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Stressful situations: modeling granular fragmentation at high pressures

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2022 Granular Gordon Research Seminar

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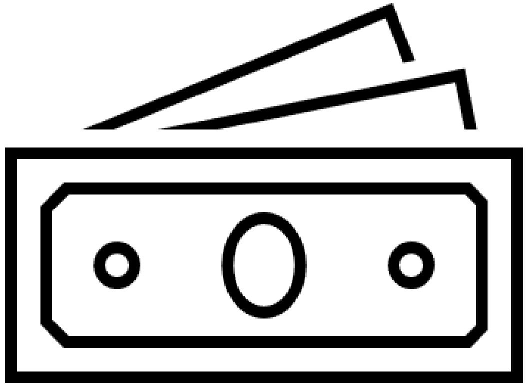
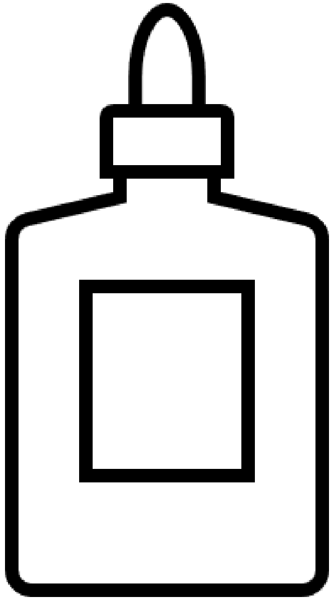
The saddest of granular matter

Do you buy a new mug or fix it?





It depends.

~~How much did you love this mug?~~

How many pieces are there?

Factors affecting the number of grains

1. ~~The strength of the mug~~
2. The number of times you dropped it
3. The size of the mug
4. The impact velocity

How can we quantify each factor's impact?

Simulating granular materials at high stresses

Far from rigid limit, assumptions of discrete element method fail
Contacts are no longer independent, grains can deform/fracture

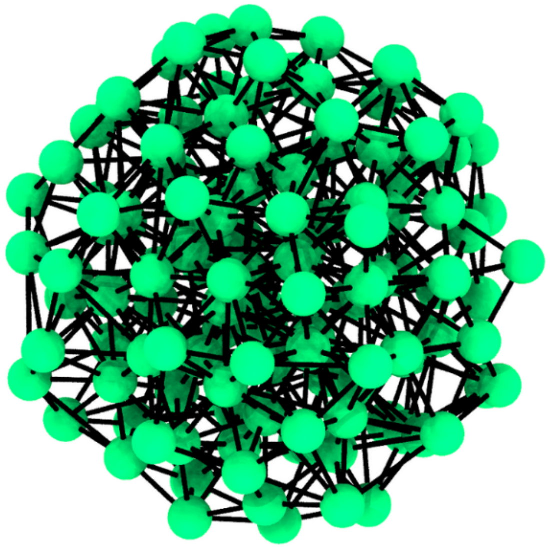
⇒ Need to simulate sub-granular resolutions

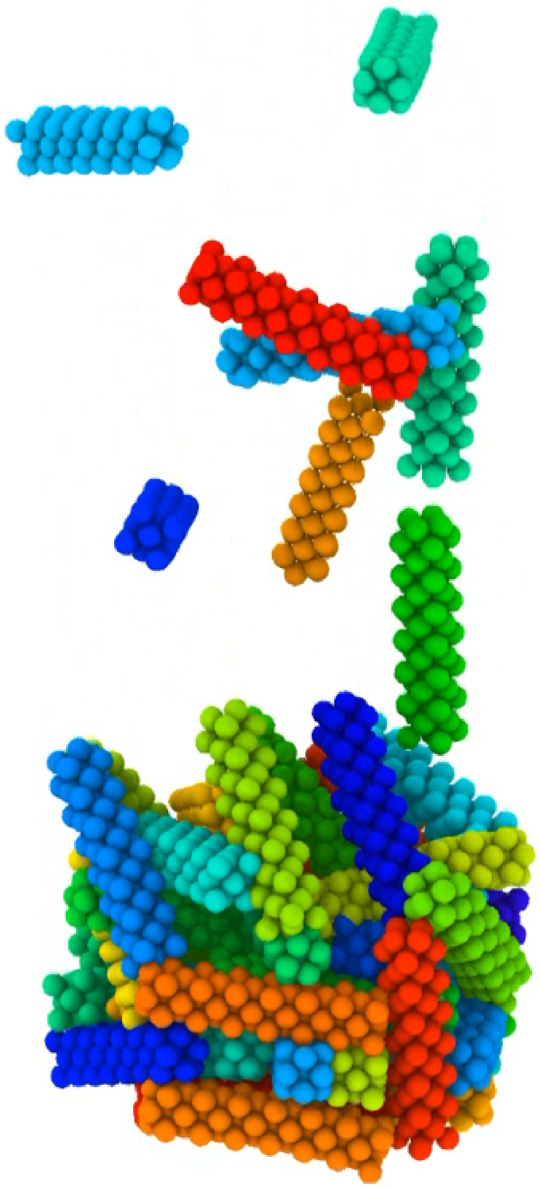
Bonded particle model (BPM) connects particles with breakable springs, solve Newtonian equations while obeying symmetries

