Applications of large-scale discrete element models in deformation and fracture of brittle solid and particulate systems

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Joel T. Clemmer, Dan S. Bolintineanu, Jeremy B. Lechman

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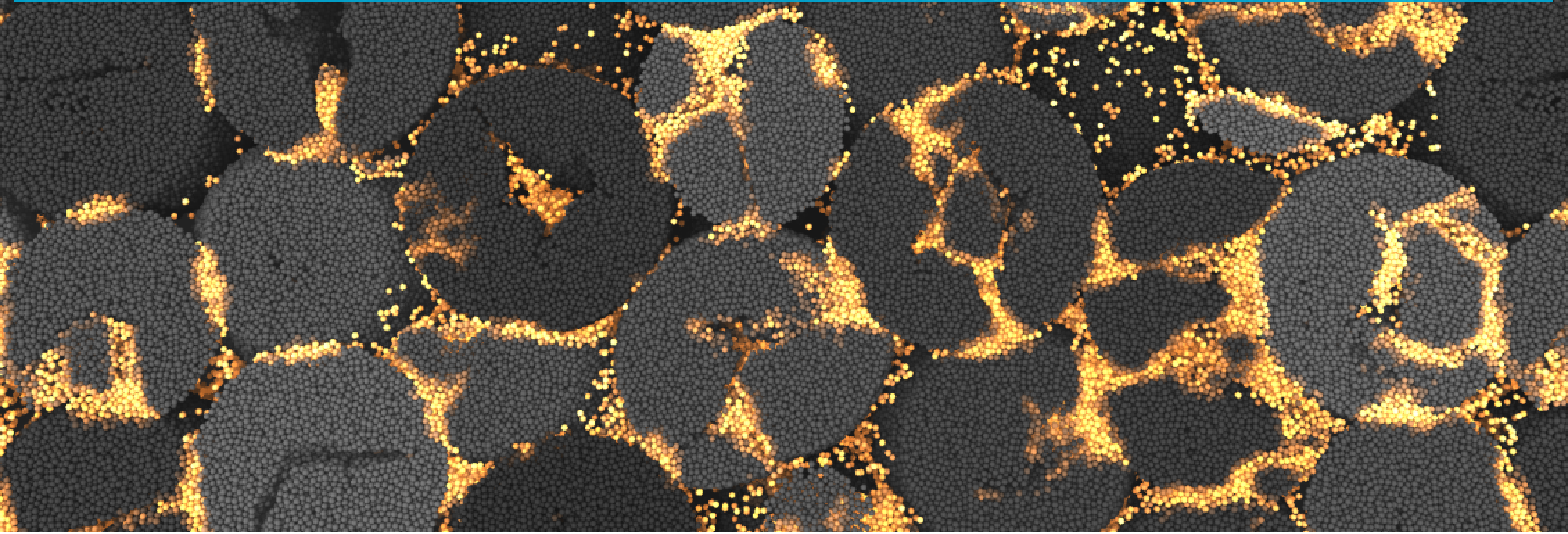

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Fragmentation of Brittle Material

Loading brittle solids and particulates activates many complex processes including:

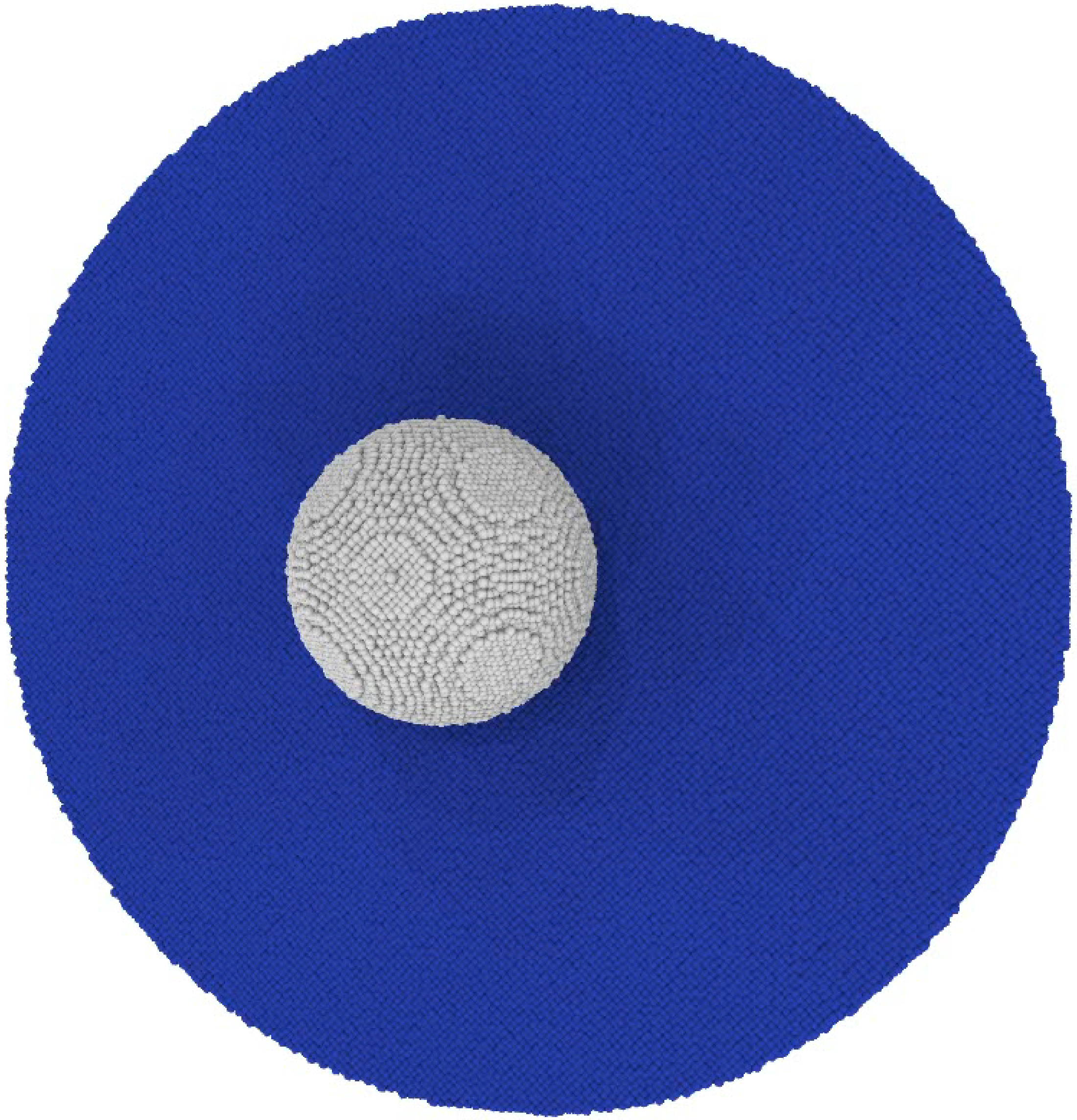
- Deformation
- Crack nucleation, growth, and coalescence
- Fragmentation
- Material flow

These phenomena present in many natural and industrial systems:

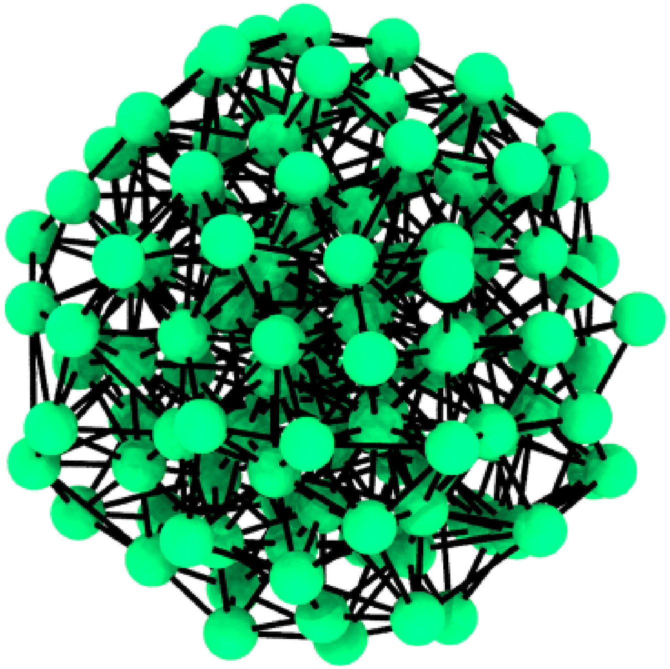
- Tectonic motion
- Ballistic impacts
- Powder compaction/grinding

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

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



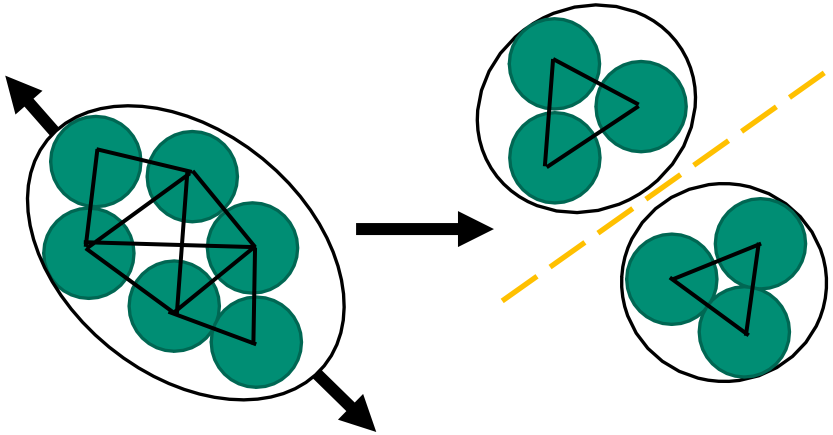
Bonded Discrete Element Model (DEM)



- 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



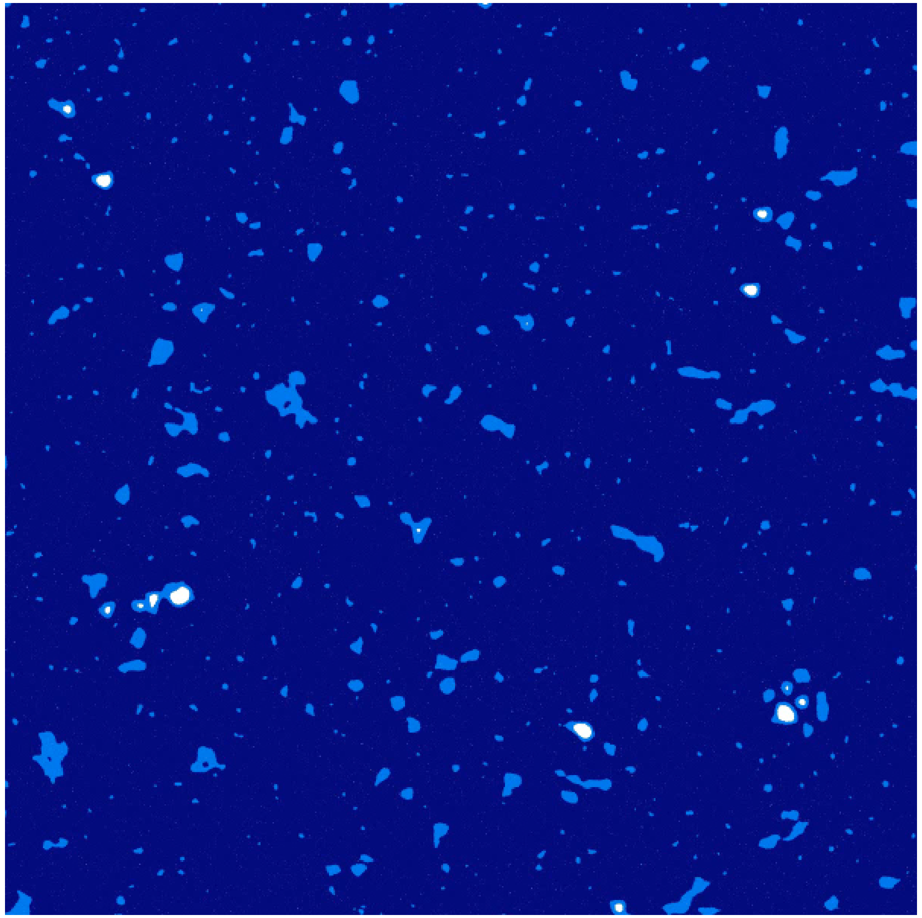
- Can adjust bond parametrization to calibrate material properties (elastic moduli, fracture toughness)

