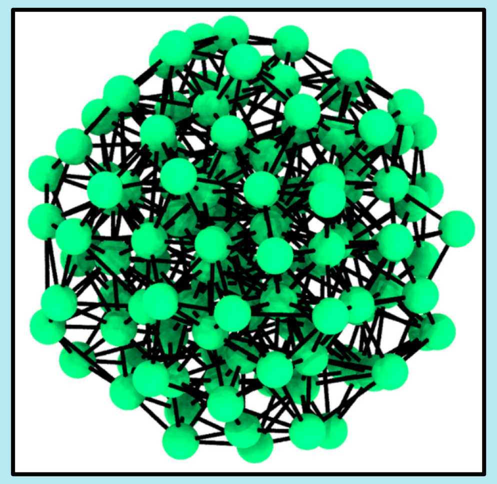
Stressful situations: modeling granular fragmentation at high pressures

Introduction

Many practical applications of granular materials are far from the zero-pressure limit of jamming including industrial processes such as grinding and die filling as well as geologic phenomena such as earthquakes, asteroid impacts, and ice floe collisions. In these systems, fracture creates an evolving population of grains that play an important role in the macroscopic response. To explore this high-stress regime, we use a bonded particle model to capture fracture and represent a wide range of material properties. We focus on two problems: the fragmentation of sheared solids and high-pressure granular compaction to explore both macroscopic responses and the microscopic statistics of individual grains.

Bonded Particle Models

Represent solids or grains as a collection of point particles connected by a network of pairwise, breakable springs to capture elastic deformation and fracture



Spring properties set material behavior:

- Dashpots can introduce viscoelasticity
- Add history-dependence for plasticity
- Breakage criteria affect fracture profile

  E.g. brittle cone/wing/Kalthoff cracks

Can adjust Poisson's ratio using an EAM-like approach:

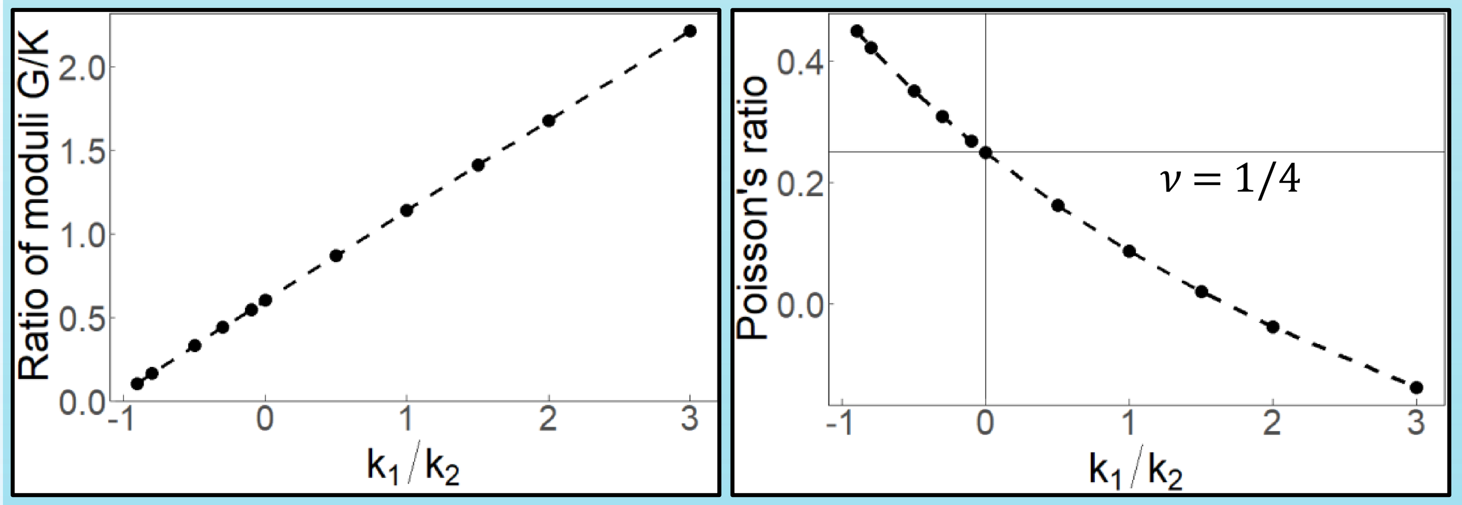
$$F(r,V) \sim \boldsymbol{k_1}\frac{r-r_0}{r_0} + \boldsymbol{k_2}\left(\left[\frac{V}{V_0}\right]^{1/3} - \frac{r}{r_0}\right)$$