Equilibrium length of bond = initial length → stress-free initial state

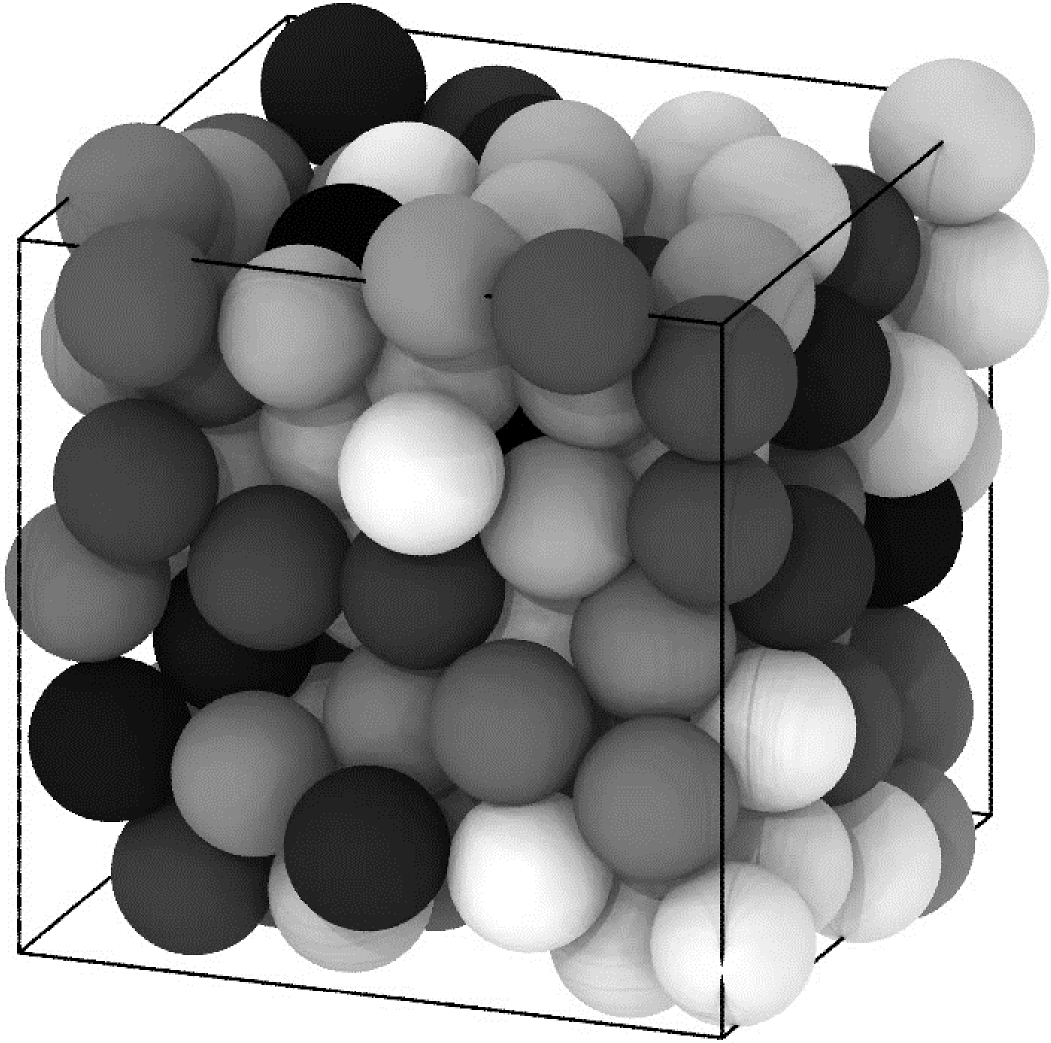
Can model:

- Soft, squishy grains
- Arbitrary shapes/sizes of grains
- Fracture and fragmentation

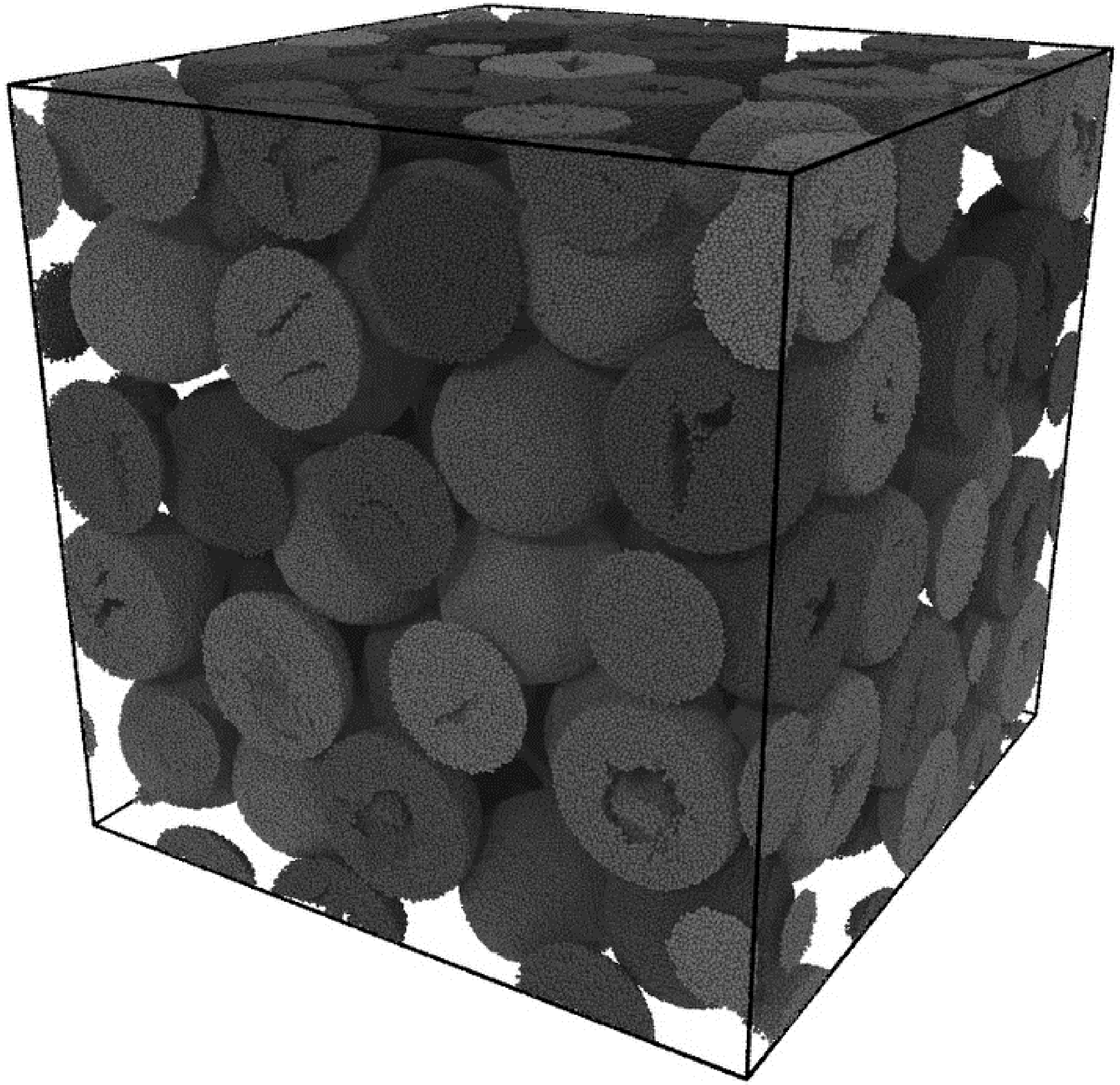




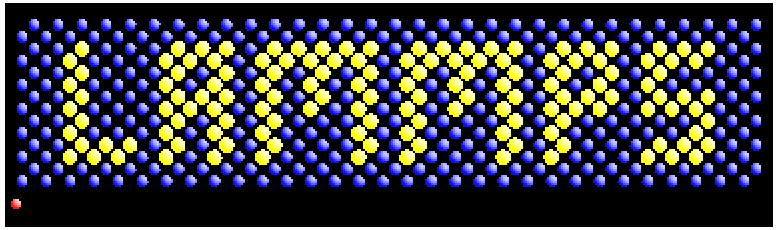
Compaction using traditional discrete element method