- Many flavors of bonds for different applications, currently implementing in LAMMPS

Advantages 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

Application 1: Solid Fragmentation

In confined granular flow, dilation is limited
 ⇒ Grains may need to break to rearrange

Distribution of grain sizes, often power law:

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

Comminution may be scale invariant:

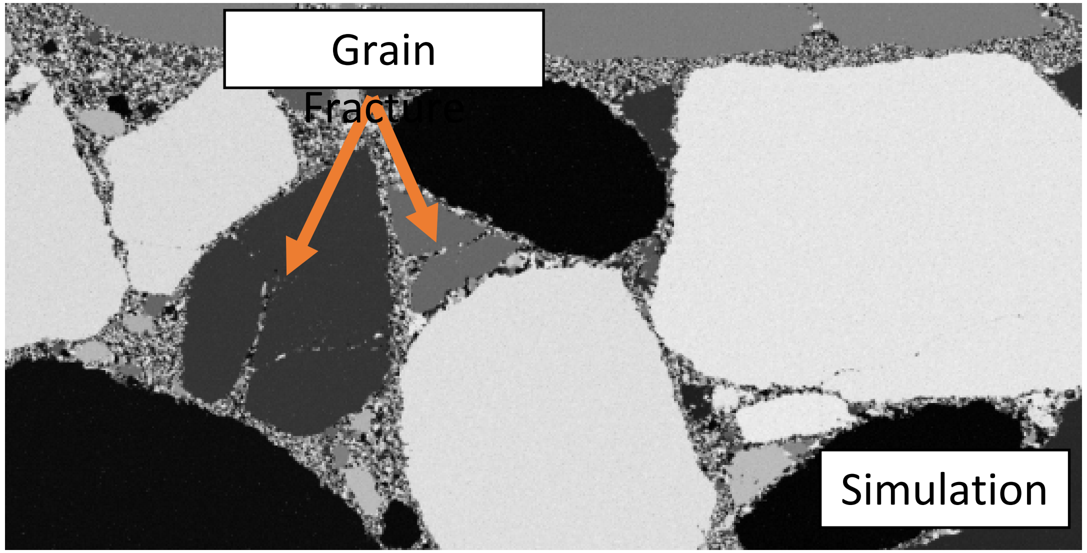
– How does $N(M)$ evolve with strain?

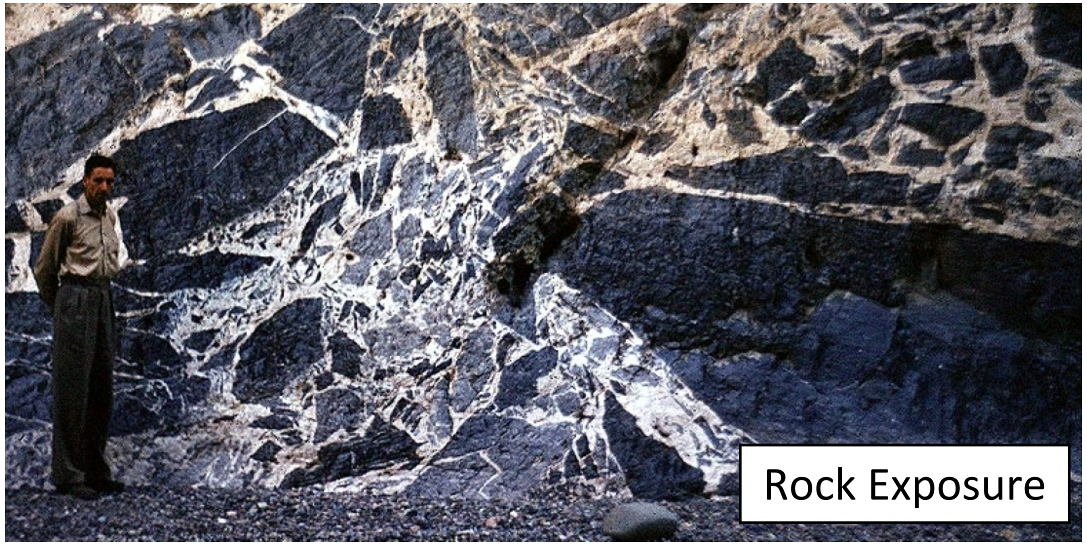
– What is the equivalent to a steady state?

– What is the impact of rate/material properties?

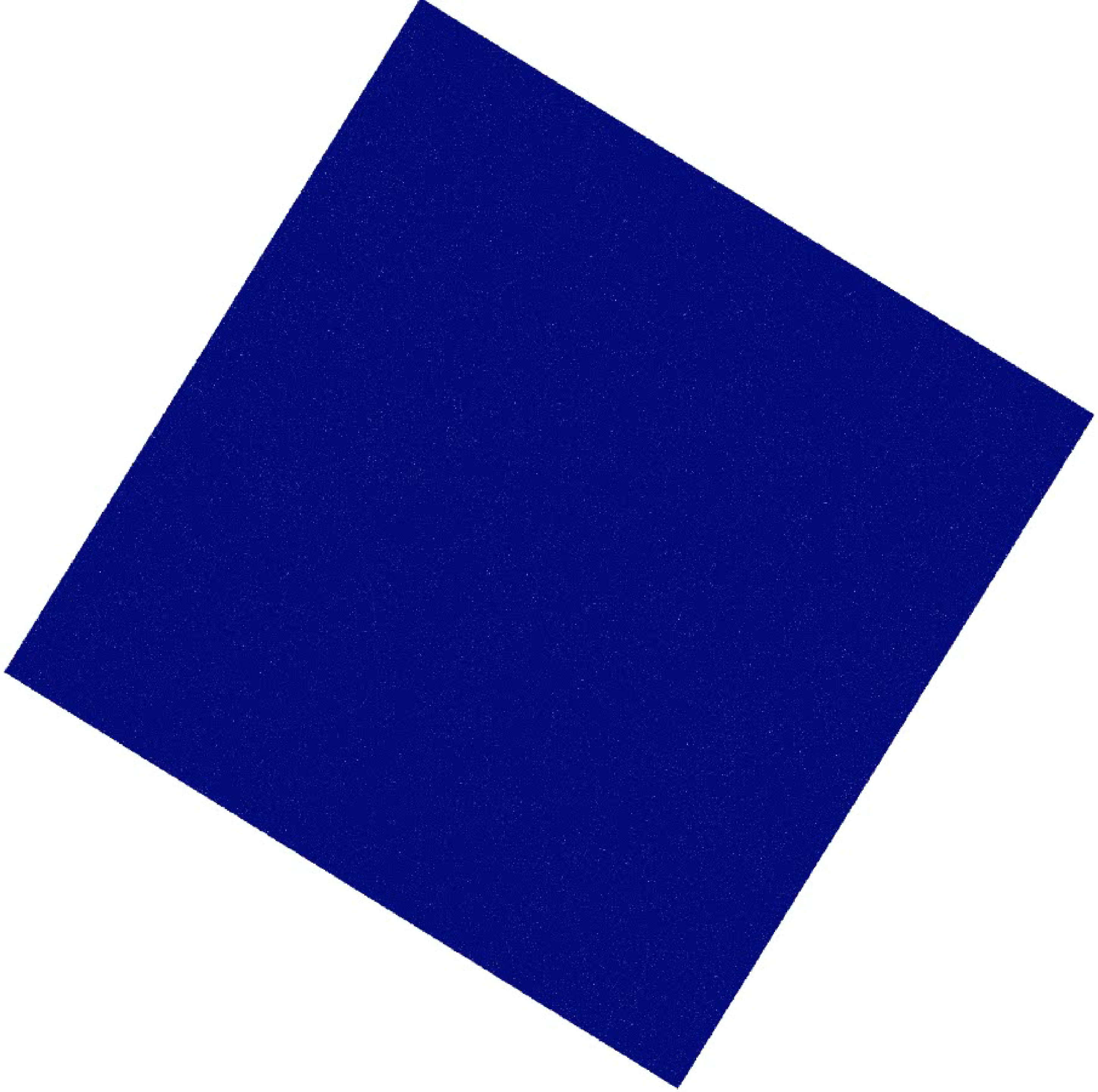
– Is this an instance of criticality?

Explore using bonded DEM (Clemmer, Robbins 2021)