V = local volume of particle pair, r_0 and V_0 = initial values

First term = linear spring, **second** = deviation in volumetric strain

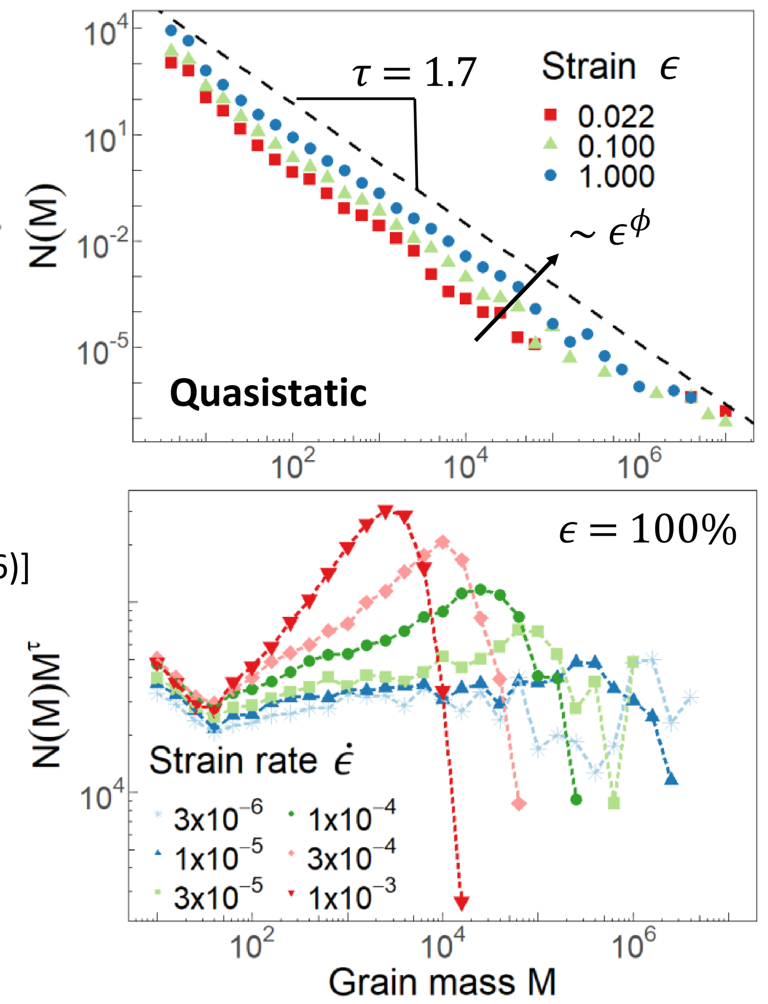
Forces are still pairwise, central-body, and equal-and-opposite

BPM package available open-sourced in LAMMPS



Generating Grains from Fragmentation

The production of grains during fragmentation is a complex and poorly understood process While simulating sheared, brittle solids in 2D, we track the number of grains of a given mass M, $N(M)$, to explore its evolution with strain and dependence on rate and system size