Compaction using bonded particle model

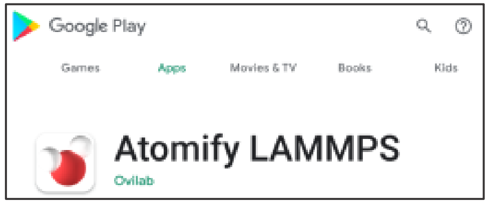


LAMMPS for granular modeling



LAMMPS (https://www.lammps.org/) is a particle-based simulation code with lots of great DEM tools and now BPM as well

It’s a flexible research platform which is fast, parallel, and open-sourced



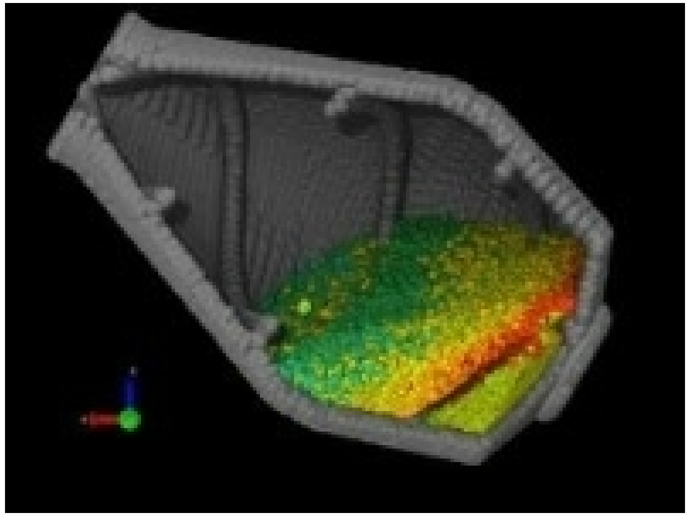
Available on the Android store (?)

Lots of active development by contributors at Sandia & other institutions

A. Kohlmeyer, S. Plimpton, D. Bolintineanu, I. Srivastava, K. Stratford, K. Hanley, T. Shire, S. Lamont, R. Berger, T. O’Connor, J. Coulibaly…

New features include:

1) BPM package with spring-like bonds and beam-like bonds
2) Updated DEM models, rolling/sliding friction (Santos 2020)
3) Options to create particles on surfaces using STL meshes
4) Computes for fabric tensor and tracking contact lifetime history
5) Efficient contact detection for polydisperse systems (Stratford 2018, Monti in prep)



A. Kohlmeyer

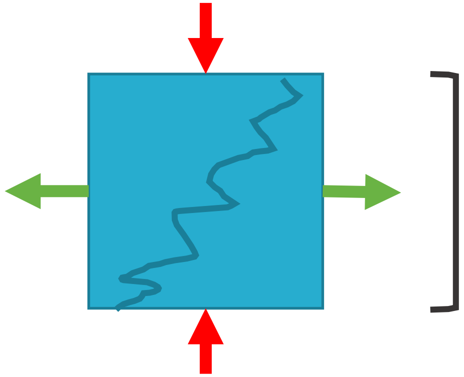
Simulations of fragmentation

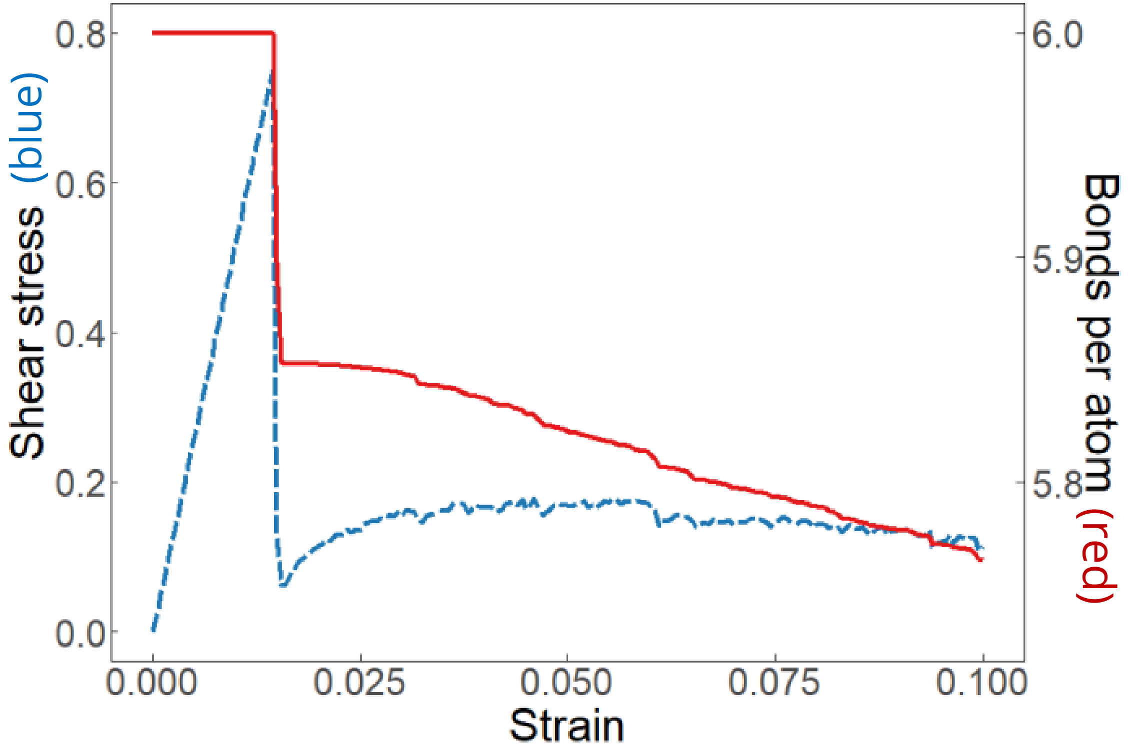
Consider a solid block undergoing shear: how does it break into grains?

