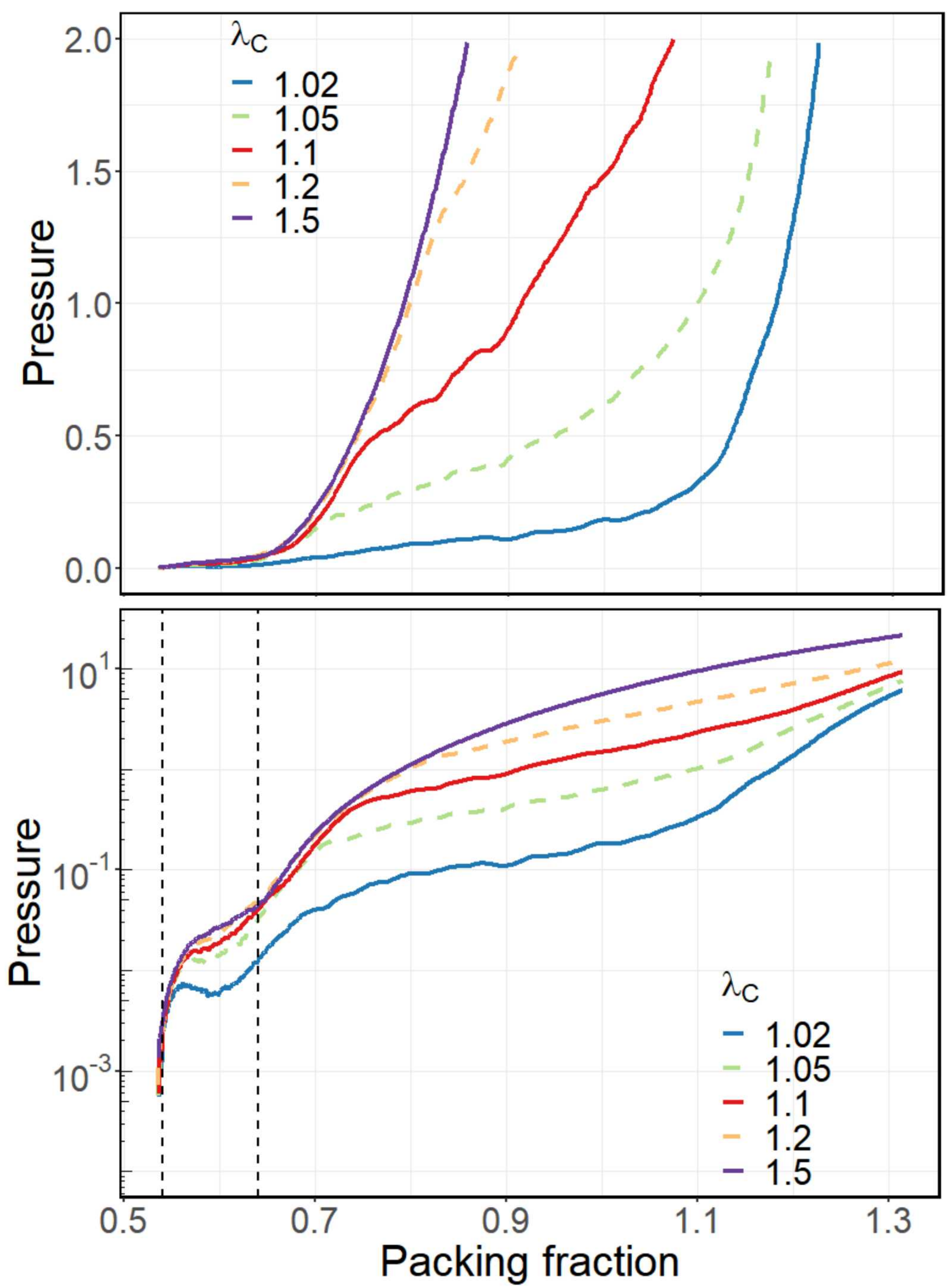
Compression Curves

Jams at packing fraction $\phi \in [0.54, 0.64]$
Intergranular friction decreases ϕ_J (Silbert 2010)

No fracture at high λ_c, only deformation,
Indicates onset of yield (particle fracture)