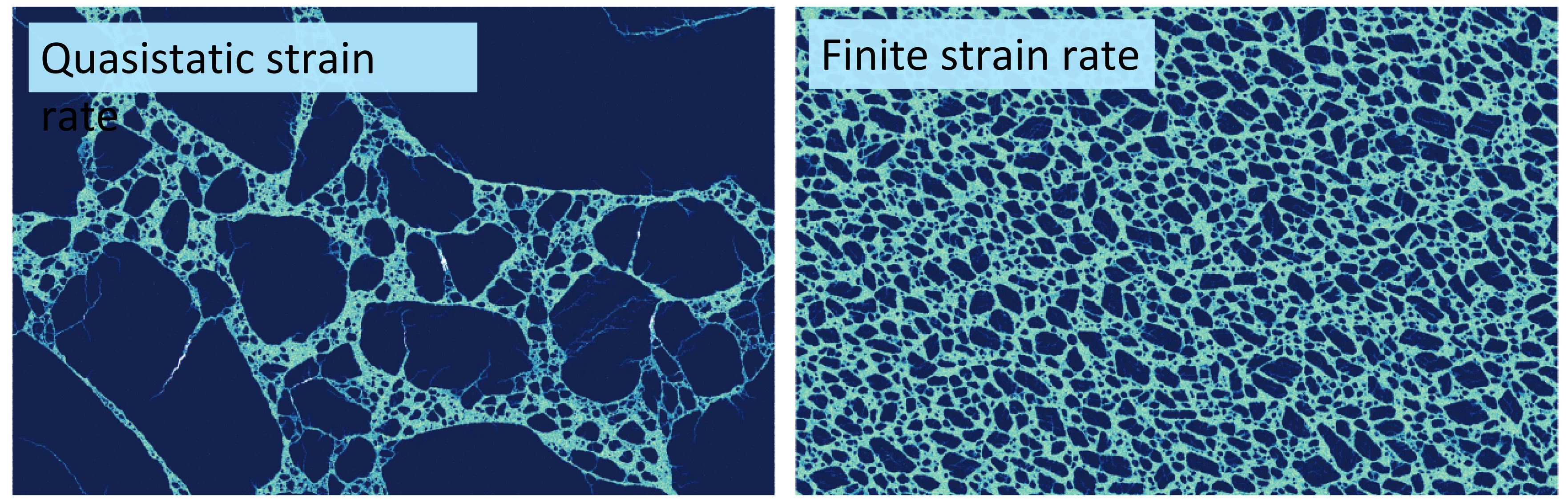


In the quasistatic limit, fracture produces a power-law distribution $N(M) \sim M^{-\tau}$ as seen in many systems [Turcotte, J. Geophys. Res. **91**, 1921 (1986)]

The number of grains grows ϵ as $N(M) \sim \epsilon^{\phi}$

At high rates $\dot{\epsilon}$, grains are finer as power laws are cutoff at a smaller mass M_{cut}

Also identify an unexpected increase in the exponent that may explain some variation in τ measured in different granular materials



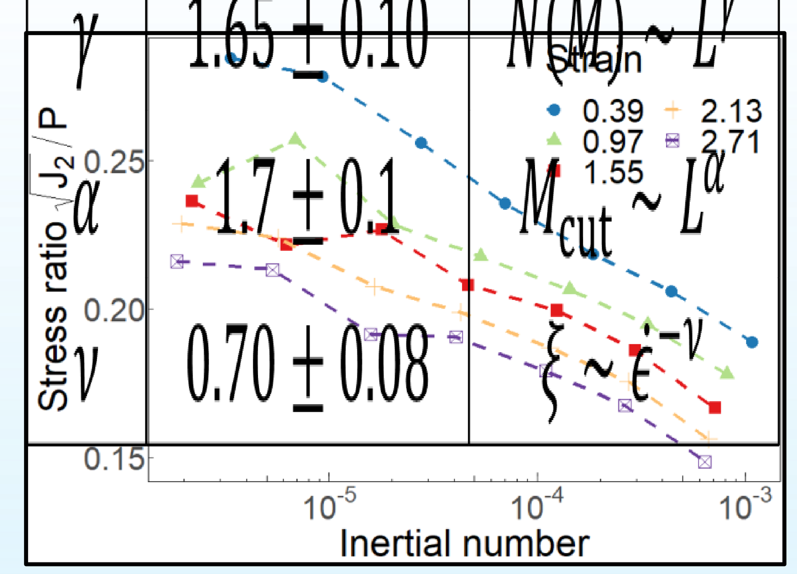
These findings resemble critical behavior where the size of the largest grain is set by a diverging length scale $\xi \sim \dot{\epsilon}^{-\nu}$ with a fractal exponent α: $M_{\mathrm{cut}} \sim \xi^{\alpha} \sim \dot{\epsilon}^{-\alpha\nu}$

τ	1.7 ± 0.08	$N(M) \sim M^{-\tau}$
ϕ	0.55 ± 0.07	$N(M) \sim \epsilon^{\phi}$
γ	1.65 ± 0.10	$N(M) \sim L^{\gamma}$
α	1.7 ± 0.1	$M_{\mathrm{cut}} \sim L^{\alpha}$
ν	0.70 ± 0.08	$\xi \sim \dot{\epsilon}^{-\nu}$

For 2D systems of different sizes L x L, we measured exponents that govern the scaling of $N(M)$ with L and $\dot{\epsilon}$ using finite-size scaling techniques

Such characterizations are important as $N(M)$ significantly affects the packing and rheology of granular systems