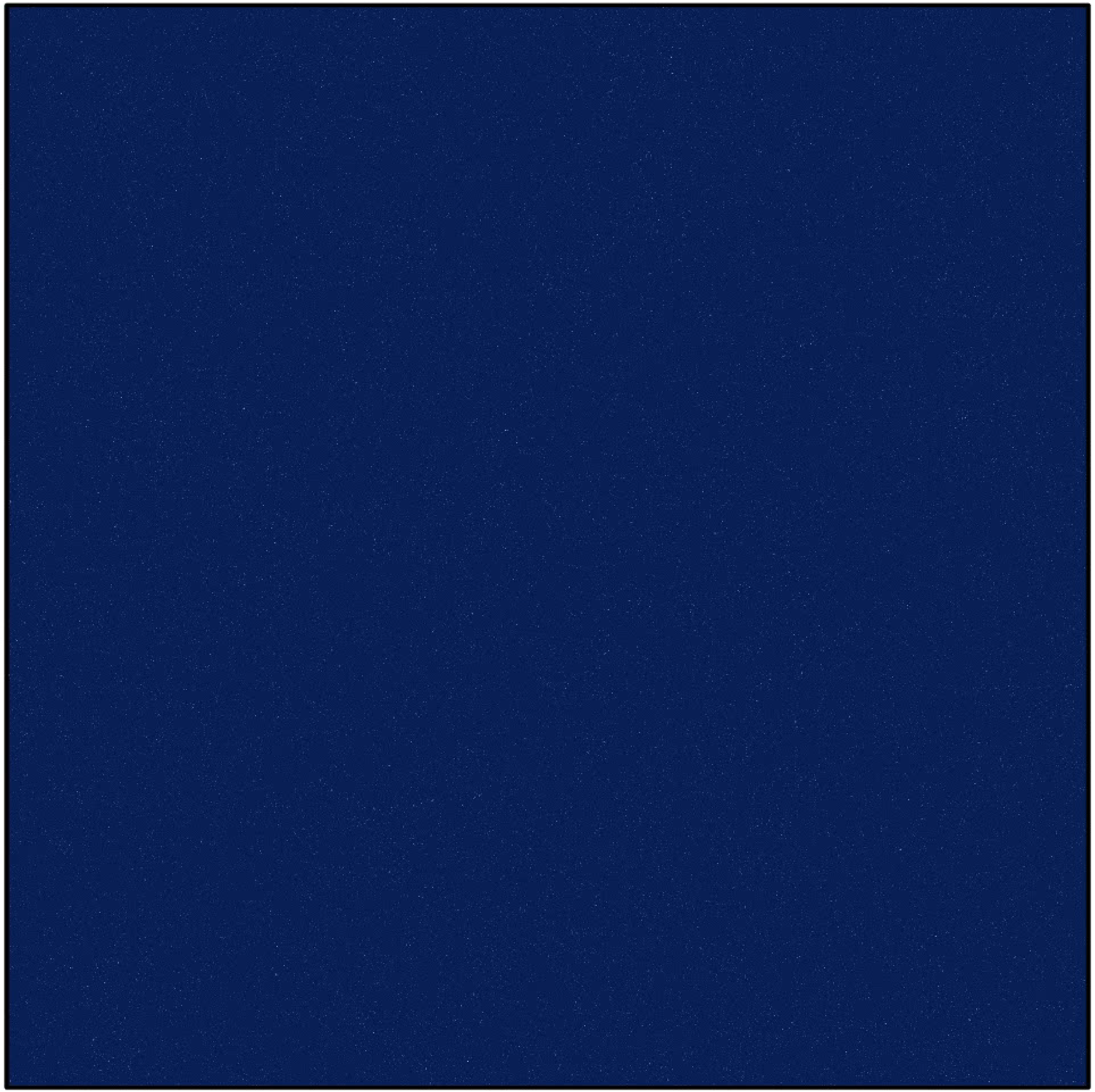
Work started at JHU with Mark Robbins, now finishing at Sandia

Set up:

- 2D simulations with systems of size L x L
- Up to 10 million point particles
- Bonds smoothly break at strains of 5%
- Fixed-rate $\dot{\epsilon}$ pure shear, constant volume
- Periodic, Kraynik-Reinelt boundaries (allows shear to arbitrary strains)



