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Modeling powder compaction and particle fragmentation in particulate material-based components using discrete element modeling

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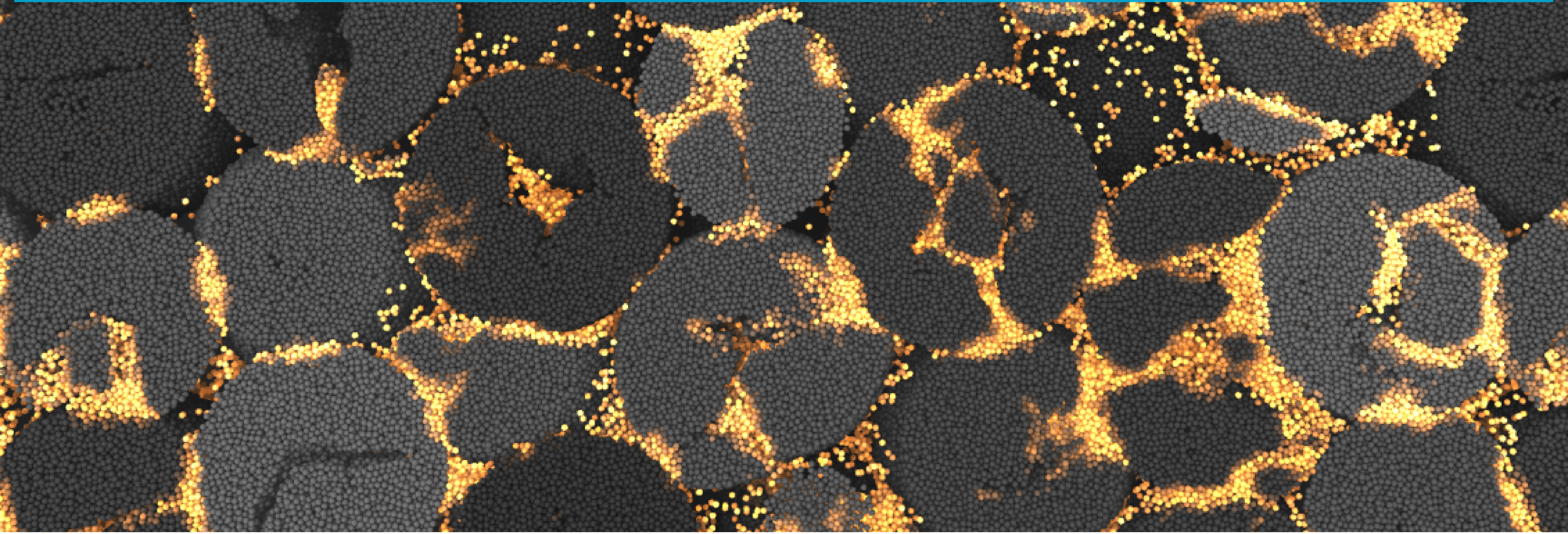

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Fragmentation of Brittle Material

Loading brittle solids and granular material activates many complex processes including:

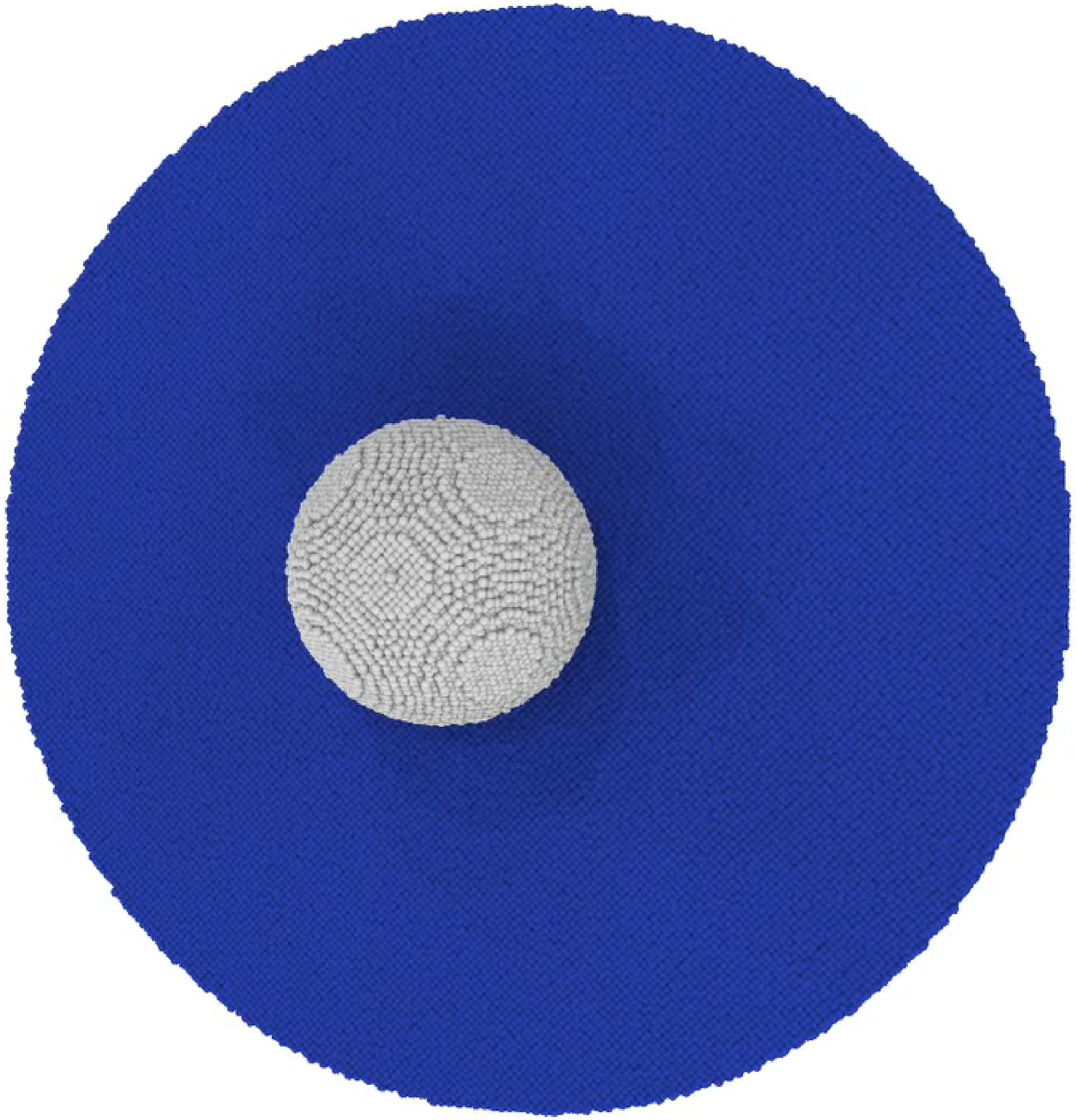
- Deformation, granular rearrangement
- Crack nucleation, growth, and coalescence
- Fragmentation -> material flow