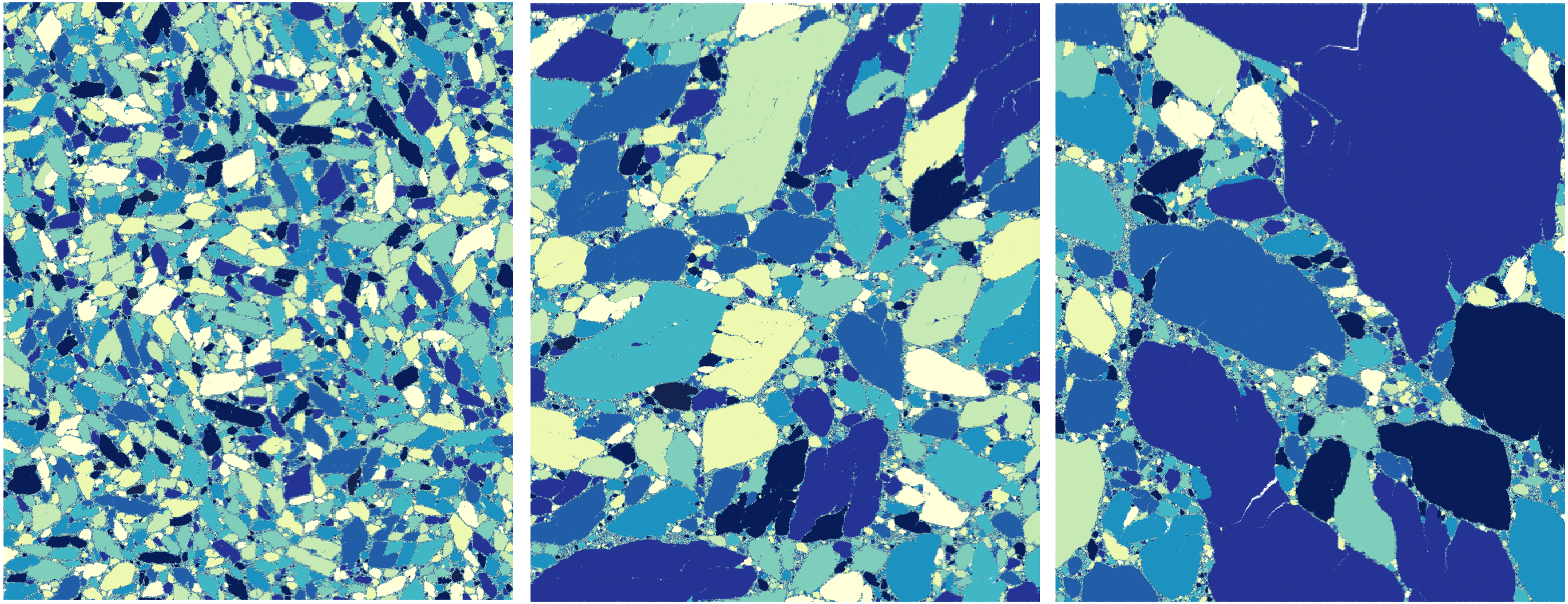


Jim Talbot – Western Washington University



Granular Medium after 150% Strain

Rate introduces characteristic length scale that decreases with increasing rate



Increasing strain rate

Rate dependent maximum grain size

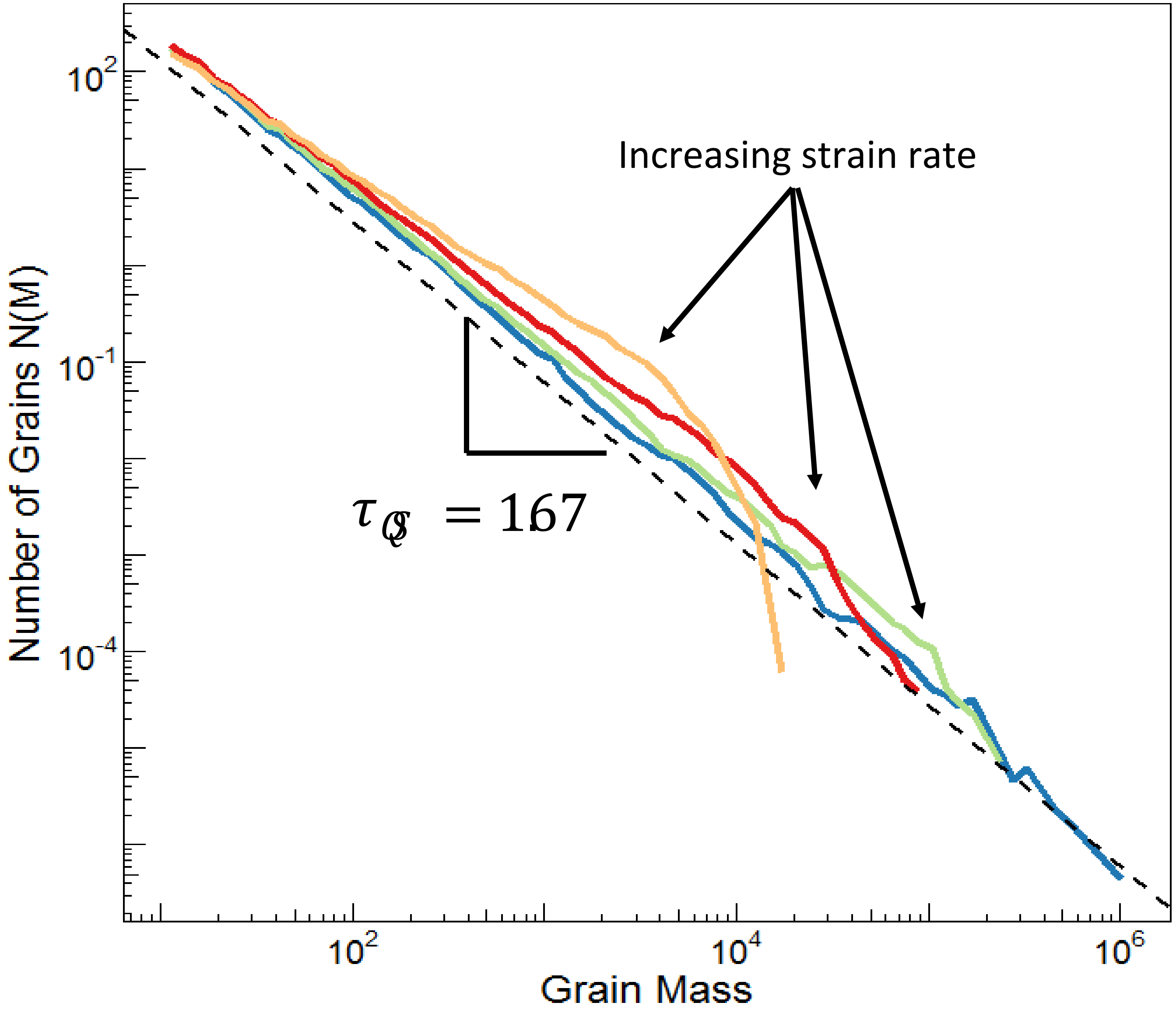
Power law extends up to maximum grain cutoff that increases with decreasing rate
See ↑ in exponent with ↑ in rate

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 partially explain variety of power laws seen in particulate materials: loading conditions determine distribution



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?
  - Are fragments power-law distributed? Critical?