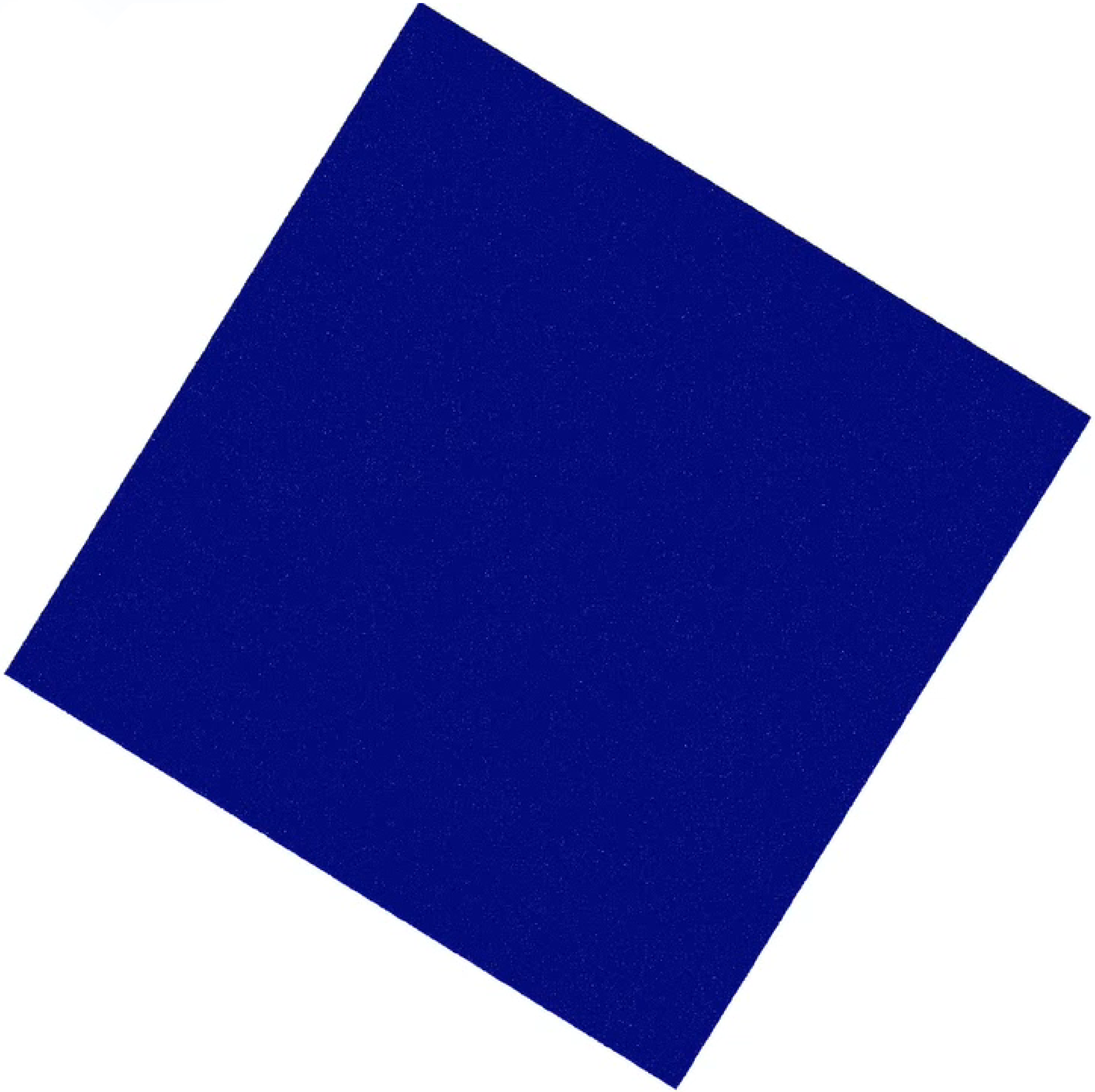




Illustrative system

2 million particles

~ quasistatic



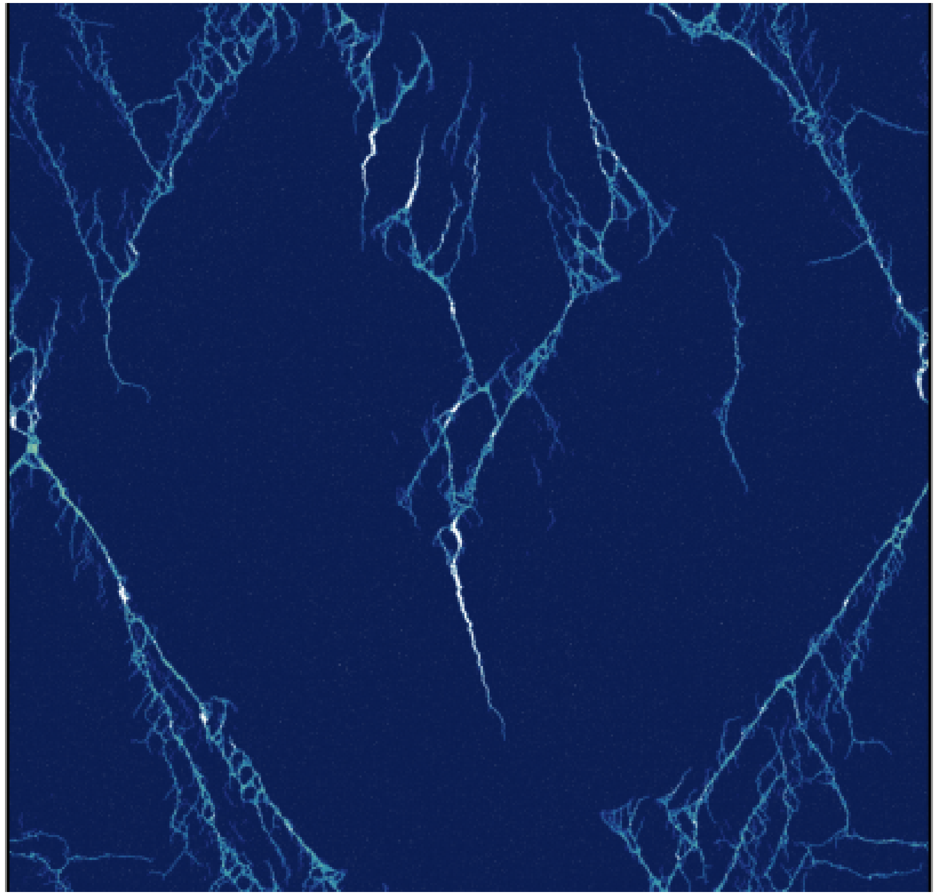
Actual simulation
KR boundaries
10^7 particles
Quasistatic

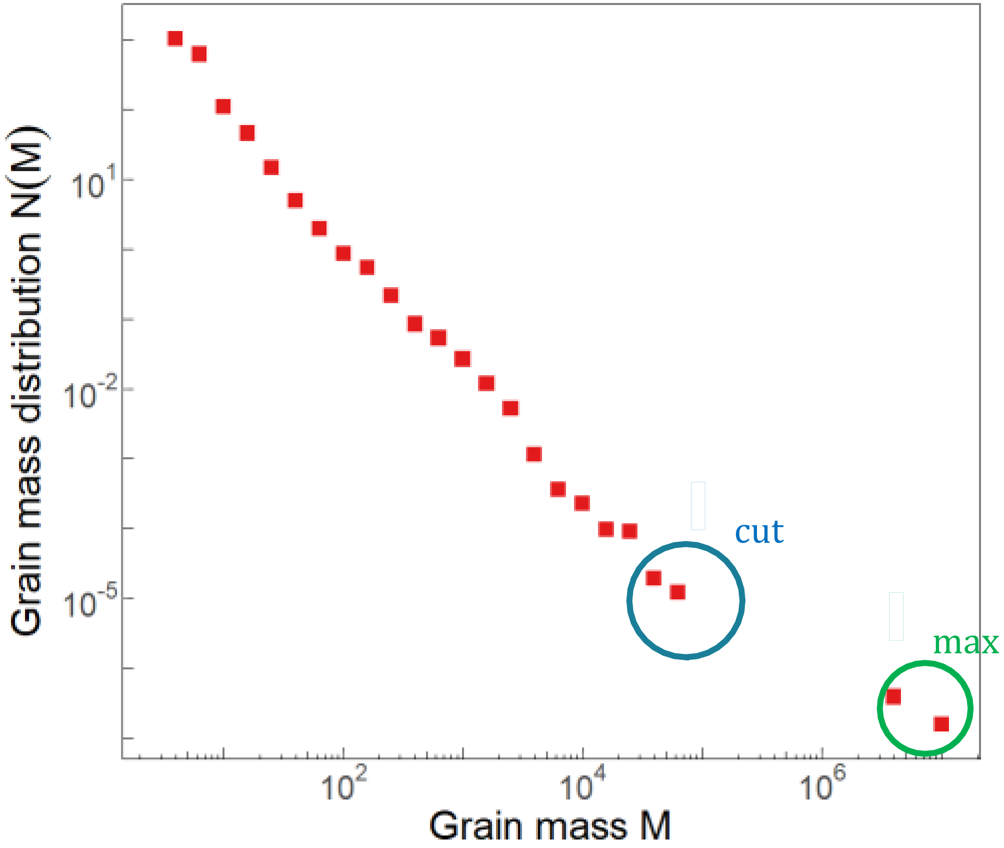
Grain size distribution in quasistatic limit

During flow, identify grains and tally # of grains of a given mass: $N(M)$

Shortly after yield, $N(M)$ looks like a power law up to $M_{\mathrm{cut}} \sim 5 \times 10^4$ particles

But majority of system is unfragmented and has a much larger mass of $M_{\mathrm{max}} \sim 10^7$ particles





Power laws in fragmentation

Power law distributions seen many times before in fragmented granular matter:

- Asteroid impacts (O'Brien 2003)
- Crushed/sheared grains (Oddershede 1993, Carmona 2008, McDowell 2002)
- Exploded egg shells (Wittel 2004)
- Fault gorges (Marone 1989, Kanamori 2004)
- Ice floes (Palmer 2006, Gherardi 2015)
- Ballistic impacts (Chen 2007, Hogan 2017, Ramesh 2022)
- …

Different exponents have been measured, e.g. $\tau \sim 1.5 - 2.2$ (Turcotte 1986)