In future extract non-affine displacement of grain center of masses (track rearrangement)

Note: ϕ exceeds 1.0 due to internal porosity and overlap of fundamental particles at very high pressures



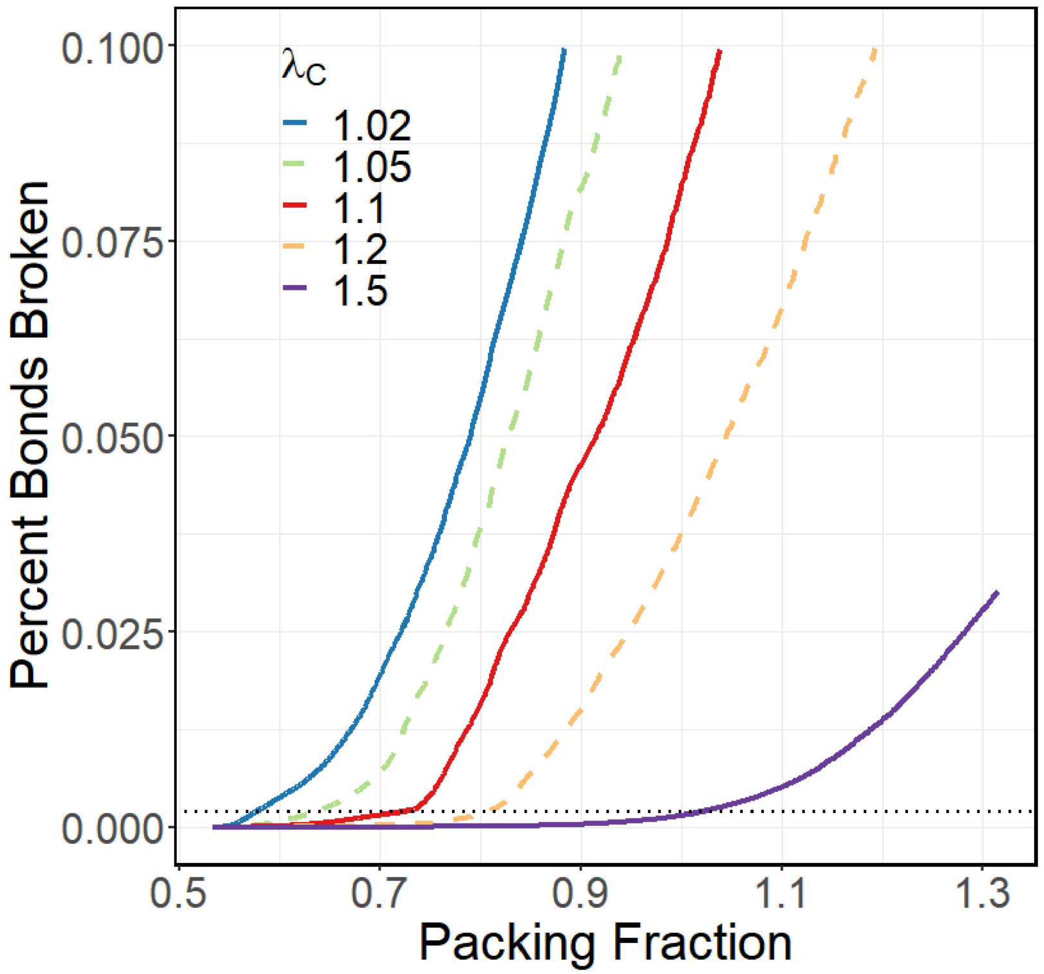
Bond Breakage

As pressure increase, bonds begin to break as granular contacts grind, accelerates when particles fracture

Estimate yield strain when 0.2% of bonds in system break (dotted line)

Yield strain at low λ_C ~corresponds to deviation in compaction curve from large λ_C