- Use bonded DEM to begin answering these questions

Uniaxial compression of microcrystalline cellulose

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

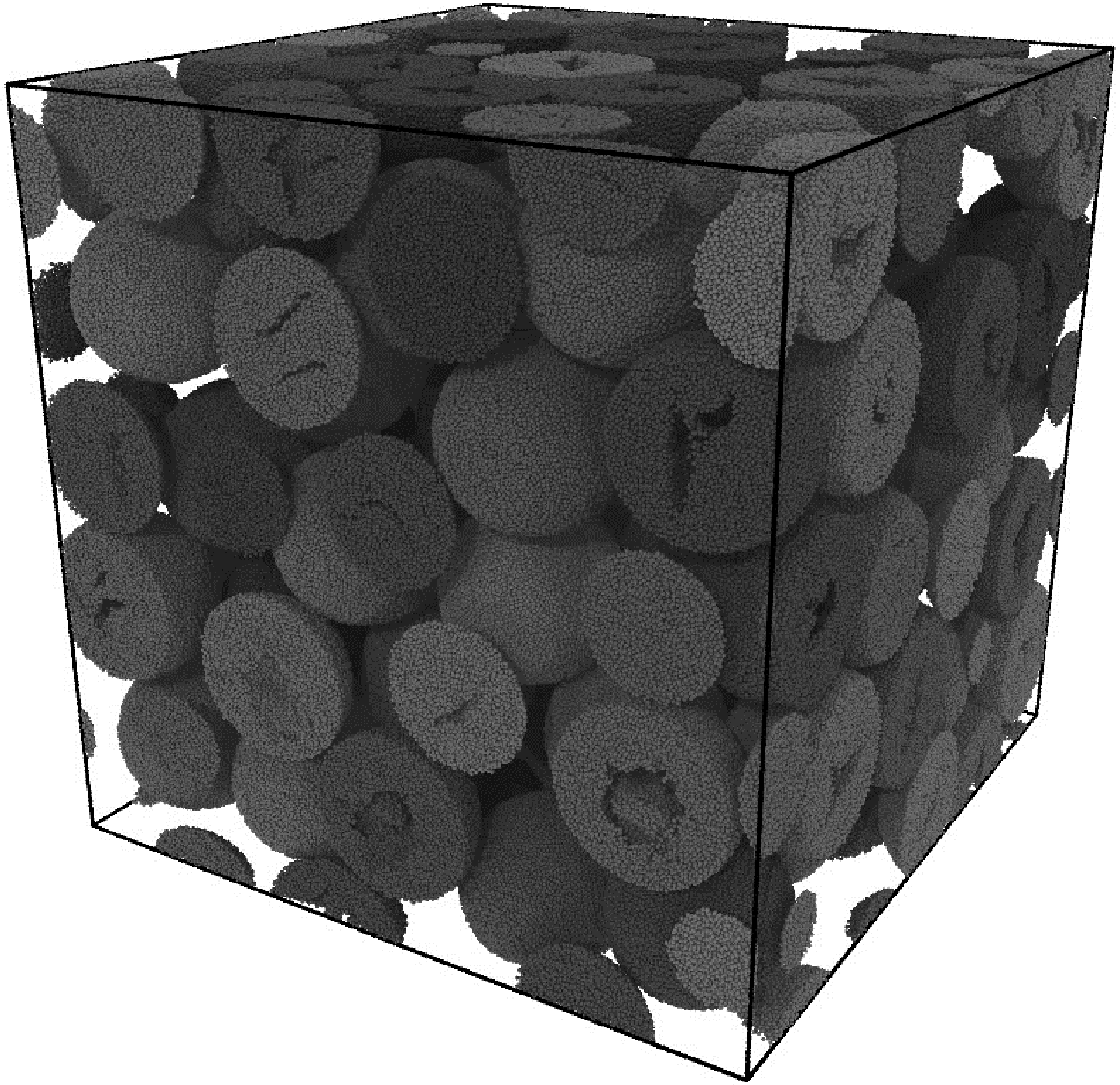
Simulations of compaction

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

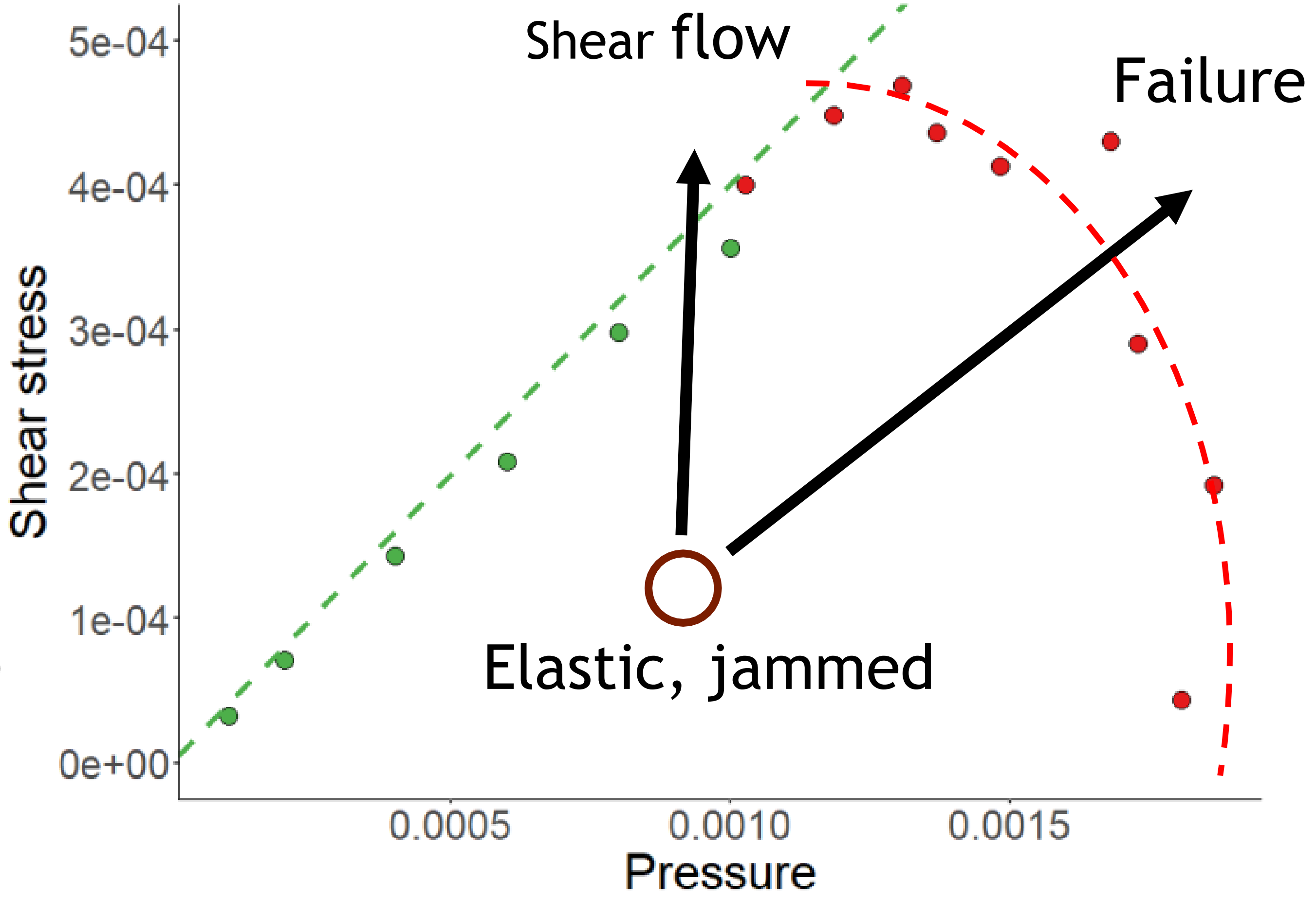


Failure as a function of shear and pressure

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

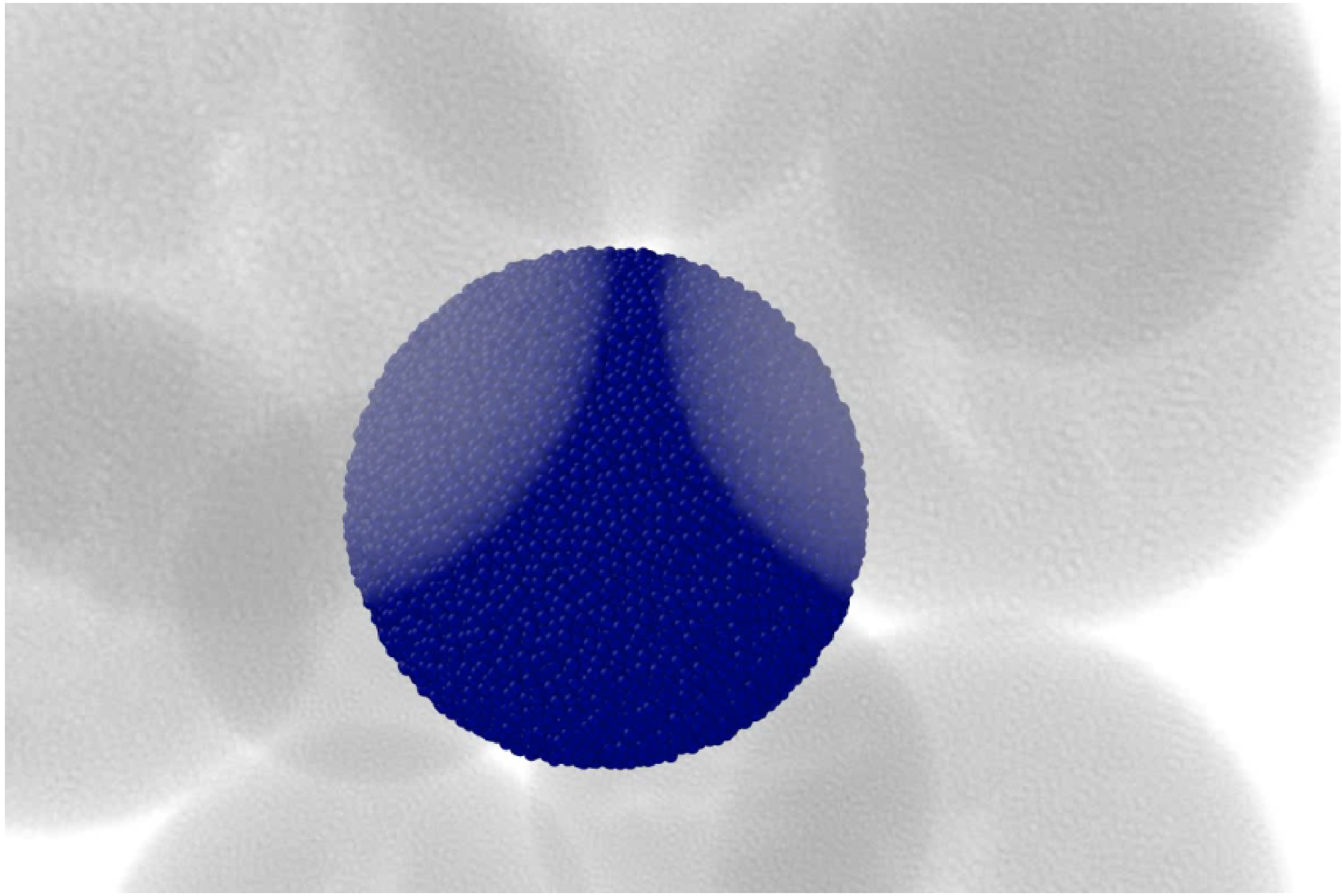
Bulk yield is set by weakest grain

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

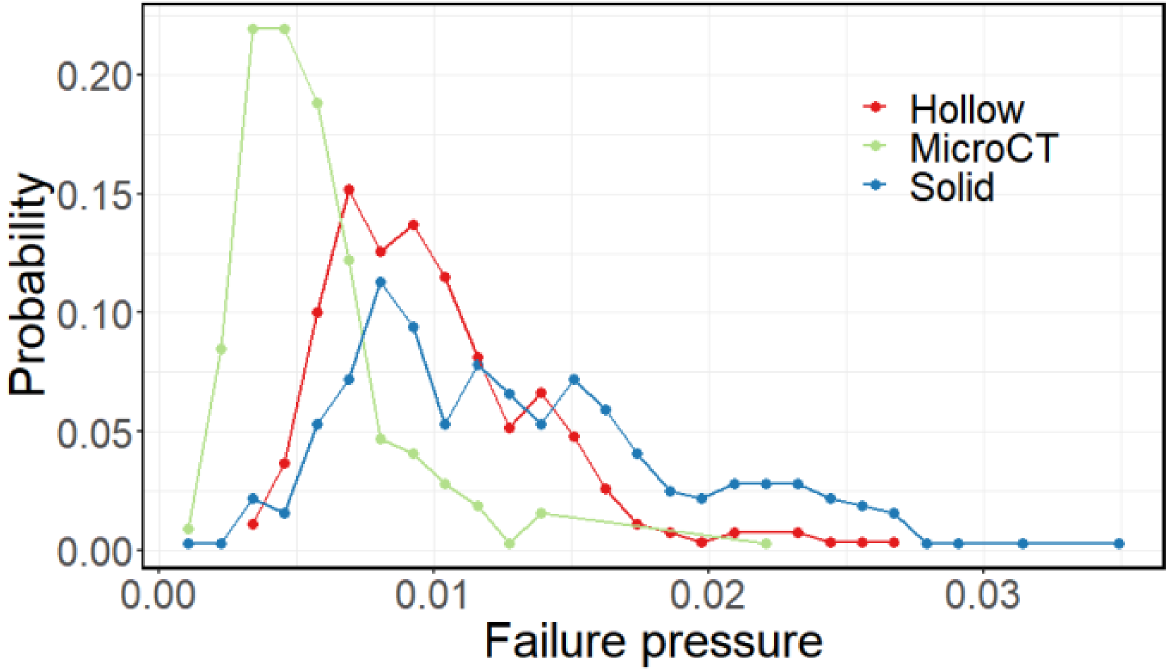
Theorized that distribution determines shape of compaction curve (Kenkre et al. 1996)

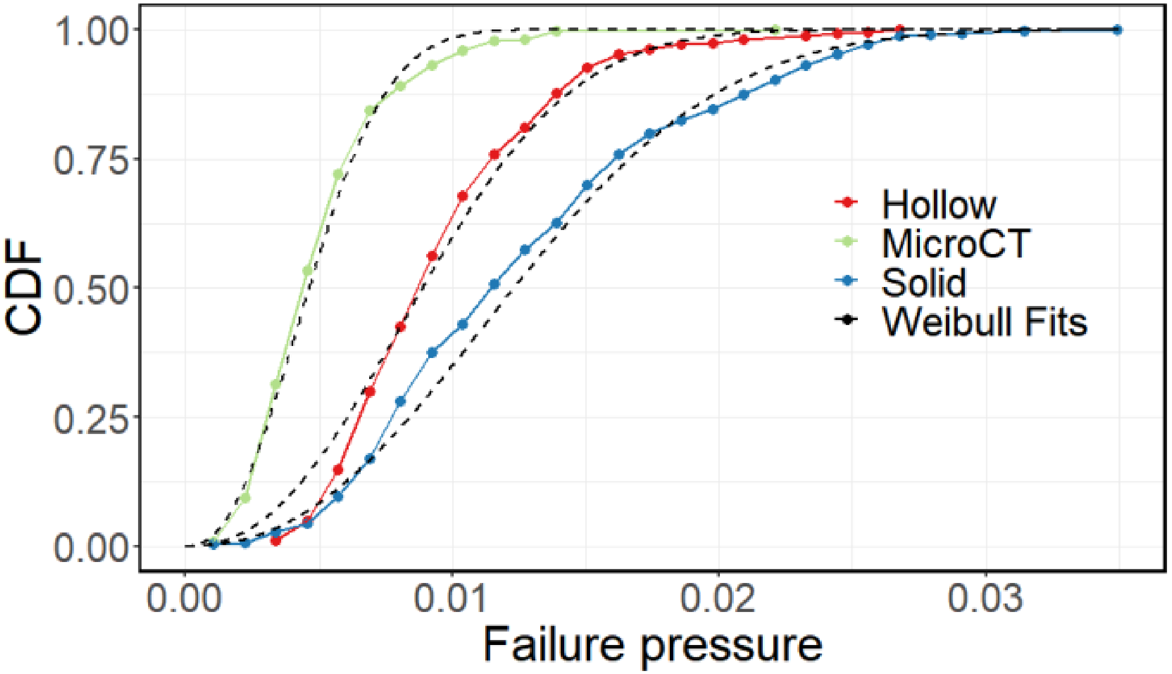
All fit well by Weibull distribution

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

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

Extra Slides

MS204: Upscaling of particle scale mechanics to continuum macroscale phenomenology

- *Many physical processes exhibit complex constitutive behavior attributable to grain (or particle) scale thermo-mechanical processes inherent to their microstructures and possible interactions with interstitial fluids. These processes often involve different length and time scales and interaction among them, requiring quantifying mechanical behaviors across the different scales and identifying connections between them. Examples of such materials may include soil and rock, pressed powders, ceramics, concrete, sprays and droplets, suspensions, among possibly others. This symposium provides a forum to present and discuss approaches for bridging particle scale mechanics to the continuum scales of interest for engineering applications both with and without effects of fluids. Topics within the scope of interest include but are not limited to:*
- *Micromechanical models with focus on associated homogenization theory for effective response,*
- *Statistical approaches of scale-bridging techniques,*
- *Data-driven multiscale modeling techniques,*
- *Microstructural and crystallographic characterizations with data reduction related to effective properties,*
- *Experimental efforts related to specific method developments.*

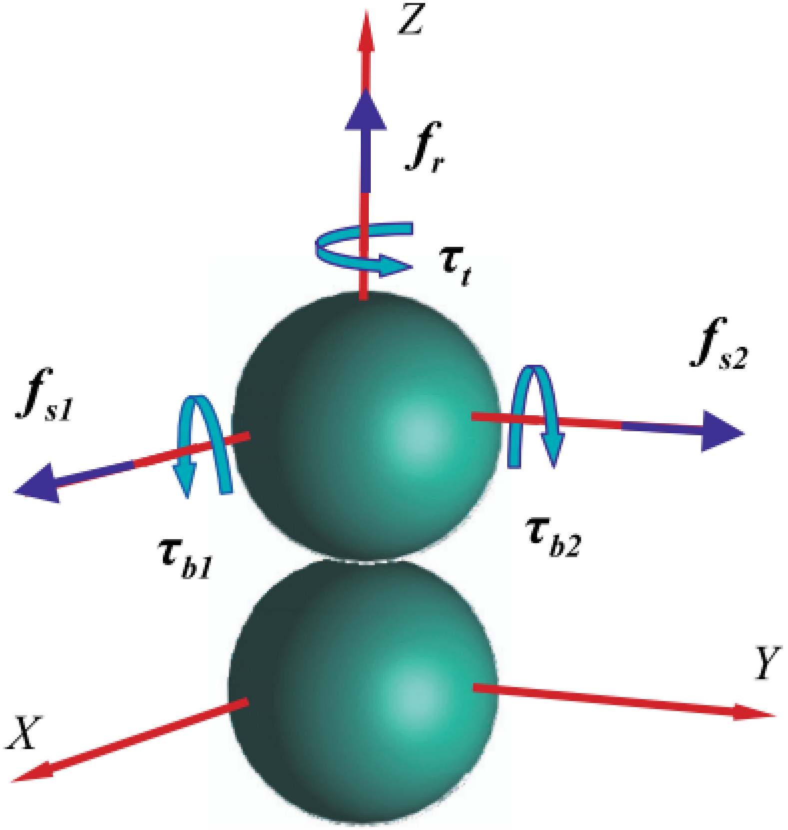
Under large loads, deformation of brittle particulate materials will eventually lead to particle fracture and failure. The process of fragmentation is very complicated and depends heavily on not only the specific conditions of loading but also on material heterogeneities such as internal porosity and local particle packing. As a solid is loaded, some set of material defects will nucleate cracks. These cracks will grow, interact, and possibly coalesce leading to failure. In order to accurately model such phenomenon, one needs to resolve the local stress field and also handle the dynamic initiation and propagation of discontinuities. Discrete element models (DEMs) are particularly well suited to these challenges. DEMs represent a solid as a collection of interacting Lagrangian points. The failure of bonded interactions between such points naturally produces discontinuities in the system. Such models have been used in a wide variety of contexts and exhibit their capabilities through the emergence of experimentally observed behavior such as the growth of wing cracks in a uniaxially compressed solid.