These phenomena present in many natural and industrial systems:

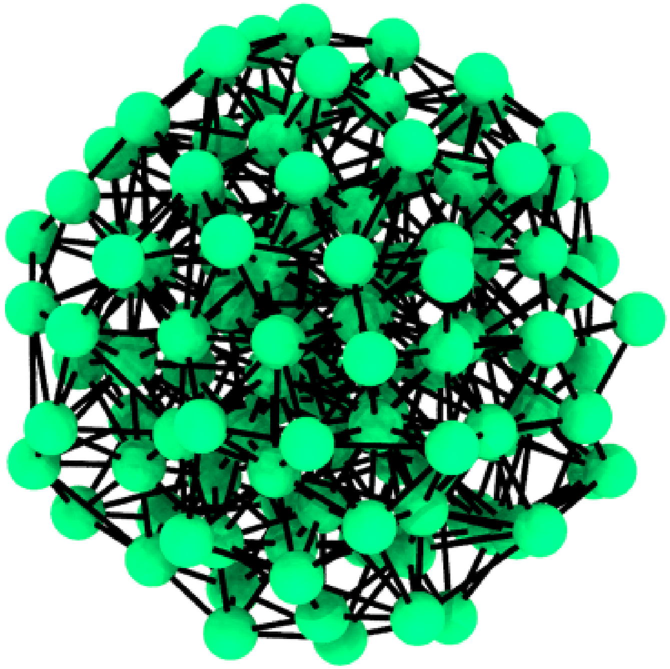
- Tectonic motion
- Ballistic impacts
- Powder compaction/grinding

Behavior depends on loading geometry, strain rates, material properties, and heterogeneities

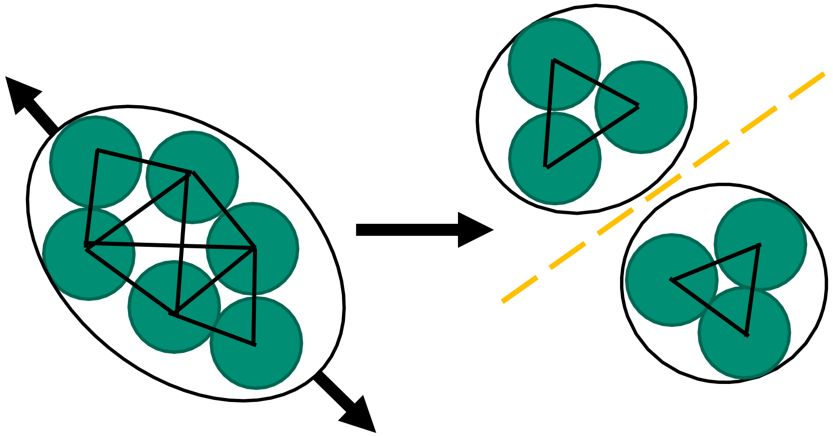
Characterization is essential for many applications
⇒ Critical need to model these processes



Bonded Discrete Element Model (DEM)



- Many varieties of DEMs for different applications, currently implementing in LAMMPS
- Typical DEMs represent coarse-grained granular systems, each simulated particle represents one grain
- In bonded DEM, solid components are represented by collection of bonded particles – network of springs represents elasticity
- Solids can fracture by breaking bonds in network
- Can adjust bond parametrization to calibrate material properties (elastic moduli, fracture toughness)



Utility of approach

Advantages of particle-based methods:

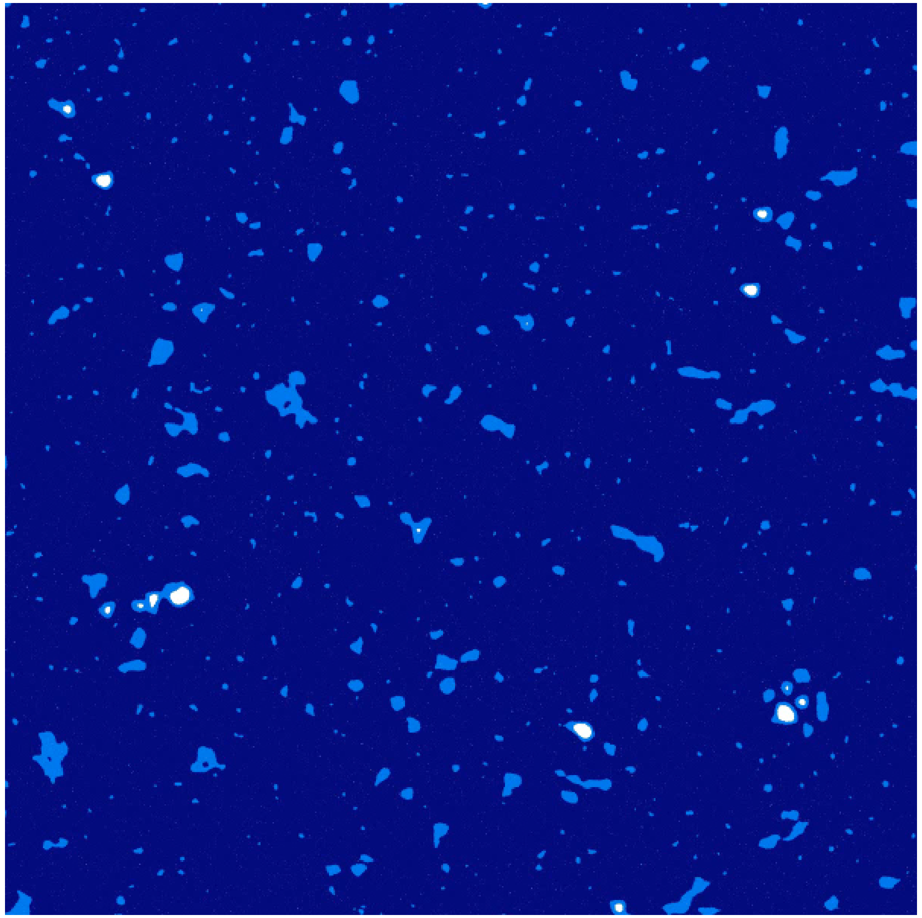
- Fragmentation is highly discontinuous process (contacts & cracks)
- Particles naturally treat discontinuities (meshfree)
- Full representation of stress field
- Crack growth set by physics/stress concentrations