Increasing $\lambda_C \Rightarrow$ increased yield strain



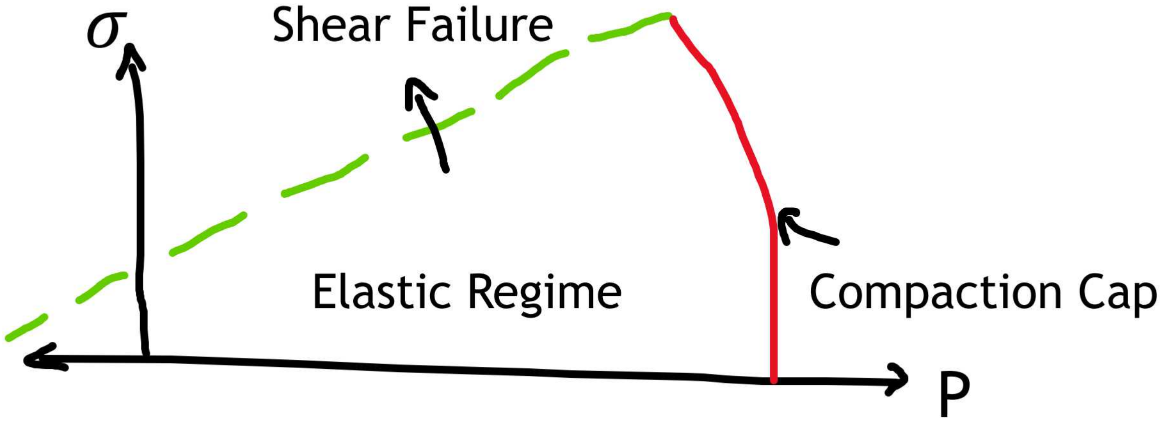
Yield Surface

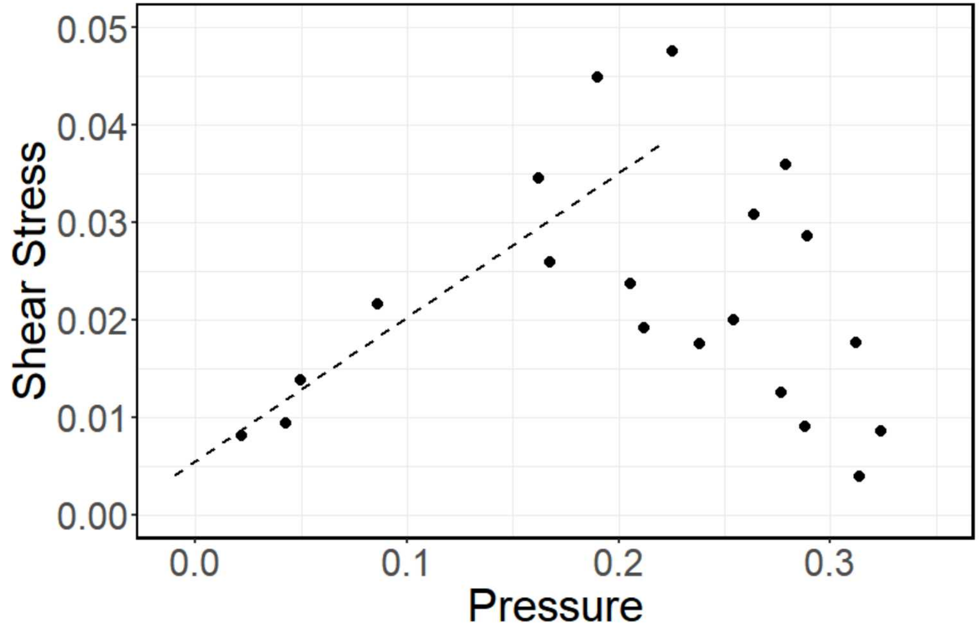
Yield surface defines extent of elastic regime
Many models exist (e.g. Drucker Prager)
Often have compaction caps at high pressures

Add additional shear loading to map out yield surface, have preliminary results for this model

Future tasks:

- Improve statistics:
  - ↑ system size
  - ↑ # of ensembles
- Test definition of yield
- Confirm no rate effects