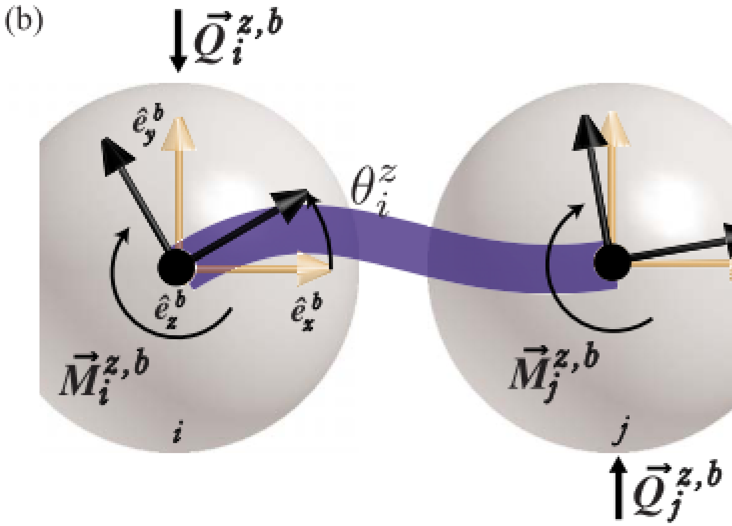
In this talk, we discuss recent work designing, calibrating, and implementing a variety of DEMs into LAMMPS, a powerful and popular codebase for large-scale, parallel simulations. A variety of applications will then be discussed to highlight the flexibility and strength of the models. These will include studies of rate effects on the density of crack nucleation and the subsequent damage accumulation in uniaxially compressed solids as well as granular breakup in sheared solids. The sheared solids are found to approach a critical state in the limit of small strain rate which is characterized by a power-law distribution of grain sizes. We focus on the problem of granular compaction which is relevant in many industrial processes such as tableting. At high pressures, fracture of grains is the primary mechanism of densification and produces complicated distributions of irregular particles. We start with uniform packings of spherical grains and simulate applying a variety of loads at different rates to study yielding as well as the evolution of the stress, porosity, and grain size distributions.

Variety of DEMs

Carmona, Wittel, Kun, Herrmann 20(
Andre Iordanoff, Charles Neauport 2(

Wang Mora 2008



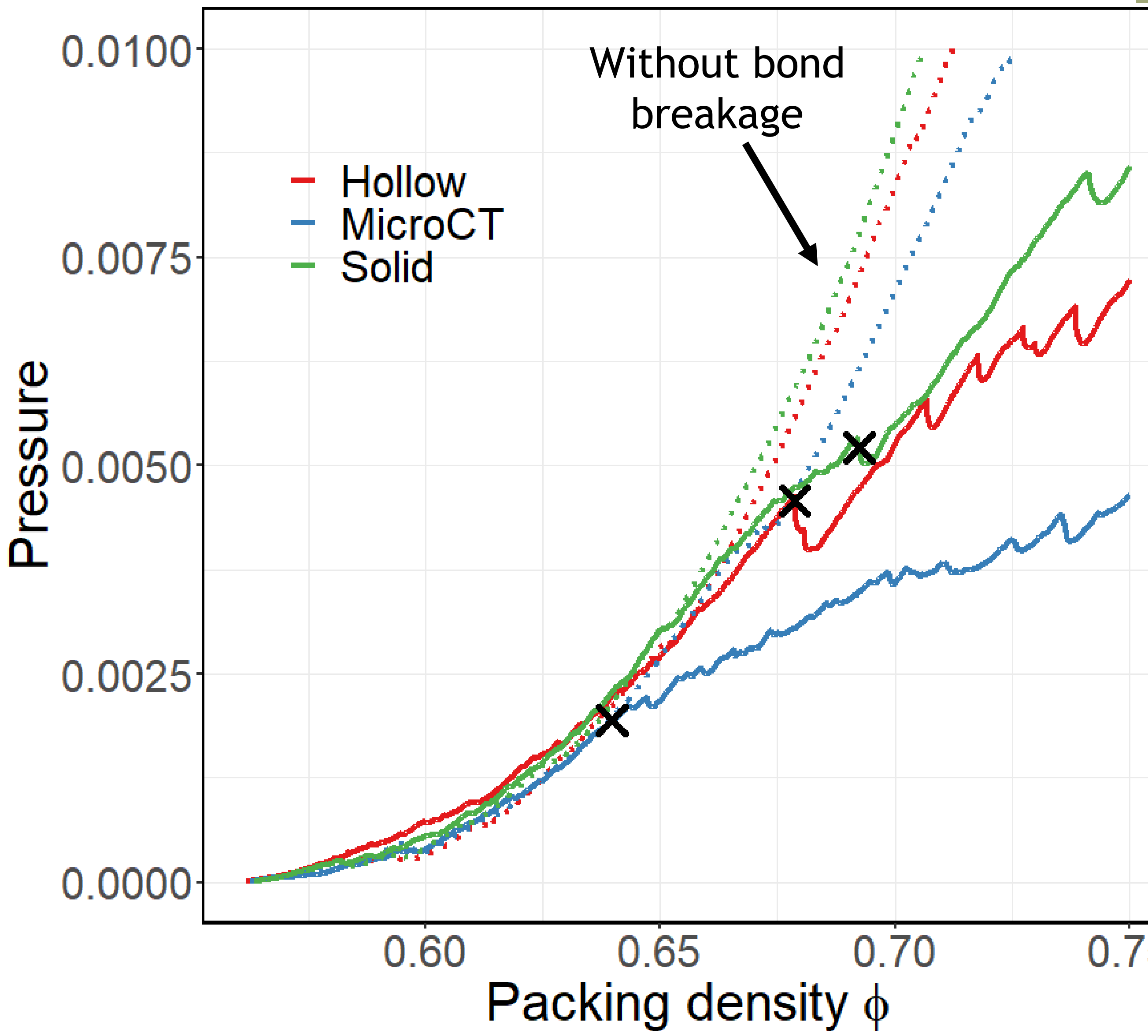


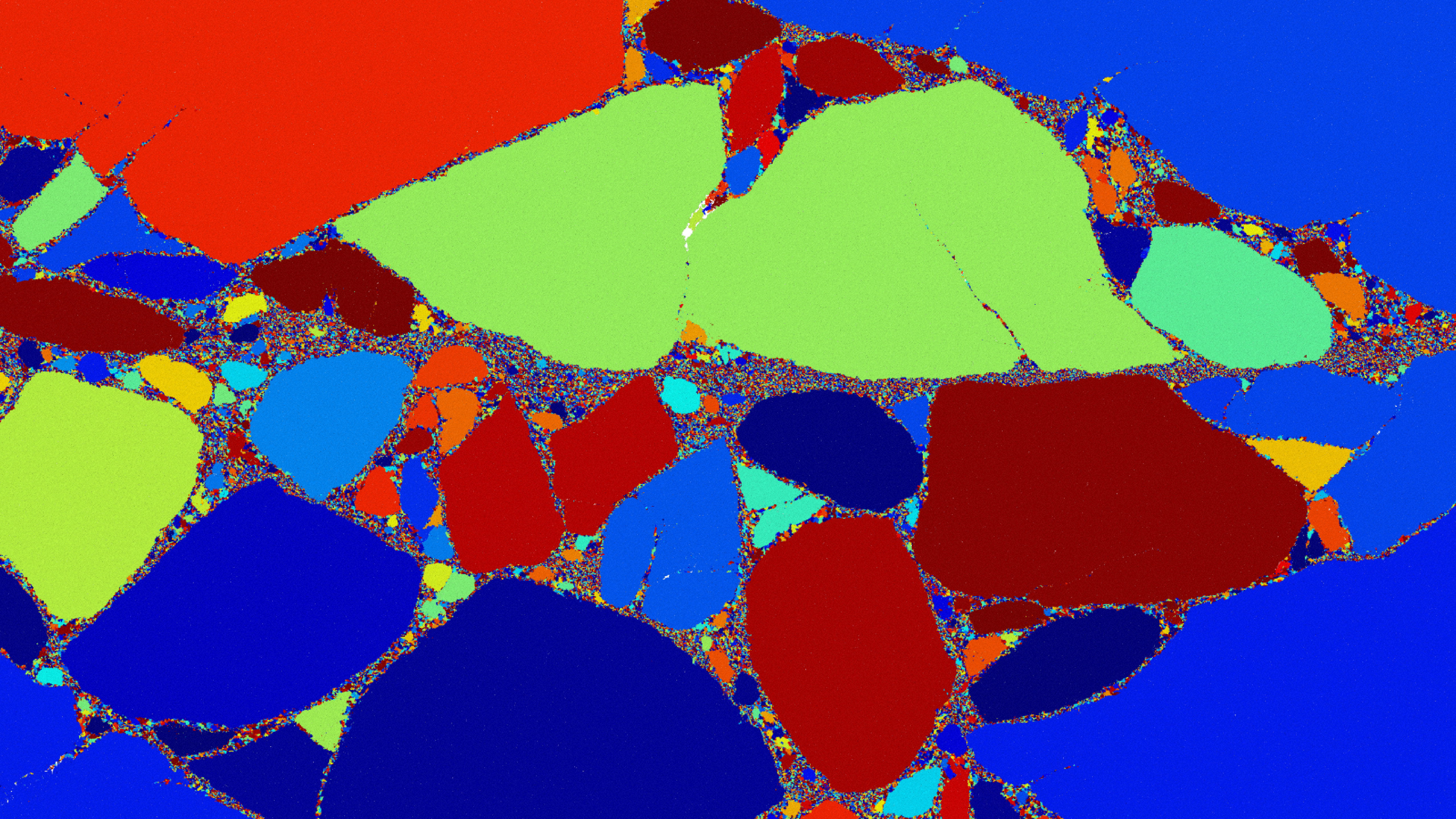
Compaction curves

Pressure rises at packing density $\phi \sim 0.57$
Friction ↓ jamming ϕ from 0.64 (Silbert 2010)