Advantages of DEM:

- Minimally produces emergent fragmentation
- Efficient, can simulate large systems/resolutions

Ideal for studying trends and testing models

Uniaxially compressed solid w/ defects



Application 1: Solid Fragmentation

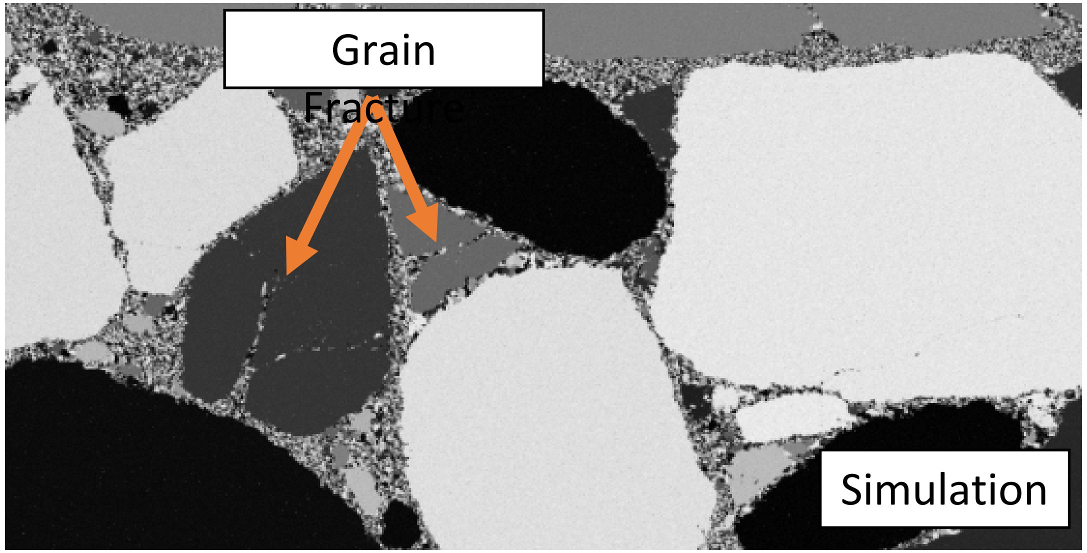
Under shear, solids fragment leading to granular flow where grains continue to break down: comminution

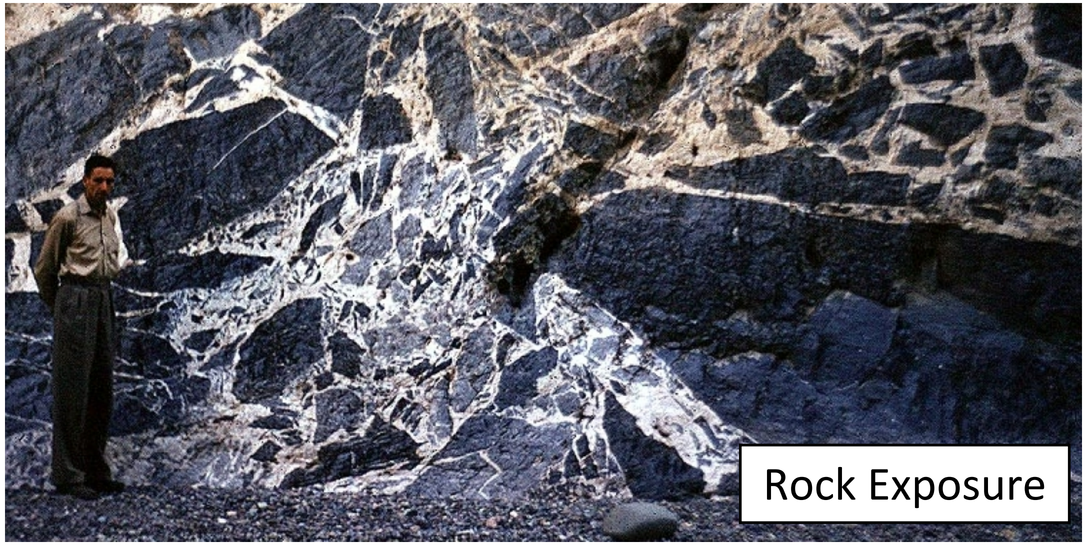
Distribution of grain sizes, often power law:

$N(M) \sim M^{-\alpha}$ $\alpha \sim 1.5 - 2.2$ (Turcotte 1986)