E.g. we see an inverted $\mu(I)$ trend during fragmentation as μ decreases with I due to particles being finer at higher rates

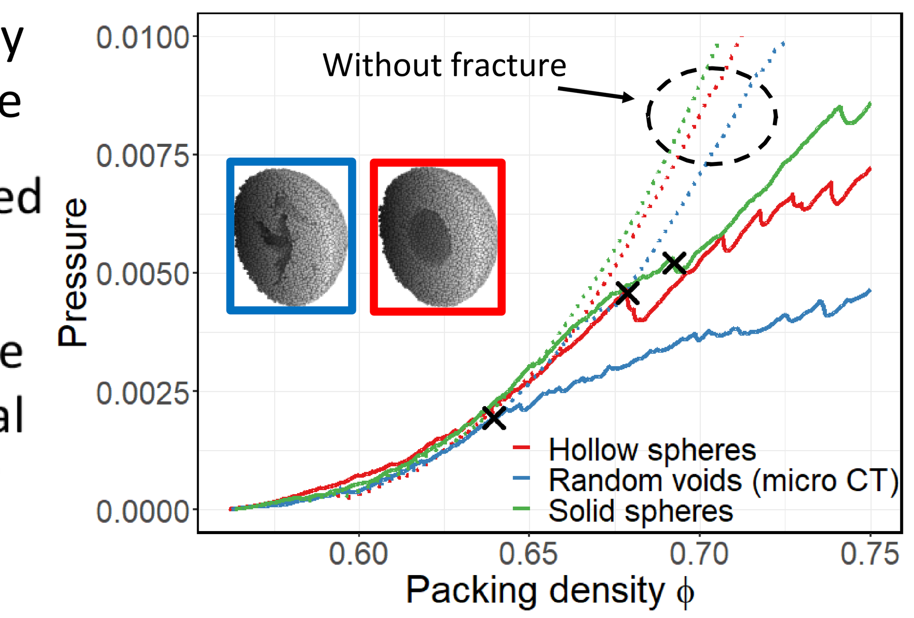


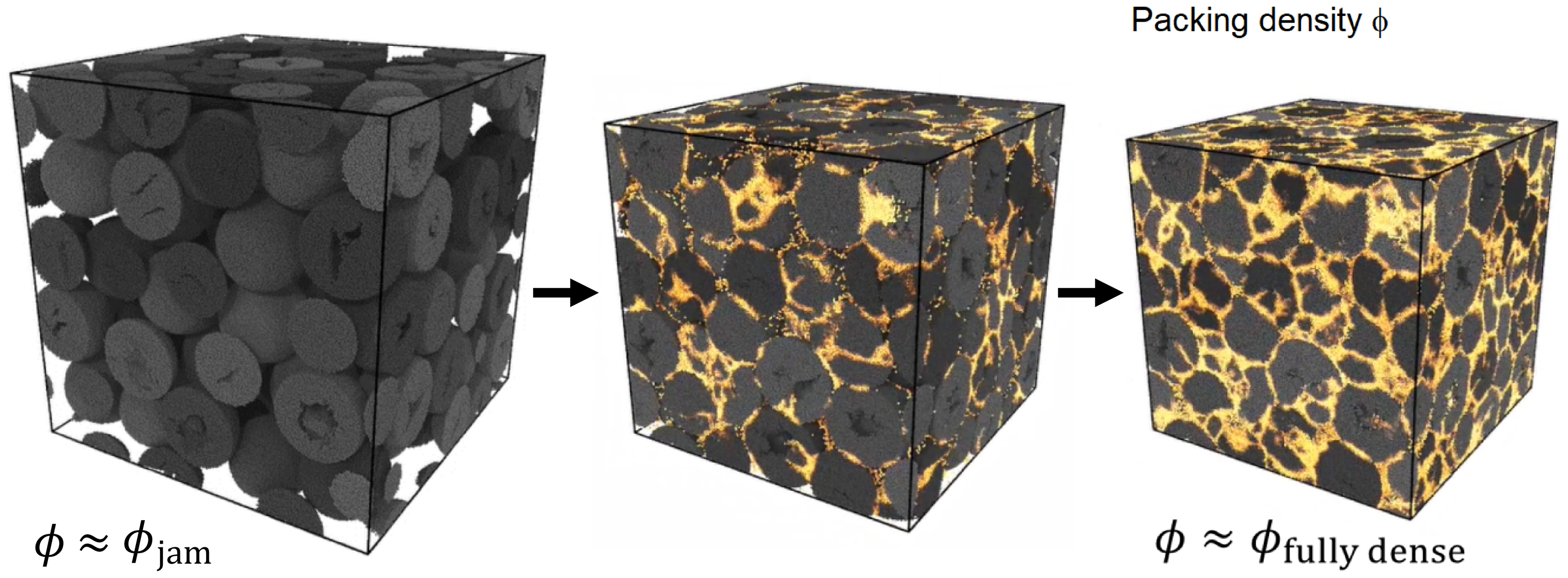
Loading of Granular Systems

For granular systems to compact to fully dense states, grains deform and fracture

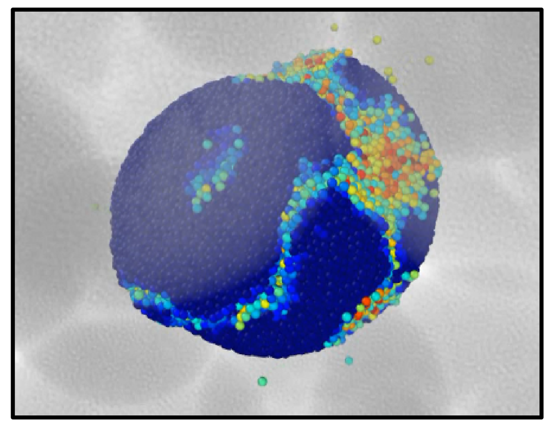
At small packing fractions ϕ see expected scaling of pressure $P \sim \phi - \phi_{\mathrm{jam}}$

At larger ϕ, see deviations – how can we link this to the behavior of individual grains and their mechanical properties?



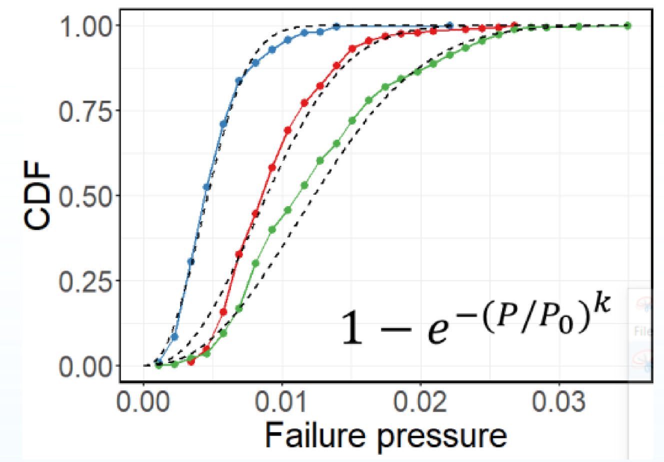


Consider sets of grains with different types of defects: no defects (solid), homogenous inclusions (hollow), and heterogeneous voids from micro CT