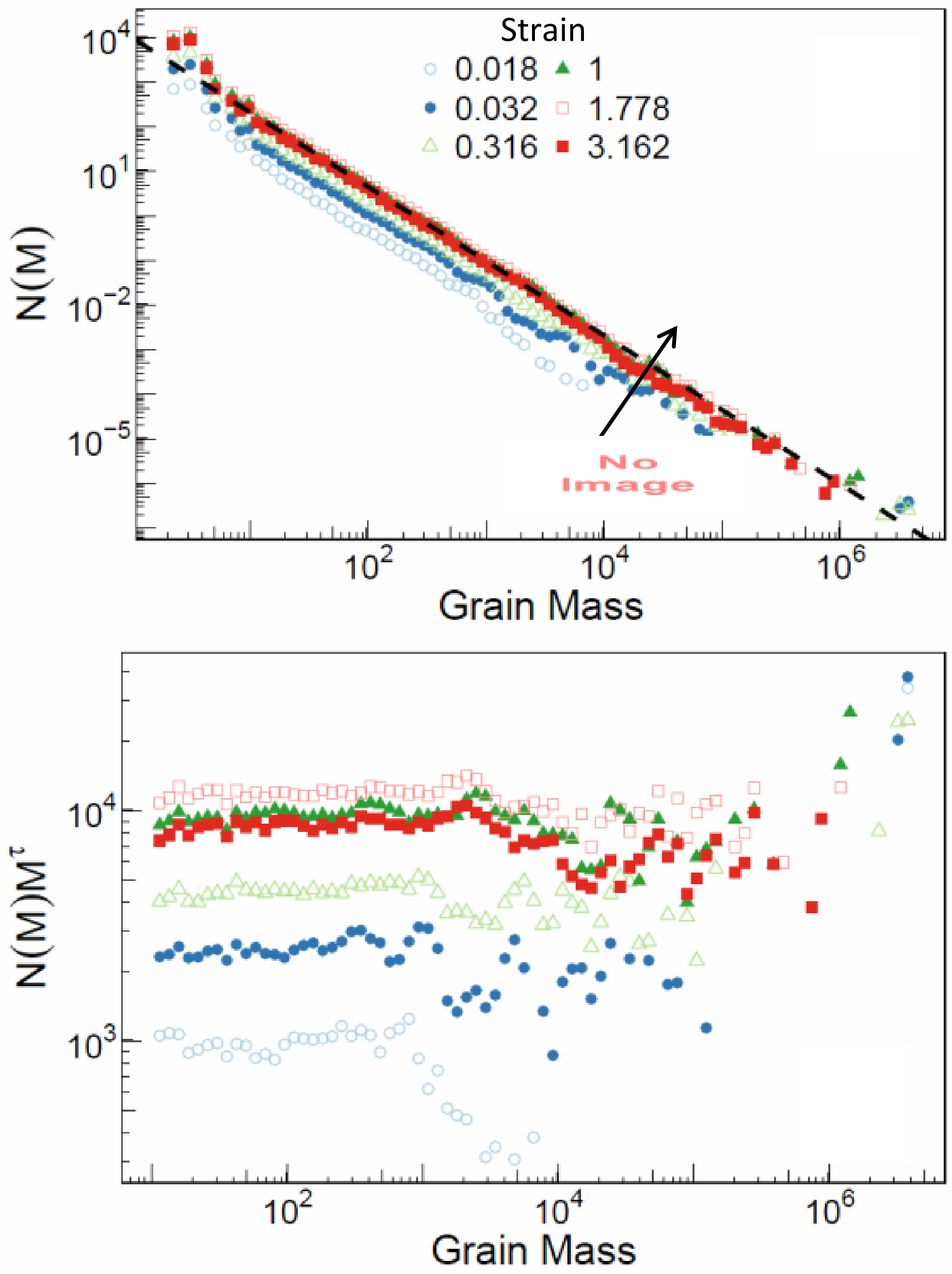
Small ϕ: see rearrangement
Large ϕ: see deformation → damage → failure
(indicated by black X's)

Can study theoretical curves without fragmentation to highlight its impact
Note: porosity reduces stiffness of system

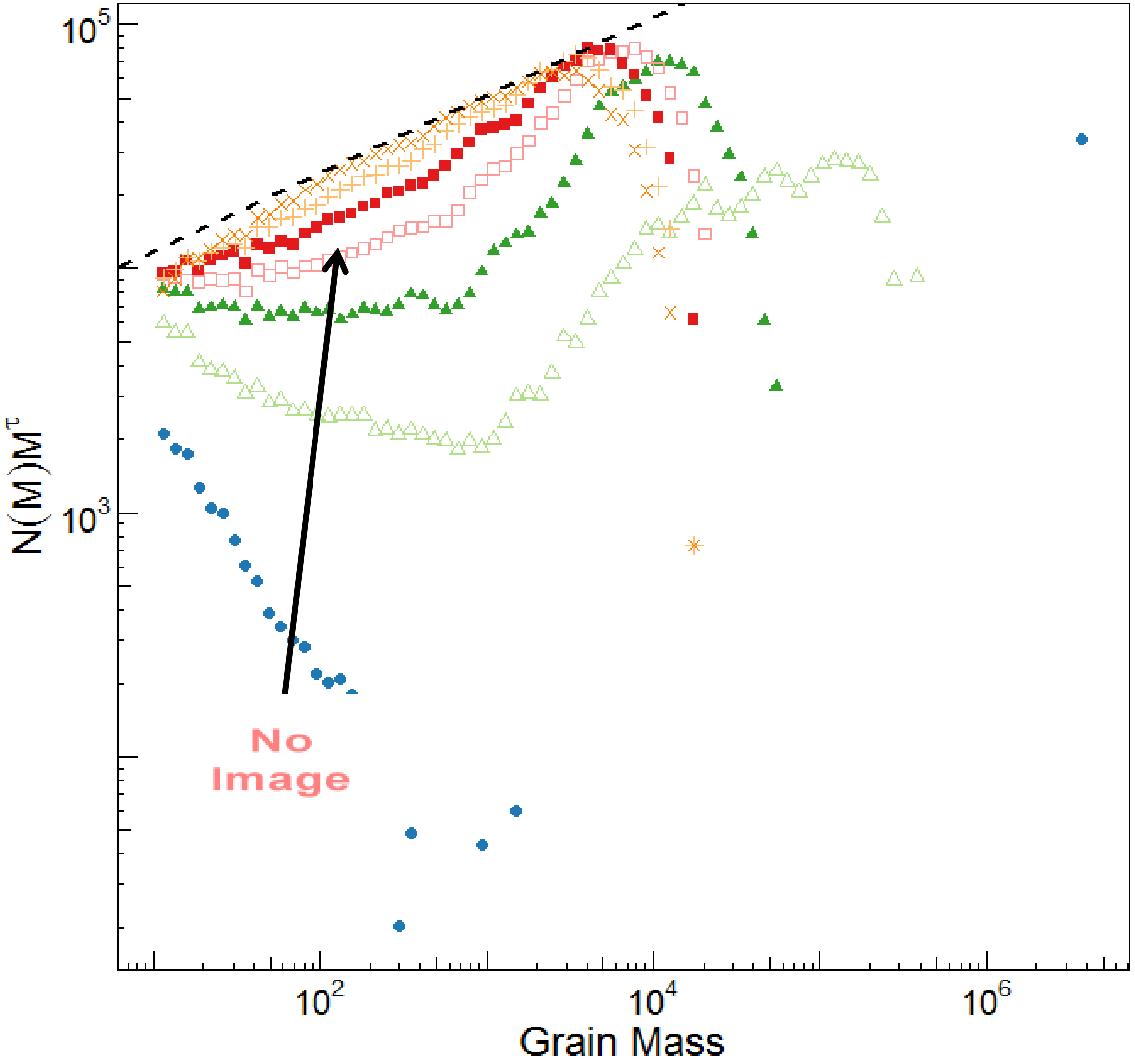




Grain Size Distribution



Rate dependent exponent



Impact Defects on Fracture - Preliminary

Study interaction of strain rate and defect density on initial failure

Use realistic initial defect distribution from micro CT scans

Moorehead et al. 2018

Track evolution of crack distribution – calculate damage

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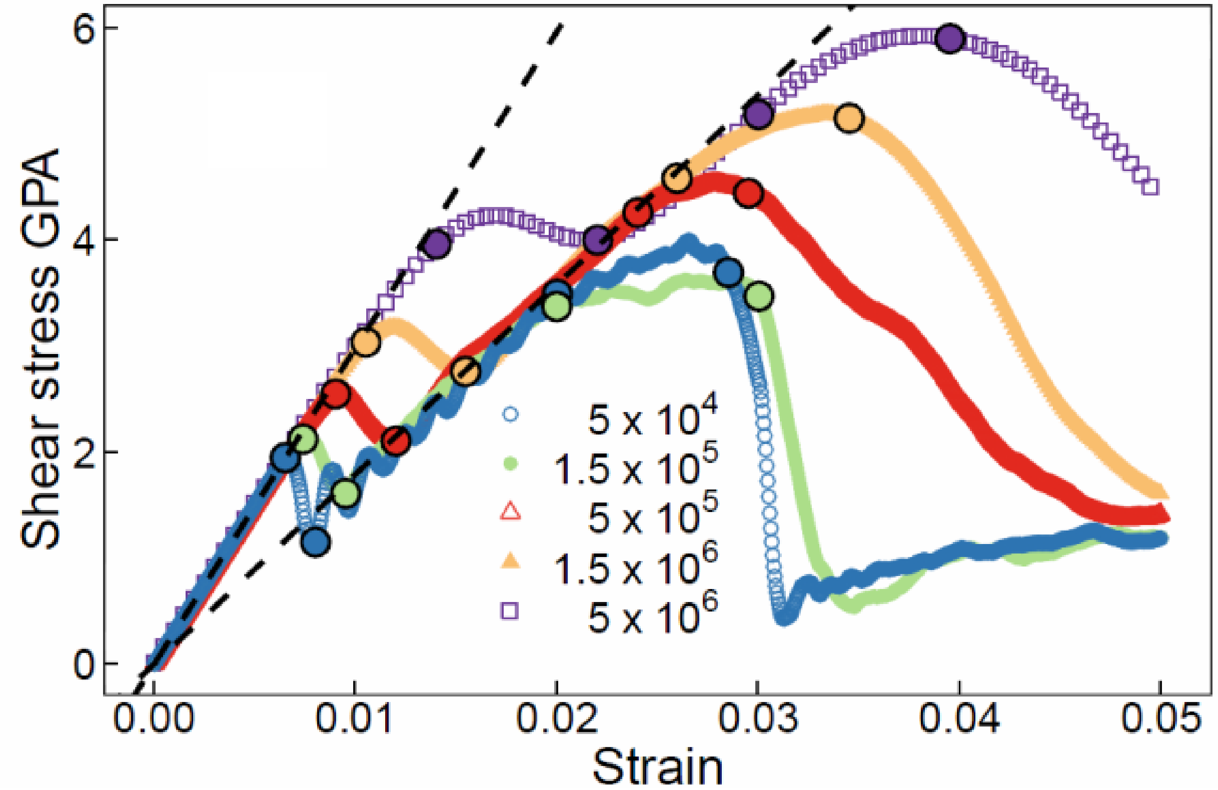
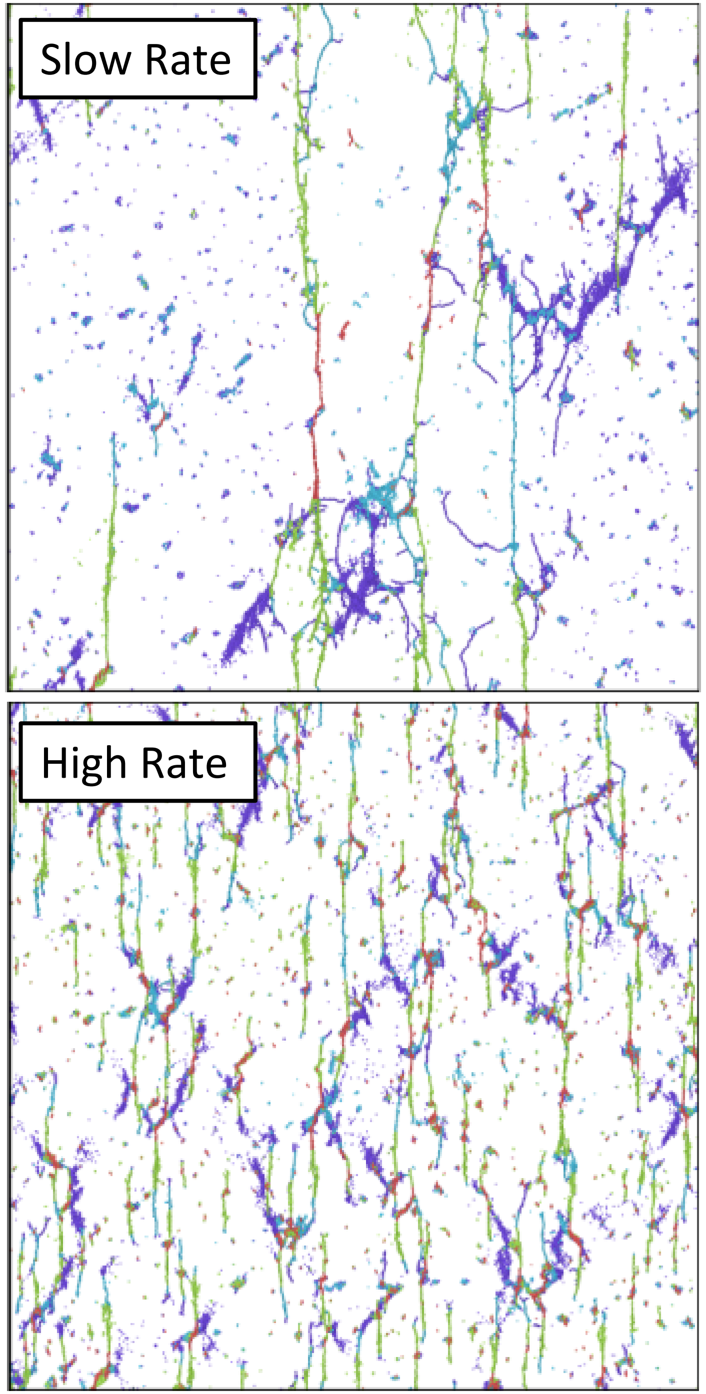
Rate Effects