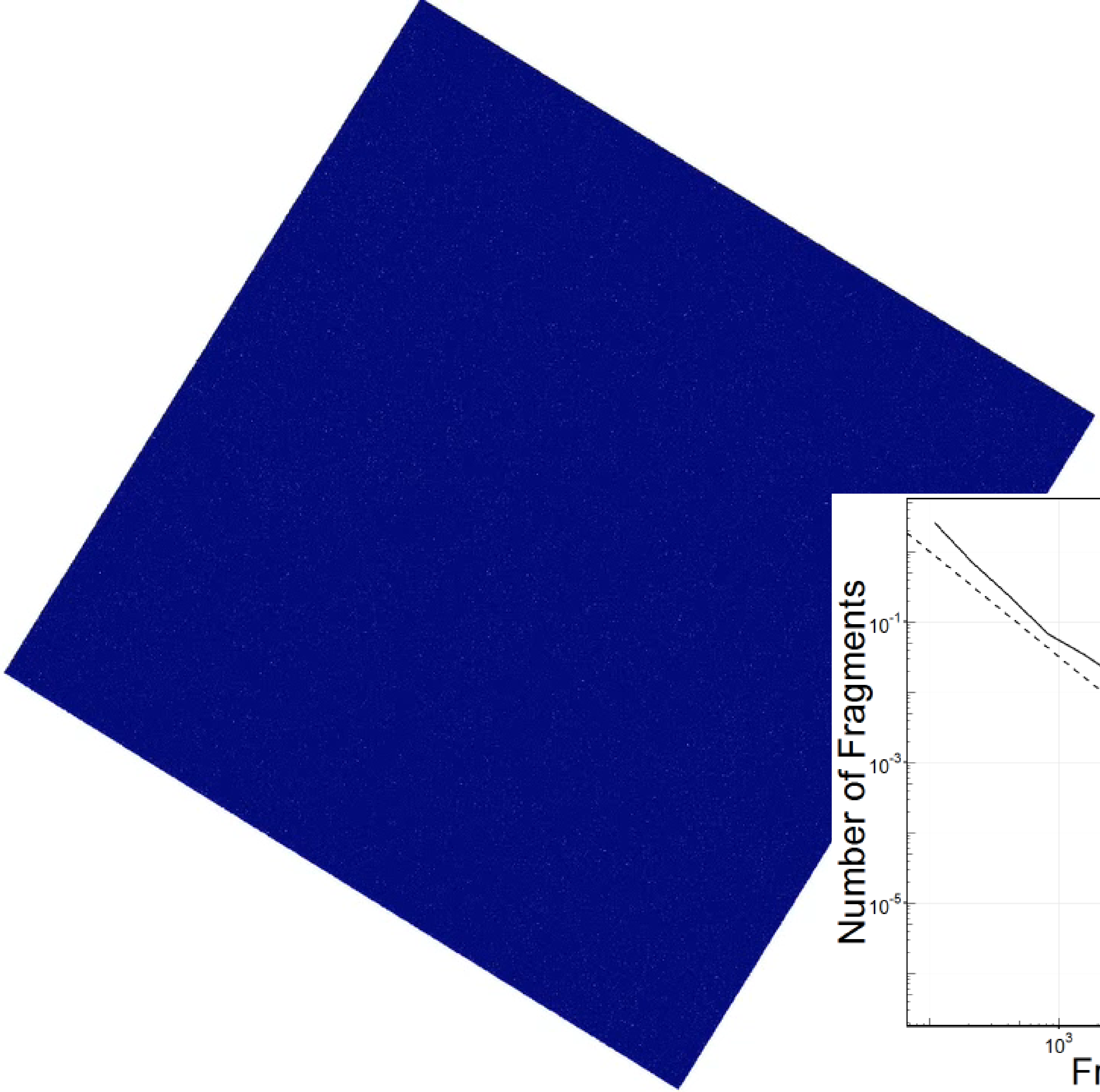
Comminution may be scale invariant:
– How does $N(M)$ evolve with strain?
– What is the equivalent to a steady state?
– What is the impact of rate/material properties?
– Is this an instance of criticality?

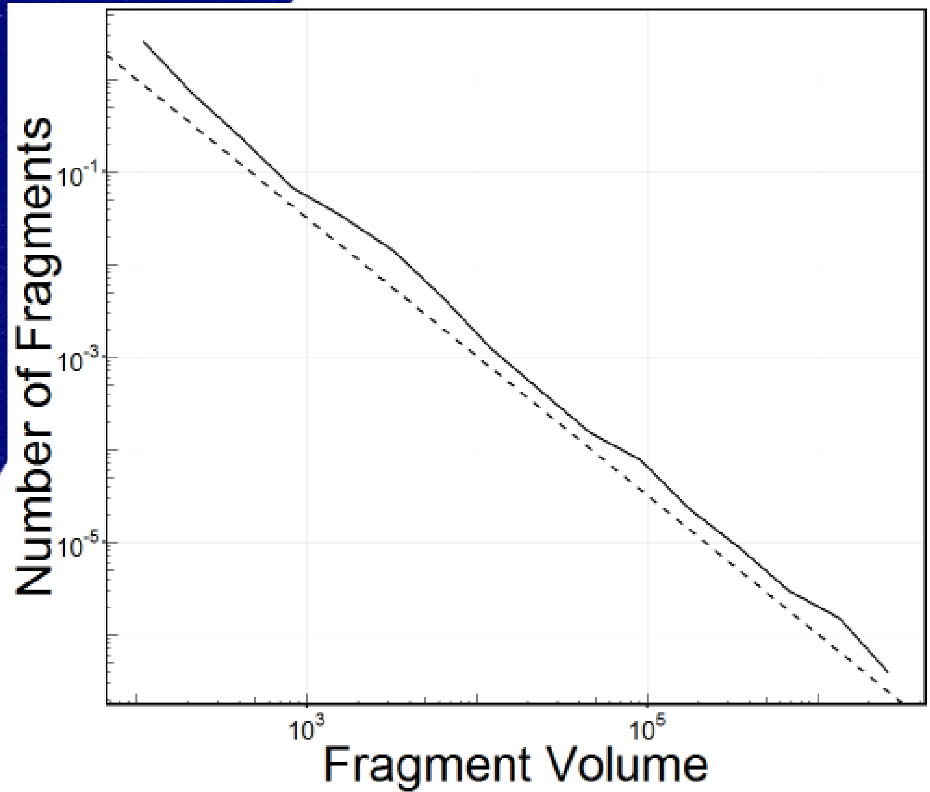
Explore using bonded DEM (Clemmer, Robbins 2021)