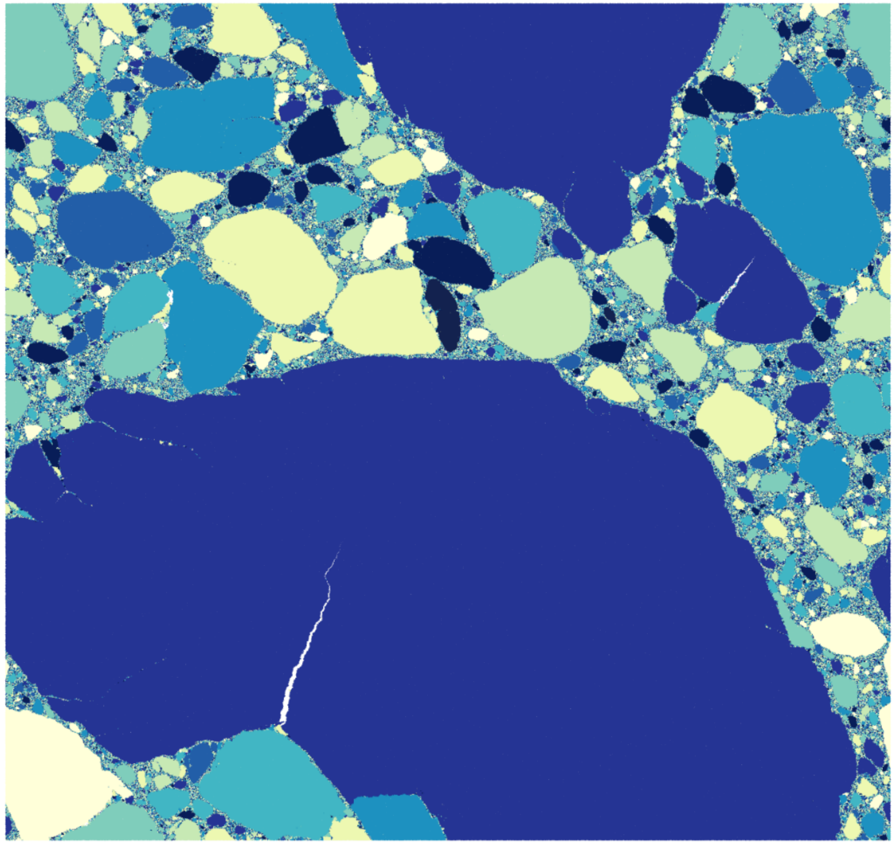
Can we improve theoretical understanding of this behavior?
Can we understand how distributions depend on strain, system size, and strain rate?

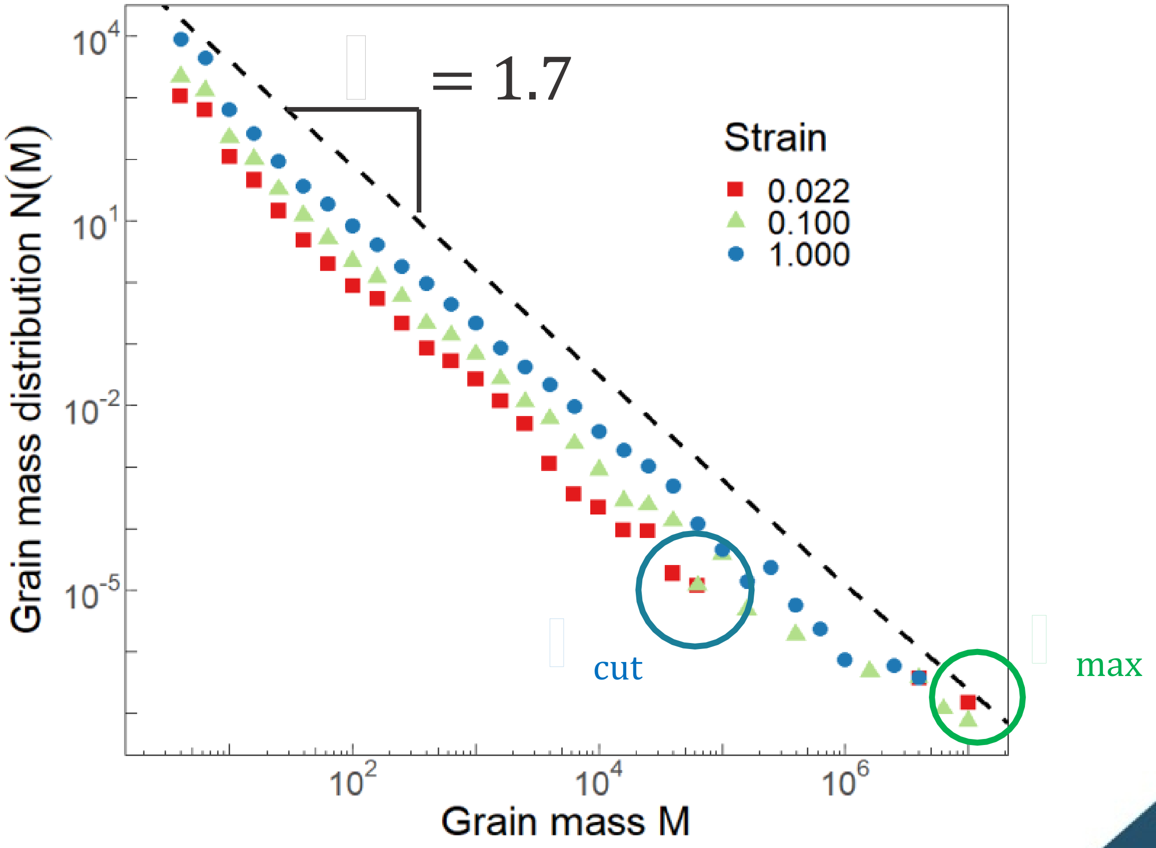
Evolution with strain

With increased strain, M_{cut} grows and $N(M)$ shifts upwards

Increase in power-law regime fueled by reduction in unfragmented material M_{max}