Measure strength of each grain by isolating it and preventing surrounding grains from breaking

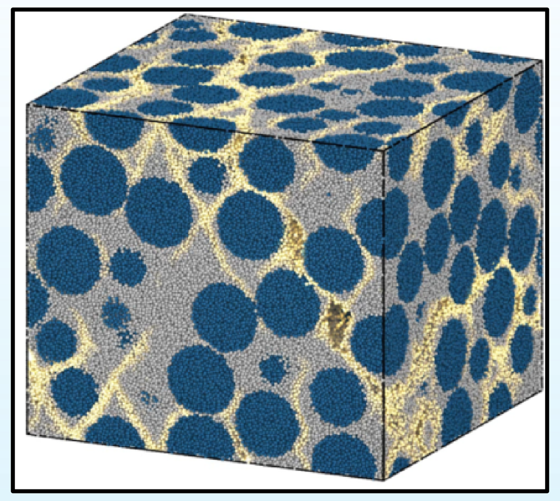
Find distributions of failure pressures are reasonably fit by Weibull curves with equivalent exponents but different characteristic pressures



Strength of a grain can depend on type of defect and local geometry (force chains/contacts)

Similarities between distributions suggests these factors may contribute in a statistically related manner and simply shift characteristic pressures

Also exploring loading of granular composites to identify how damage accumulation and failure depend on the mode of deformation as well as plastic/viscoelastic properties of the binder – early results suggest the shape of the yield surface depends on material properties of the binder



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