Jim Talbot – Western Washington University

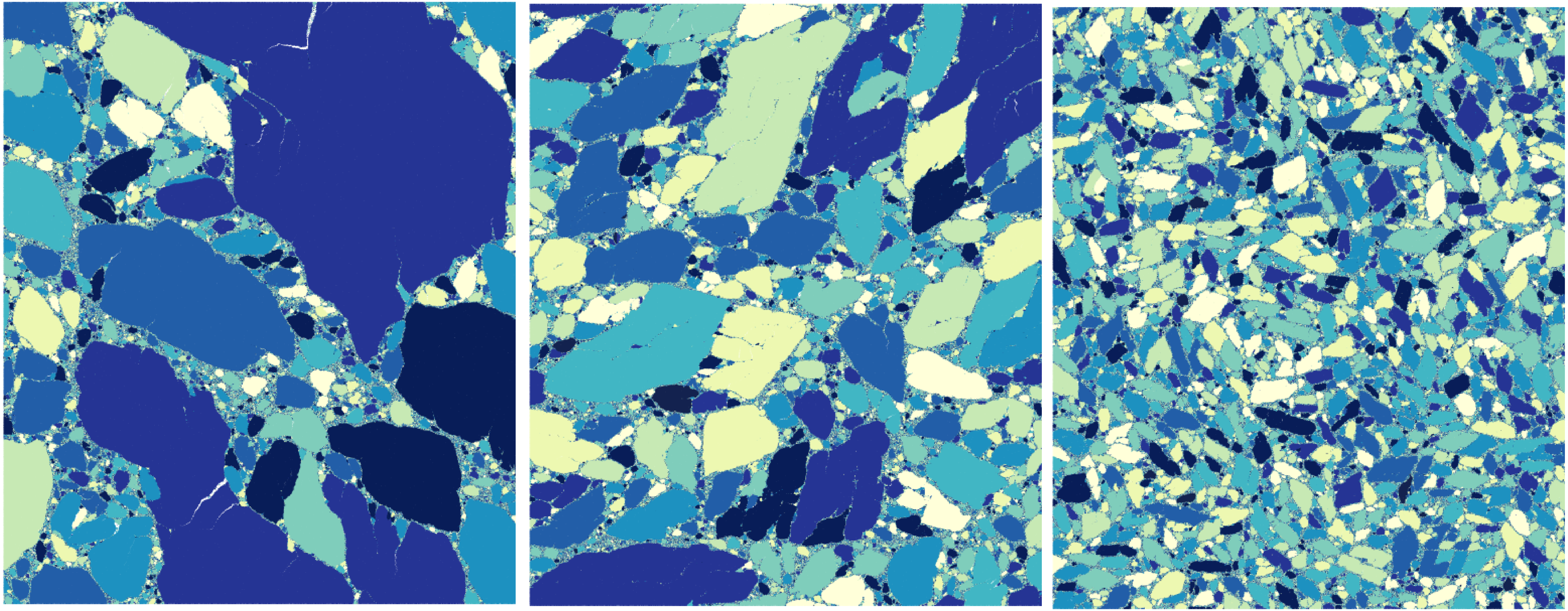




(Clemmer, Robbins 2021)

Granular Medium after 150% Strain

Rate introduces characteristic length scale that decreases with increasing rate



Increasing strain rate

(Clemmer, Robbins 2021)

Rate dependent maximum grain size

(Clemmer, Robbins 2021)

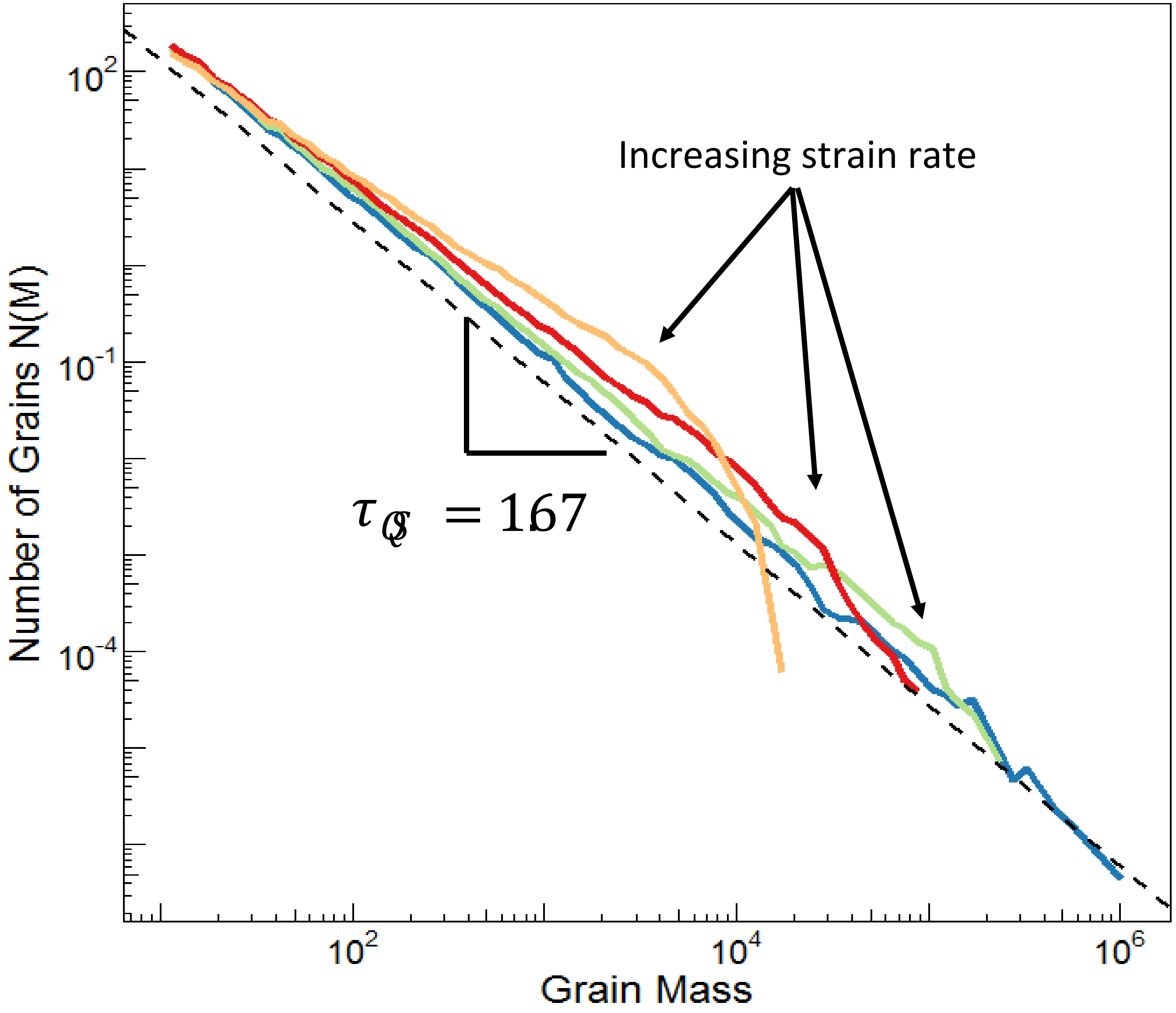
Power law extends up to maximum grain cutoff that increases with decreasing rate
See ↑ in exponent with ↑ in rate

As strain increases, power law extends to larger lengths with in QS limit

At finite rate, exponents changes with strain

No detected dependence on material properties (moduli, fracture toughness)

Could suggest loading conditions are responsible for variation in measured power laws



Application 2: Powder Compaction

Increasing pressure densifies system, different mechanisms:

- Rearrangement
- Deformation
- Fracture

Fragmentation relatively poorly understood:

- How does fracture depend on macroscopic stress?
- How does packing fraction evolve at high P?
- What's the effect of defects/porosity?