Increased strength at high rates, increased number of cracks/defects active in failure

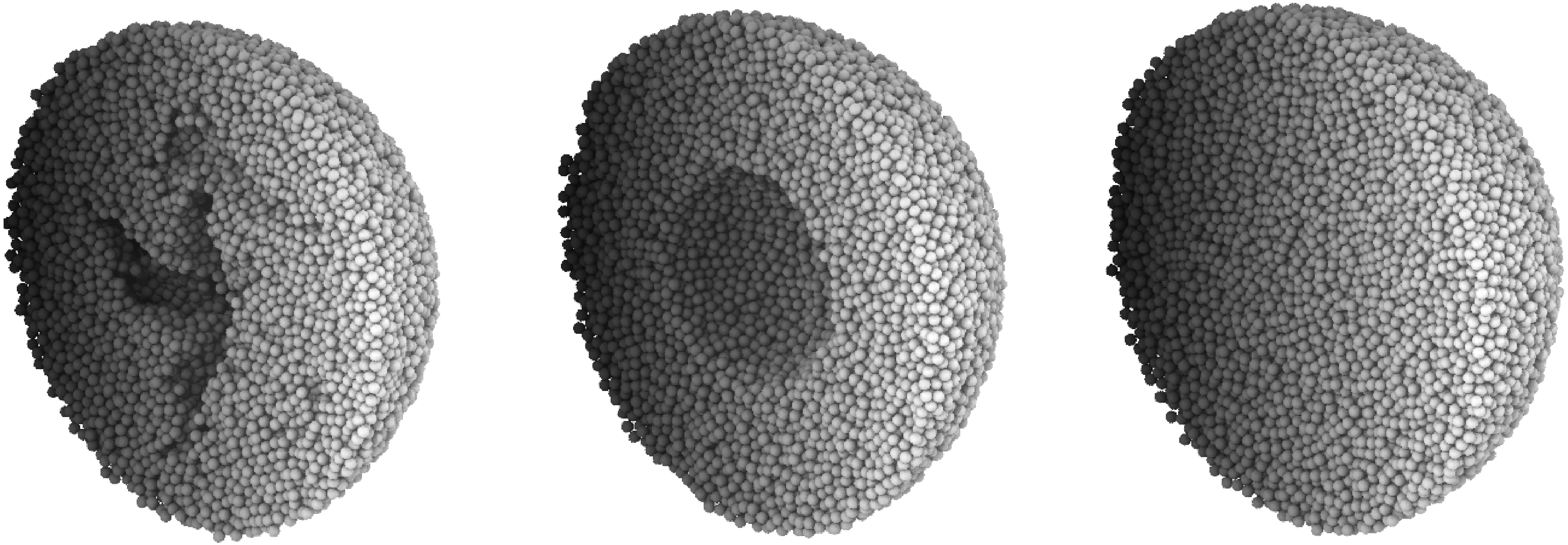




Defects in DEM Grains

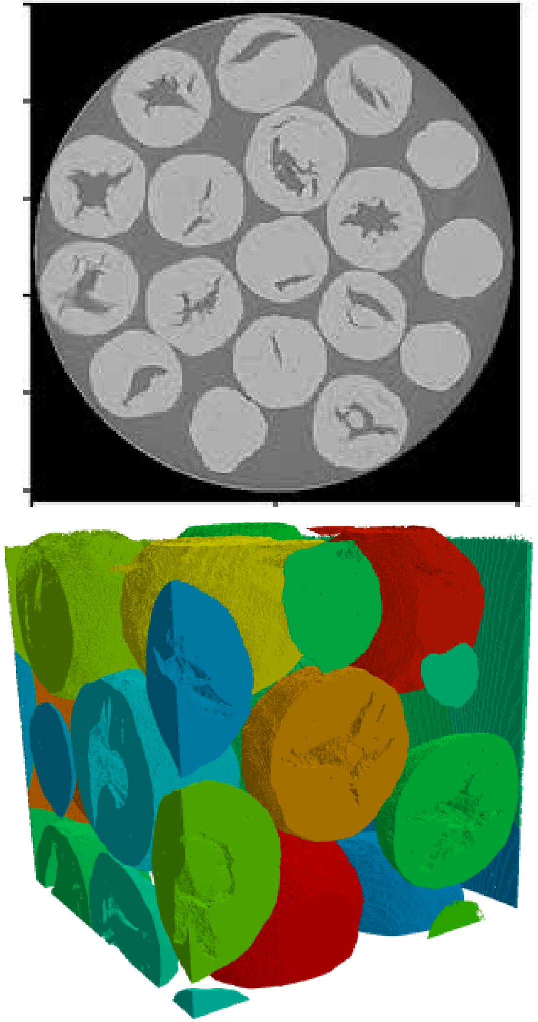
Goal: quantify effect of porosity/defects on granular strength and fragmentation

Study 3 types of grains: realistic porosity, uniform porosity (hollow), and solid

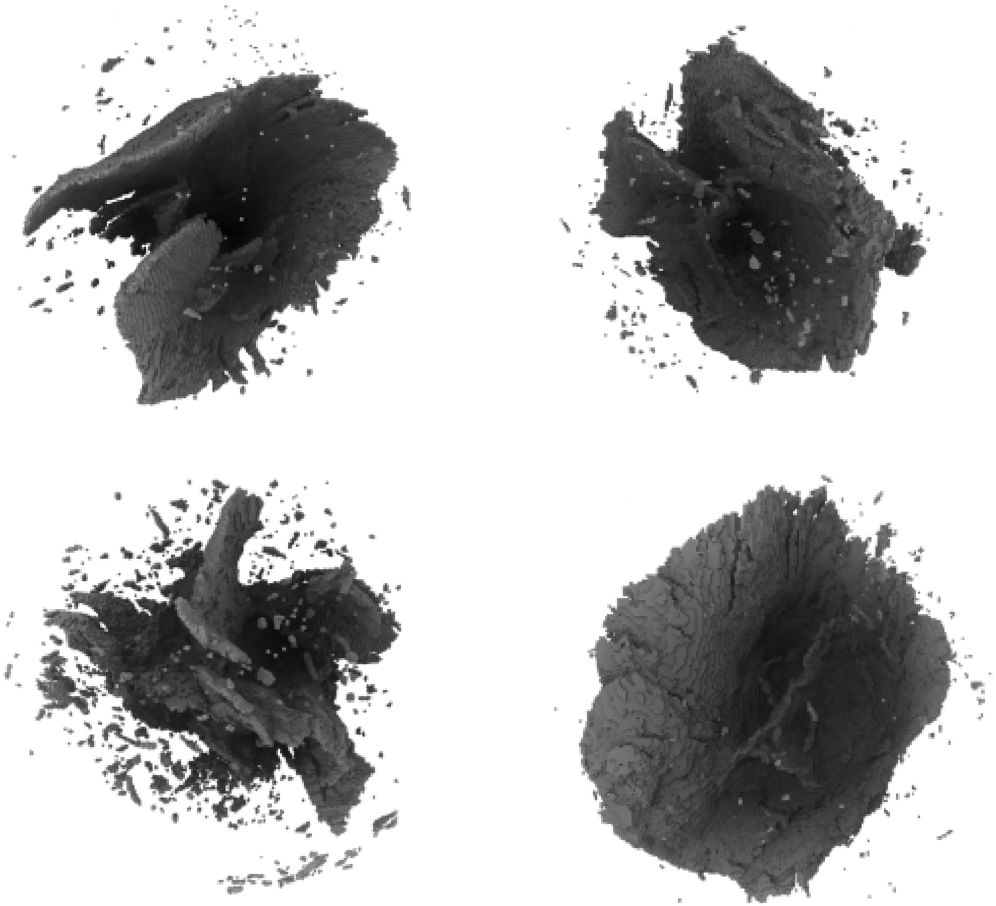


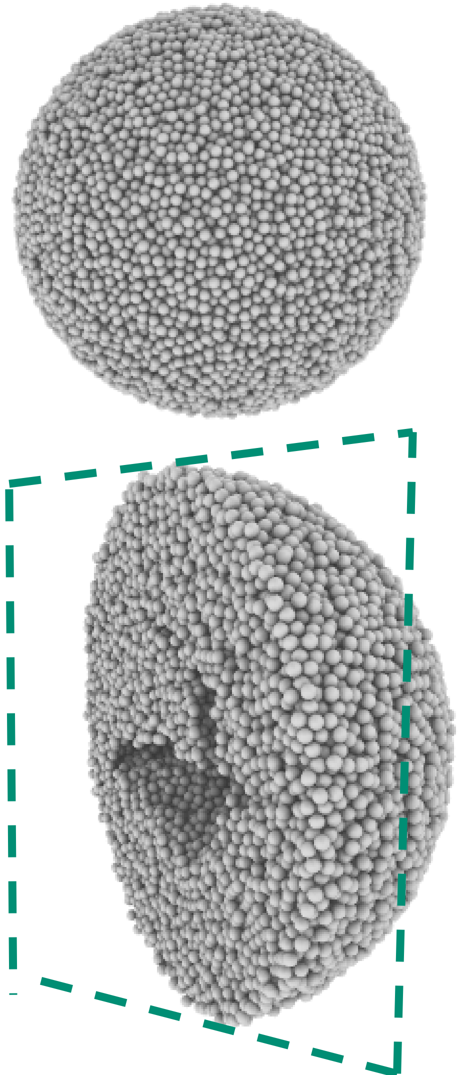
Defects Derived from Microcrystalline Cellulose

Process CT Images → Create library of internal voids → Carve out region in spherical DEM grains