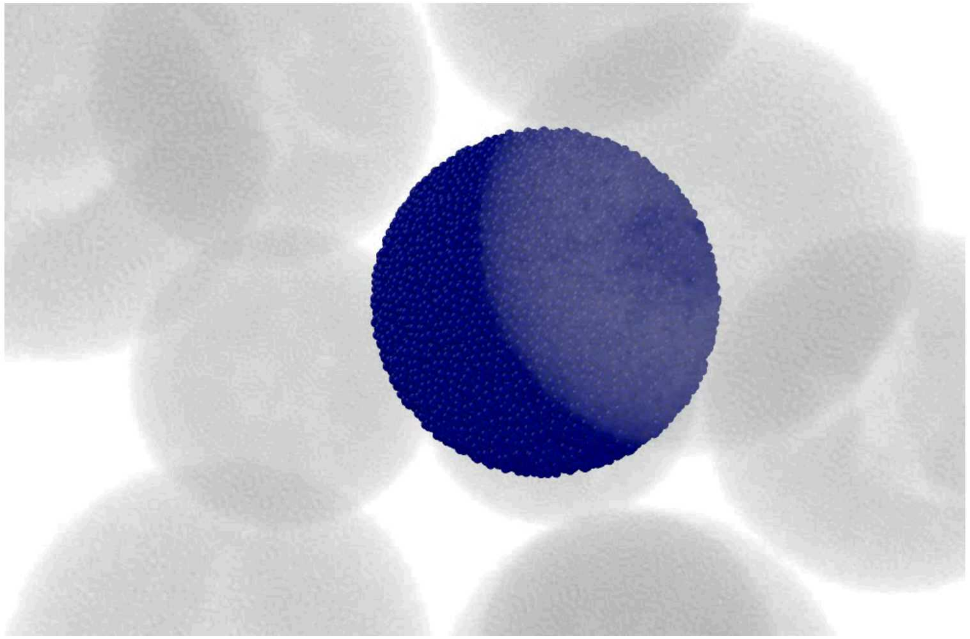


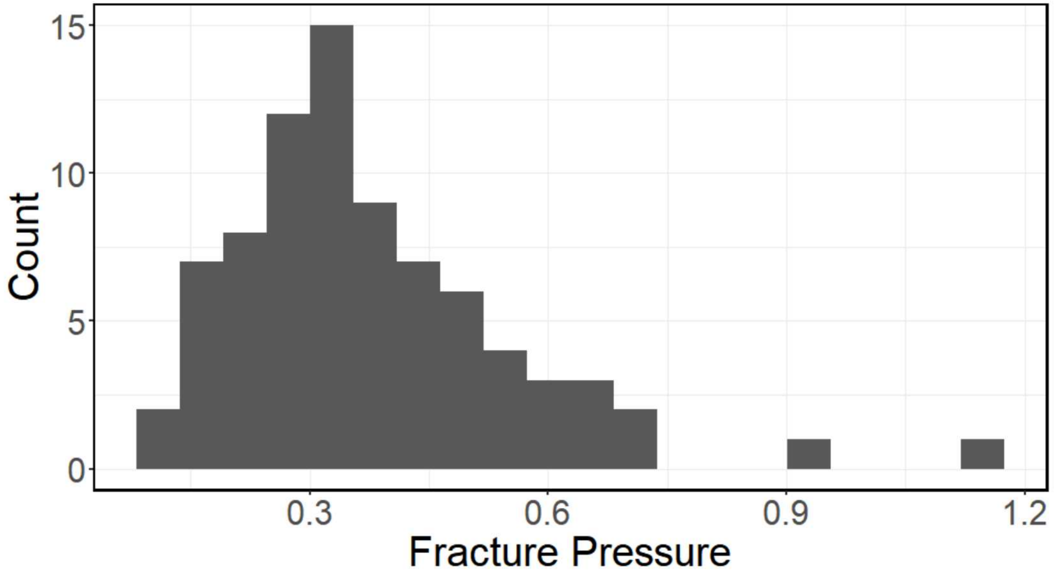
Failure Distribution

Isolate failure of individual grains by preventing surrounding grains from fracturing

Identify distribution of activation pressures to fracture grains

Shape of distribution is suggested to determine shape of compaction curve
(Kenkre et al. 1996)





Summary

Implemented bonded discrete element models to study the flow of granular matter at high pressures – can capture deformation and fracture of grains

Identified compression curves, working to map out regimes of granular rearrangement, deformation, and fracture as well as the yield surface

Began determination of pressure distribution for fracture of individual grains – hope to compare to theoretical predictions for compaction curves

Future: more data, compare results to equivalent experimental system

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