More strain, more grains

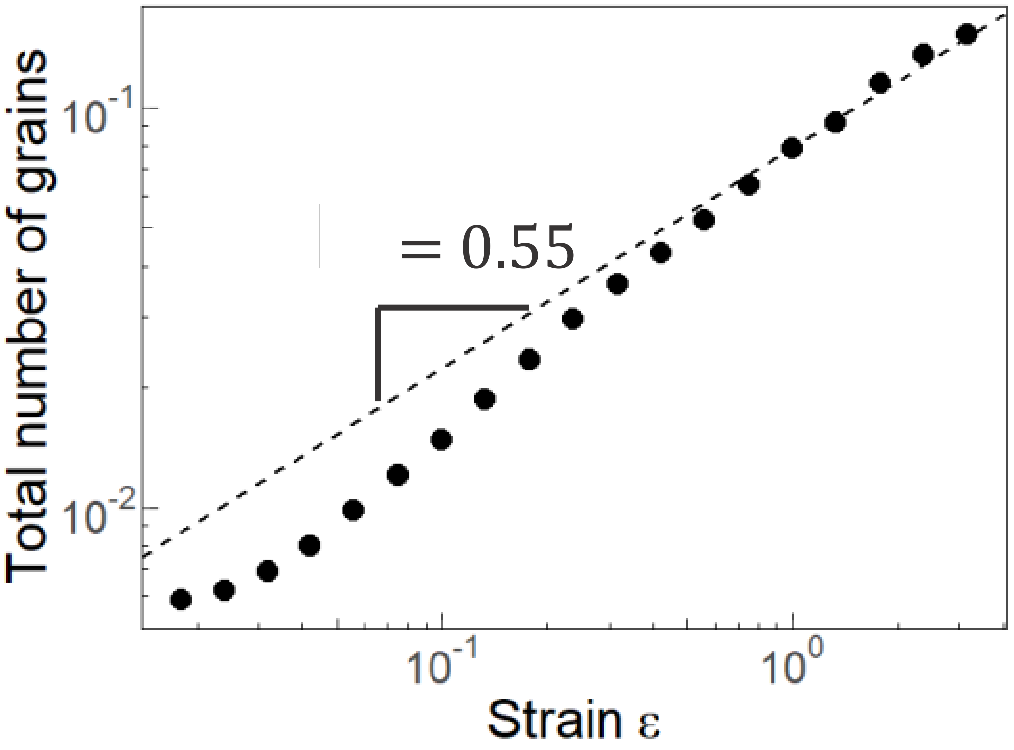


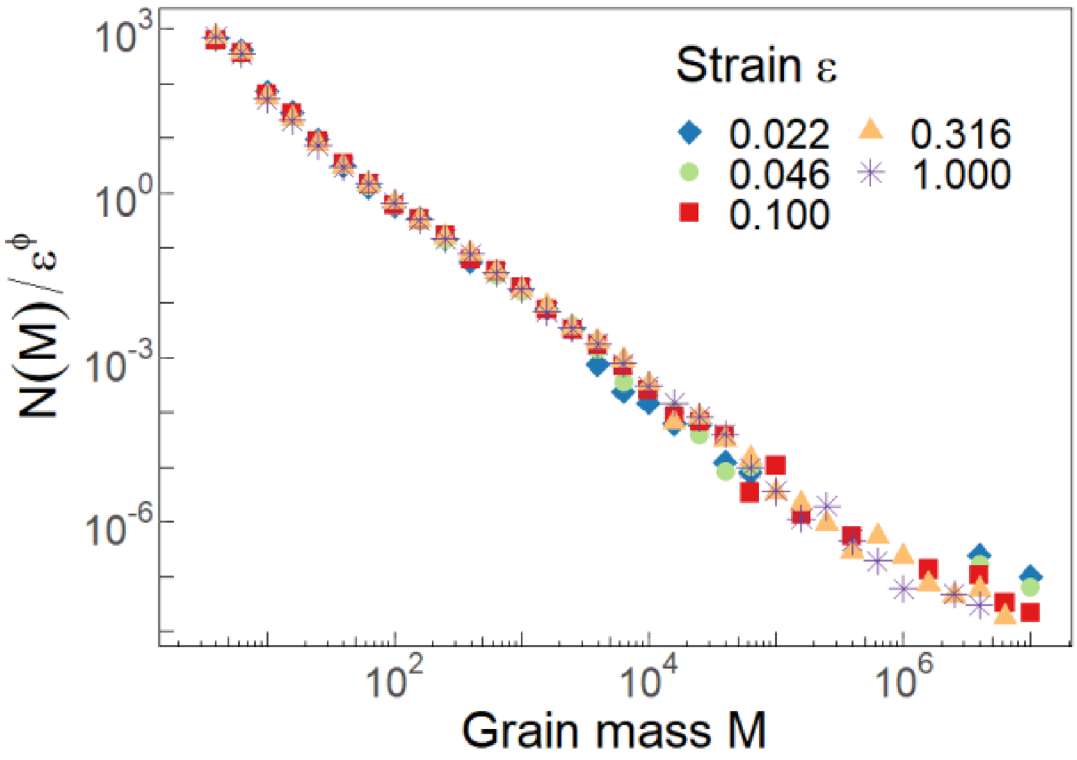


Evolution with strain

Find total number of grains in the system grows as a power of strain

⇒ Can vertically collapse curves by scaling $N(M)$ by ϵ^{ϕ}





Factors affecting the number of grains

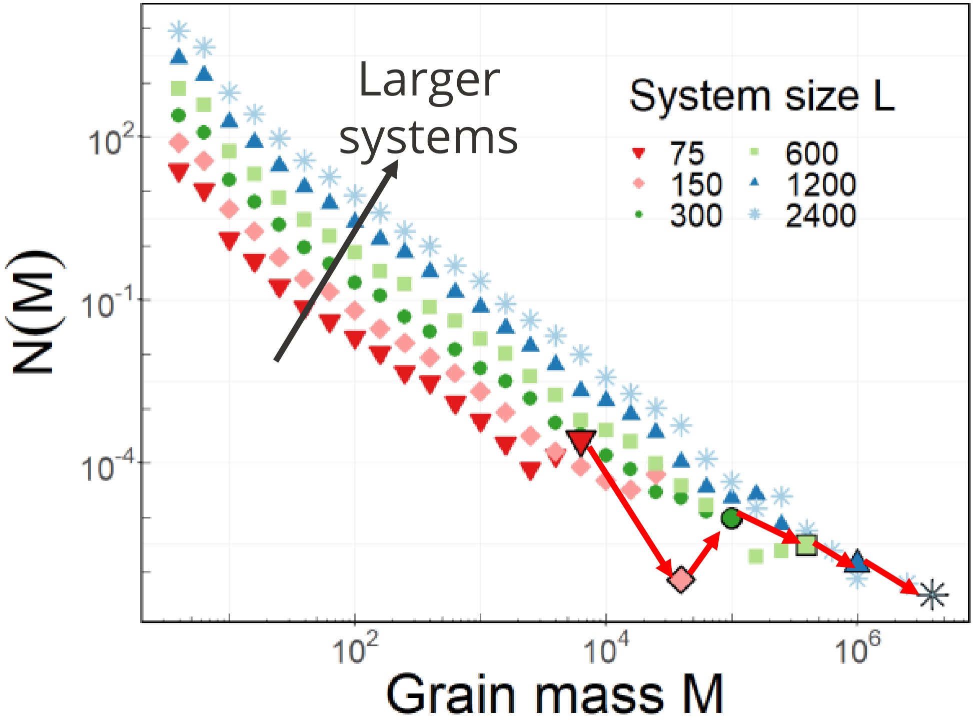
1. ~~The strength of the mug~~
2. ~~The number of times you dropped it~~
3. The size of the mug
4. The impact velocity