M. Cooper et al. (2020)

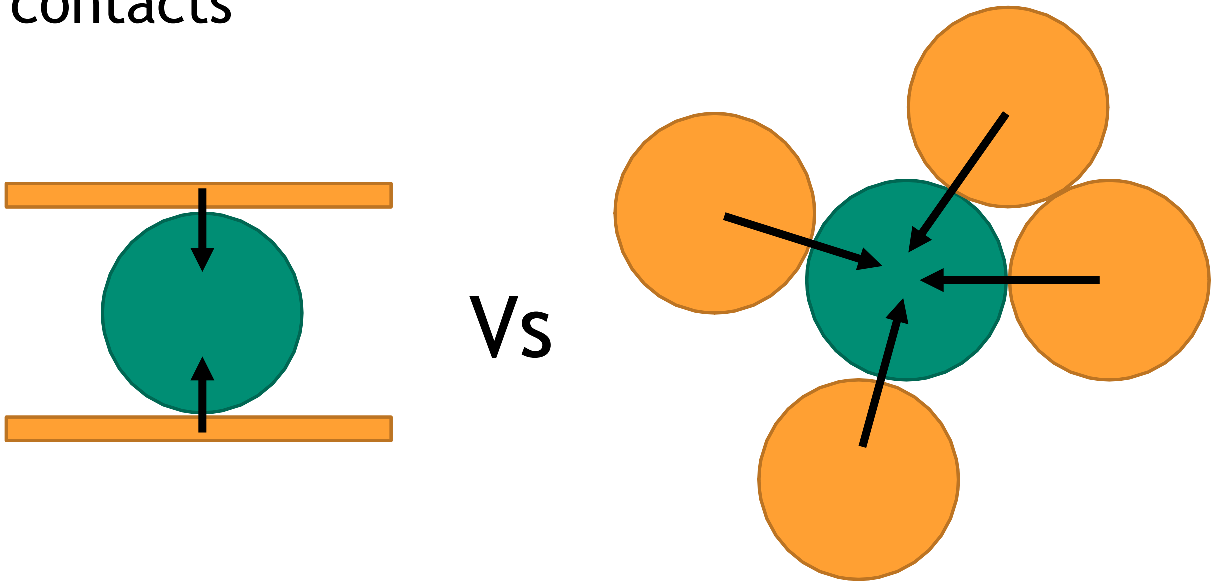




Measuring Strength of Grains

Could measure strength under uniaxial strain (e.g. Brazil test)

However, grains in a packing experience very different loading geometry: many shifting contacts



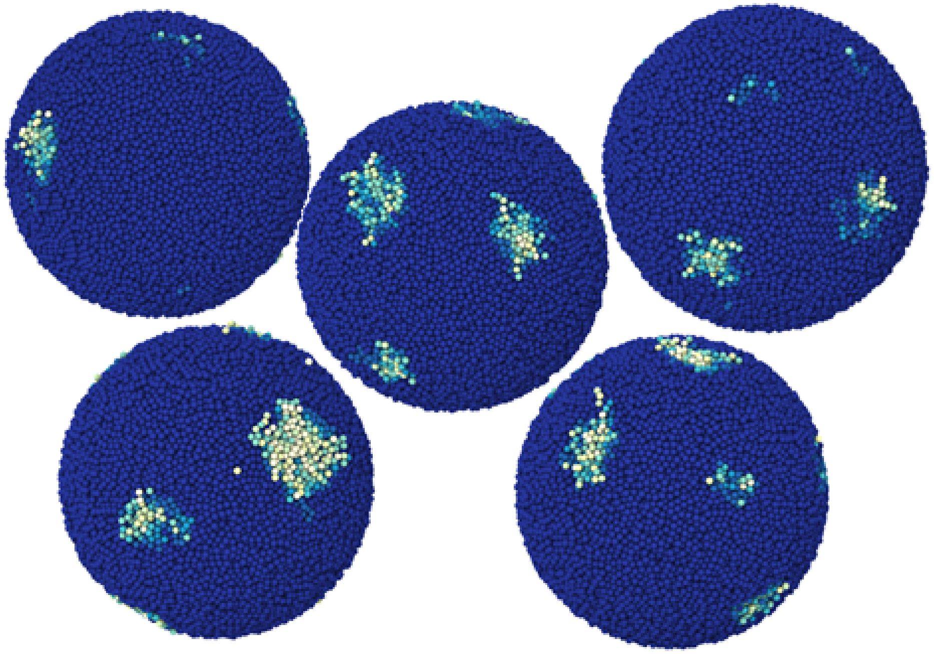
Instead focus on actual particle packings

Granular Damage in Compaction – Defining Failure

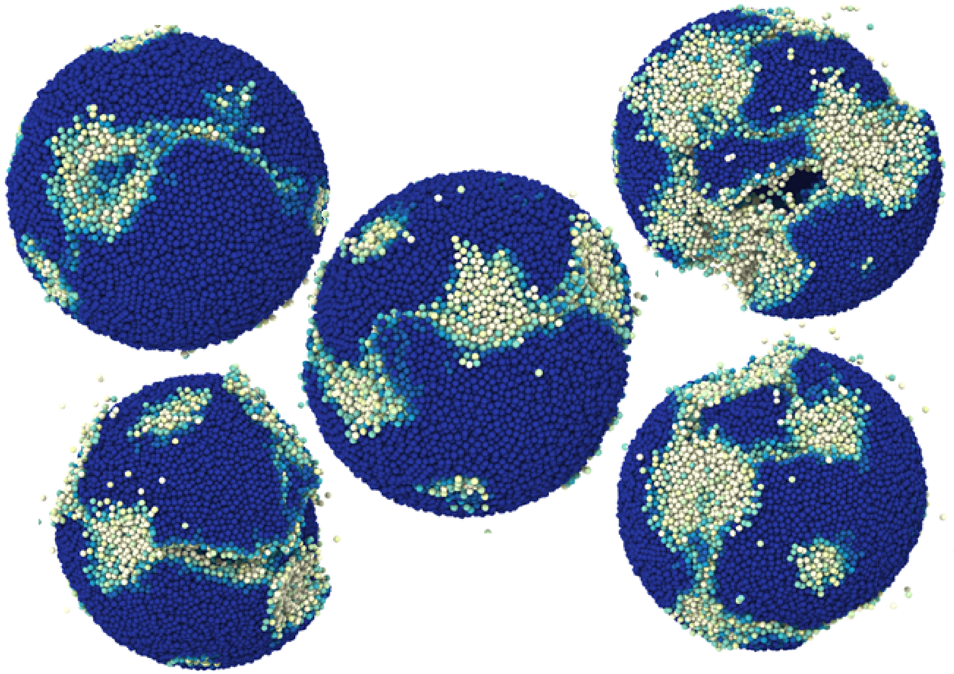
As grains slide past each other, damage (broken bonds) can occur on the local contact even at lower pressures – abrasion

At higher stresses, cracks nucleate and grow as grain fractures – our definition of failure

Abrasion



Fracture/failure



Porosity effect

Changing porosity, still see highly skewed distribution w/ long tail

↑ mean and variation for hollow/solid grains

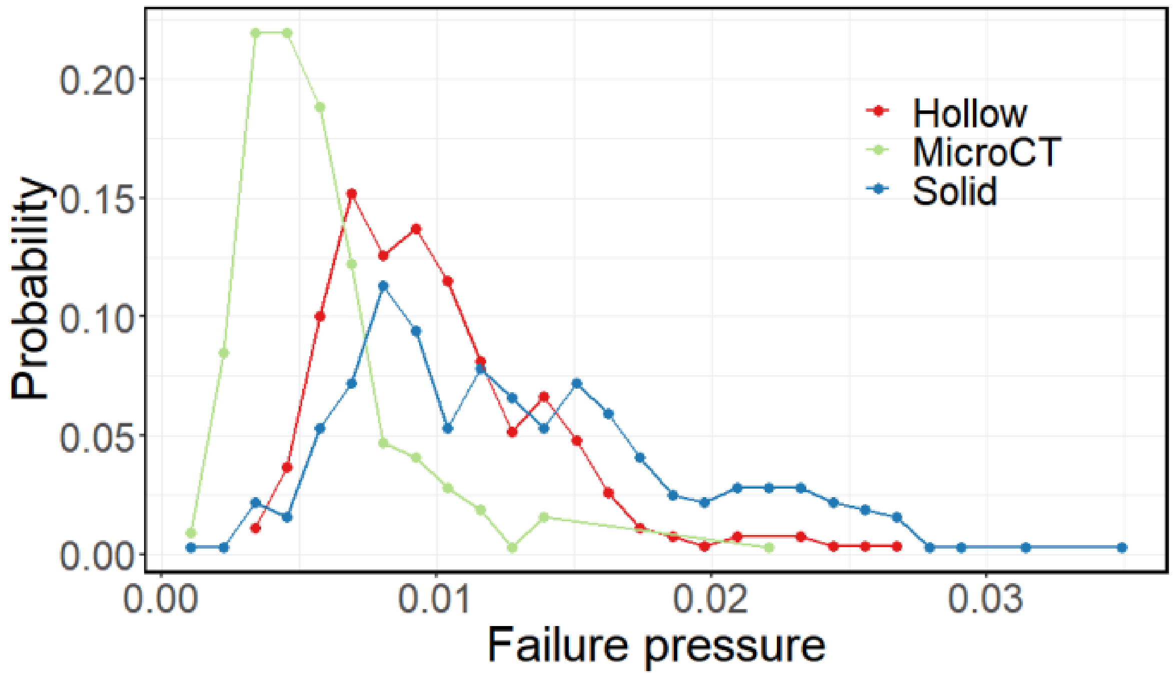
Note while solids grains generally stronger than defected, environment still very important as some solid grains are weaker

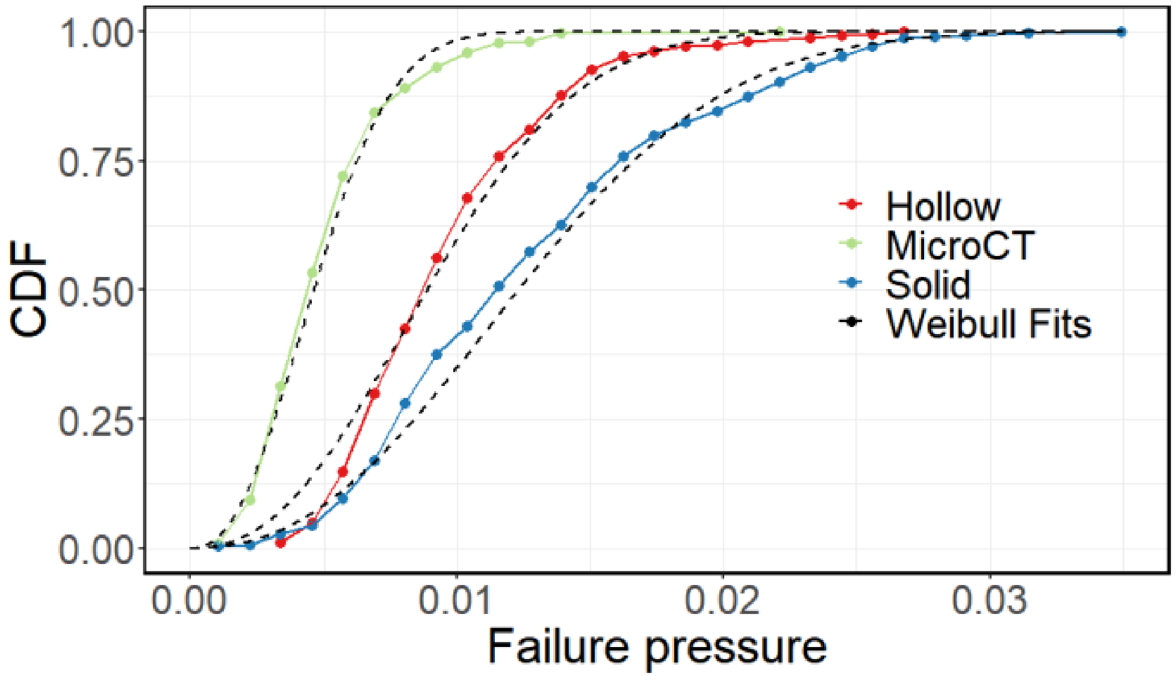
All fit well by Weibull distribution

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

Constant exponent $k = 2.3$

P_0 depends on defects





Isolating Effect of Defects

Given a fixed local environment, can we compare loss in strength due to defect?

Run compaction with identical packing configurations with defected and solid particles

Use solid strength to 'normalize' defected strength, look at relative loss of strength due to defect