Use bonded DEM to begin answering these questions

Uniaxial compression of microcrystalline cellulose

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

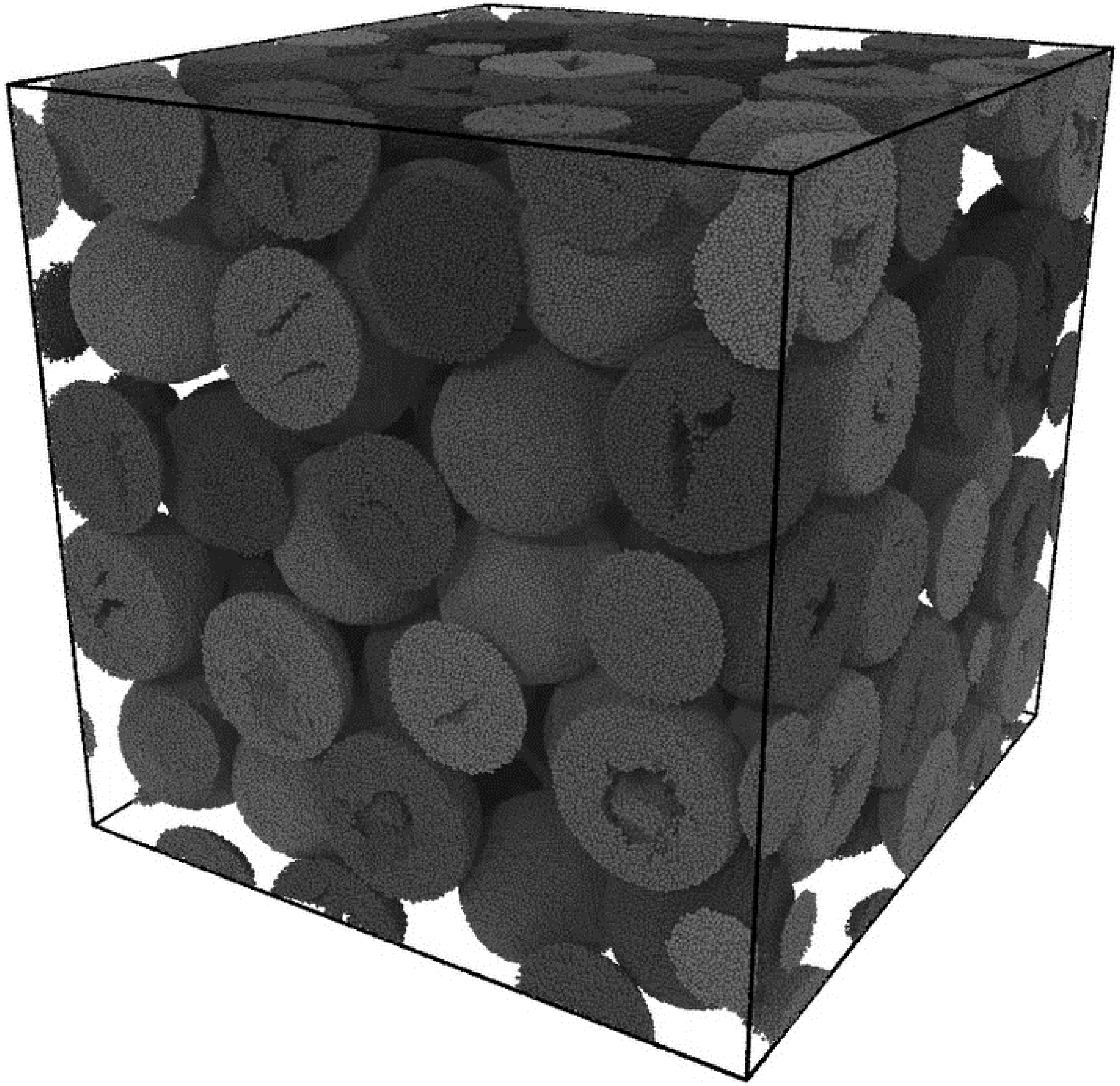
Simulations of compaction

Simulate compaction of 100 spherical grains each consisting of 45k particles

Use microCT images of powder feedstock to apply realistic defect geometries

Can identify:

- Rearrangement
- Deformation
- Failure of grains - fracture



Failure as a function of shear and pressure

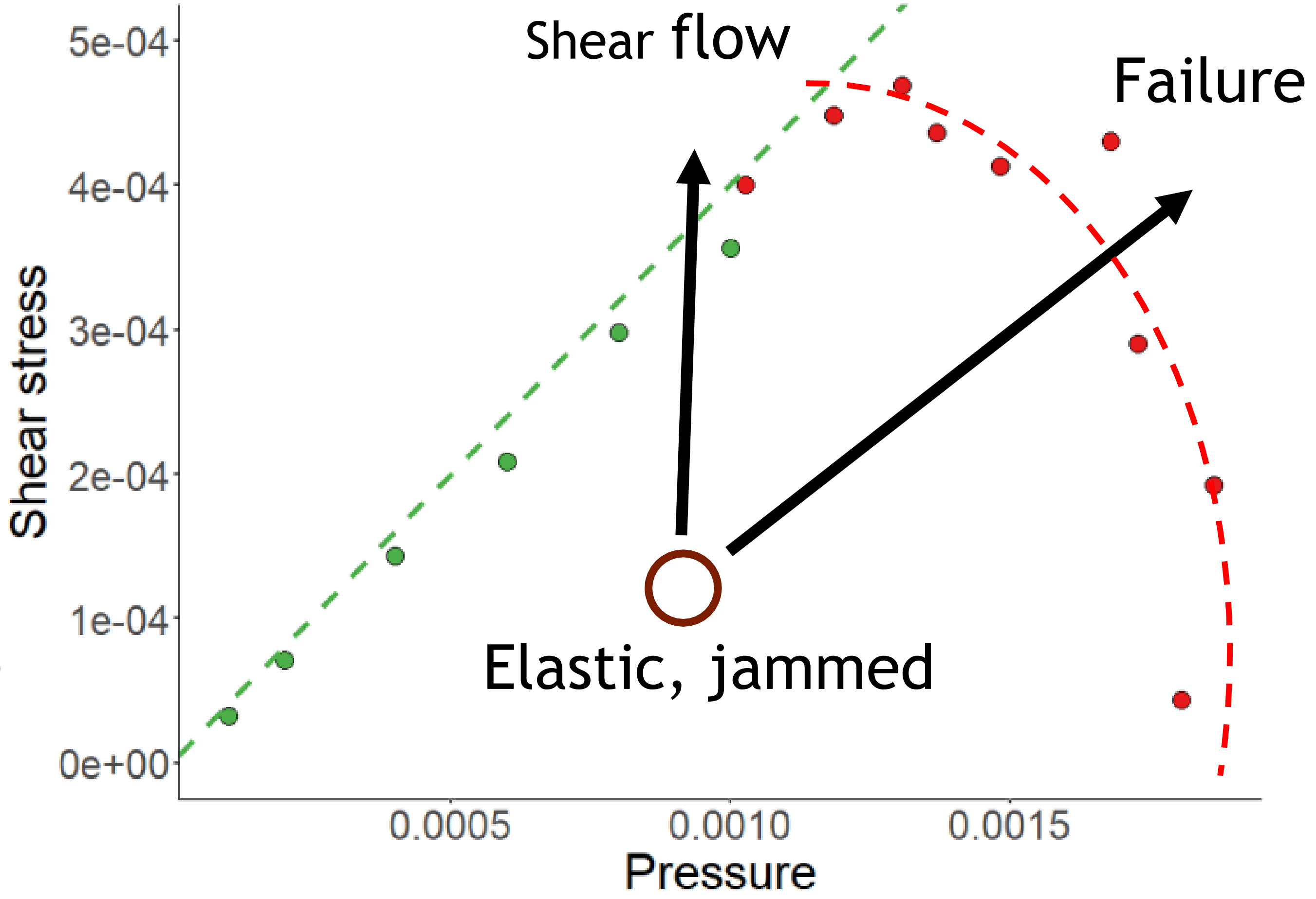
Yield surface: extent of jammed, elastic regime

Low P increase shear:

- Flows above internal friction: $\sigma/P > \mu$
- Find $\mu \approx 0.32$ - typical for materials
- No dependence on grain porosity
- No fragmentation

High P and/or shear:

- Fails at shear stress dependent pressure
- Can evaluate shape of compaction cap, e.g. Drucker-Prager



Isolating strength of individual grains

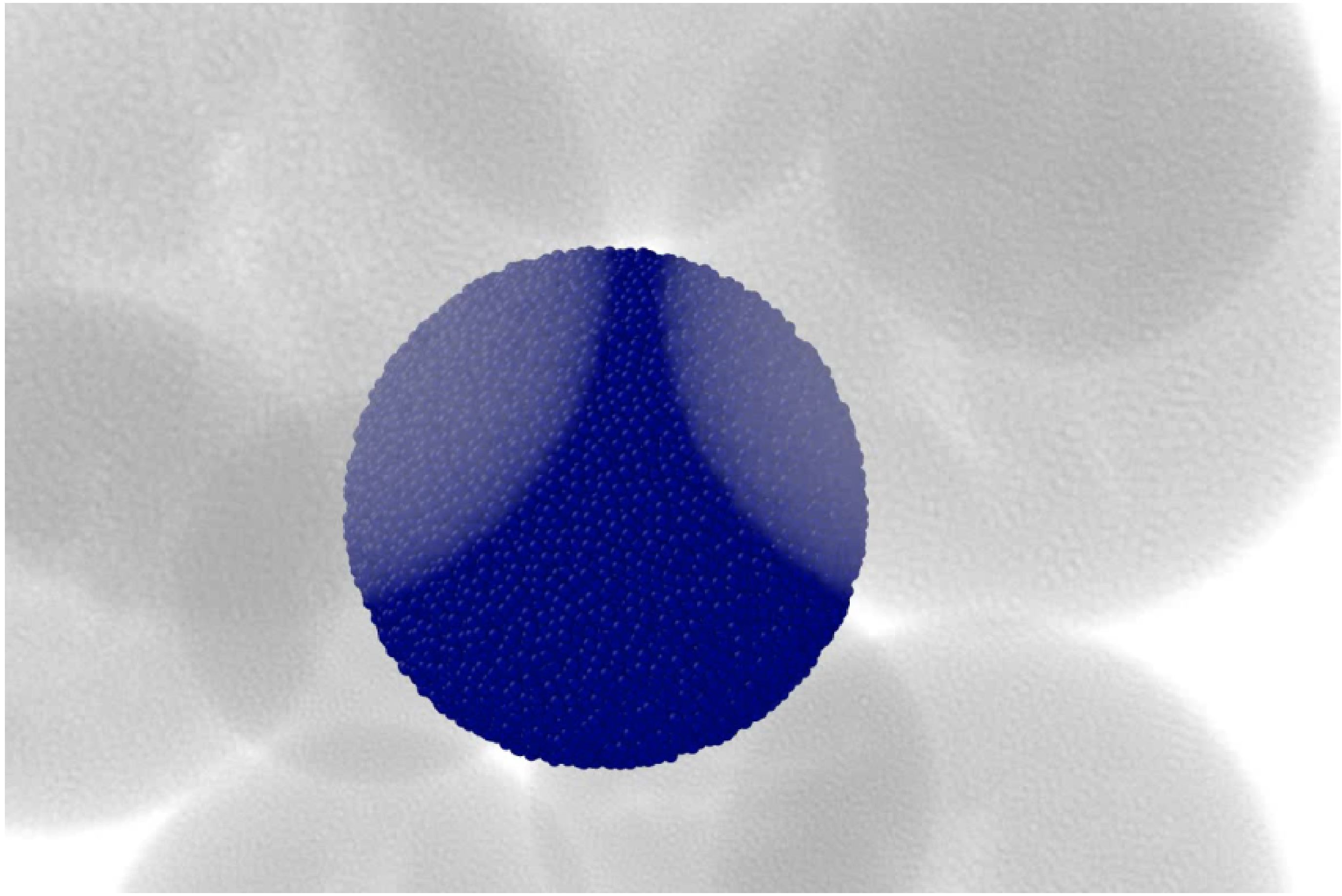
Bulk yield is set by weakest grain

Strength of a grain depends on both:

1) Internal porosity and orientation
2) Local environment
(loading geometry)

Probe variation by isolate single grain failure: preventing bond breakage in surrounding grains

=> Measure strength of every particle



Strength distribution of grains

Find highly skewed distributions
Long tail implies some grains very strong

Vary shape of defects (curve colors), can quantify reduction in strength

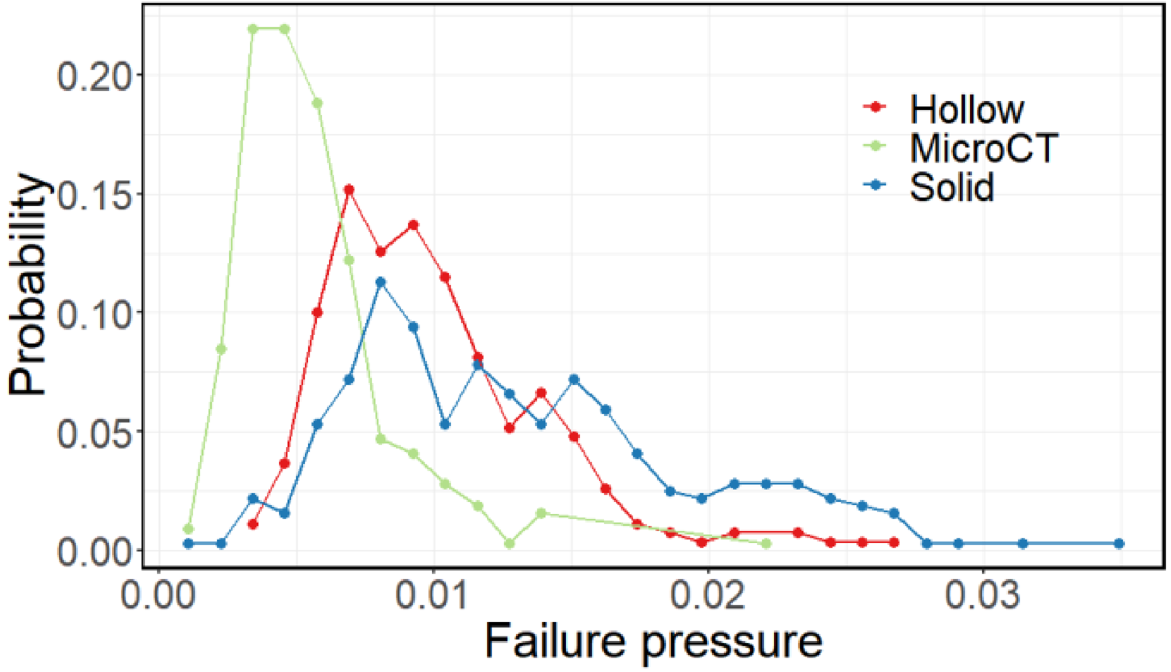
Theorized that distribution determines shape of compaction curve (Kenkre et al. 1996)

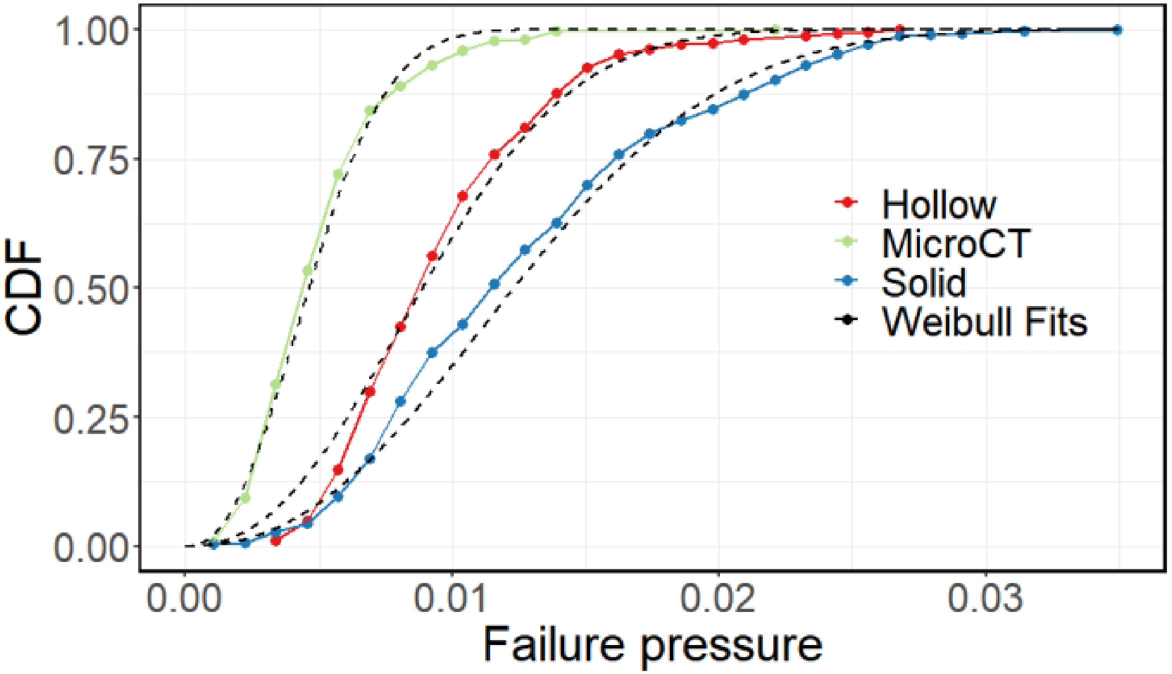
All fit well by Weibull distribution

$$\text{CDF} = 1 - e^{-(P/P_0)^k}$$

Constant exponent $k = 2.3$

P_0 depends on defects





Summary

Particle-based methods are shown to be an effective solution for the many challenges in modeling fragmentation in brittle materials

Bonded discrete element models (soon to be released in LAMMPS) can be applied to probe fundamental mechanics of comminution and granular fracture