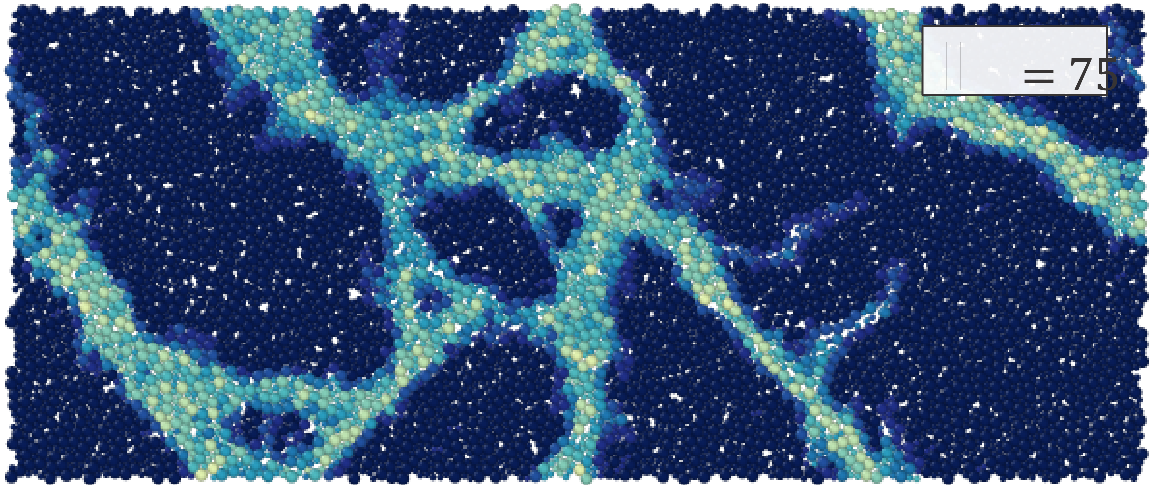
Finite size effects

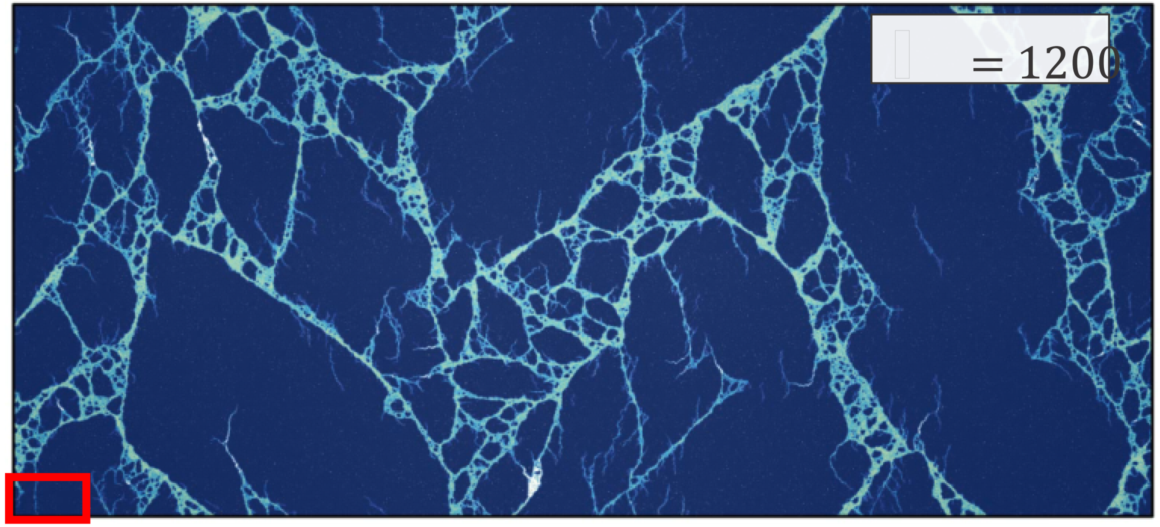
Vary system size, simulate $L = 75$ to 2400

How does distribution change?

1. Fewer grains (maybe # $\sim L^2$?)
2. Smaller grains (maybe $M_{\mathrm{cut}} \sim L^2$?)





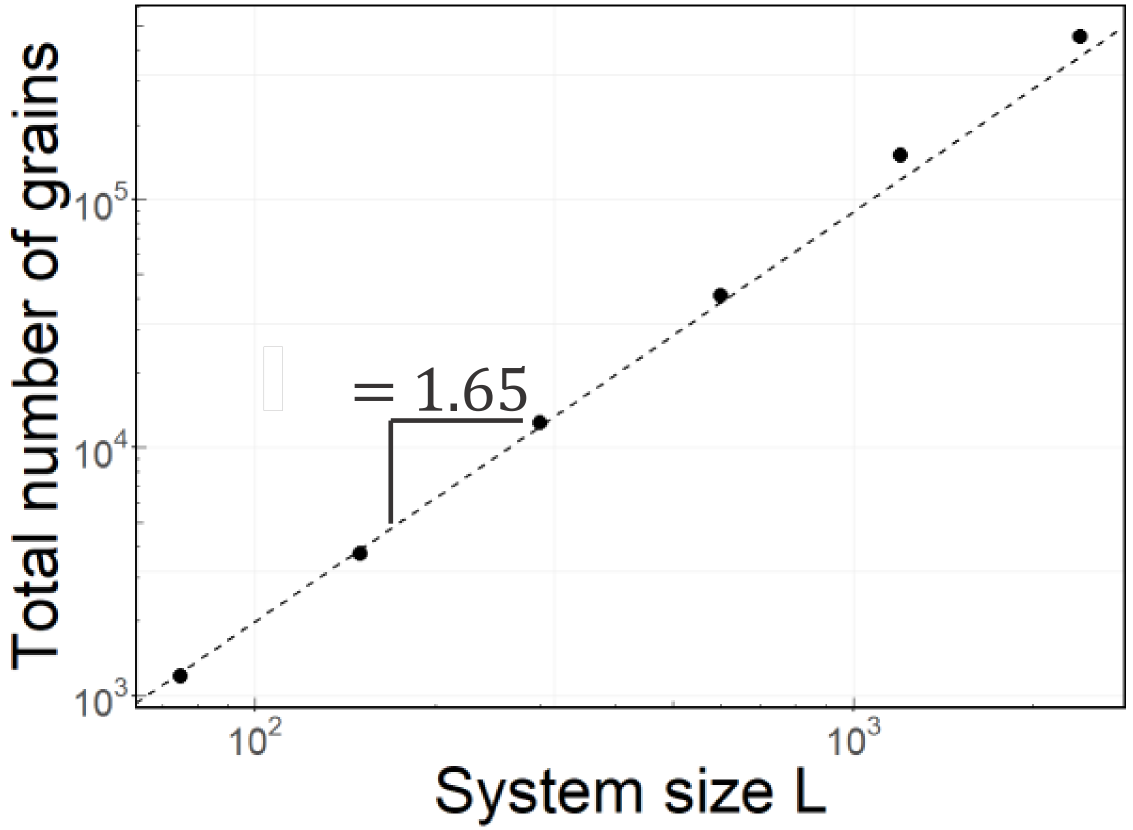


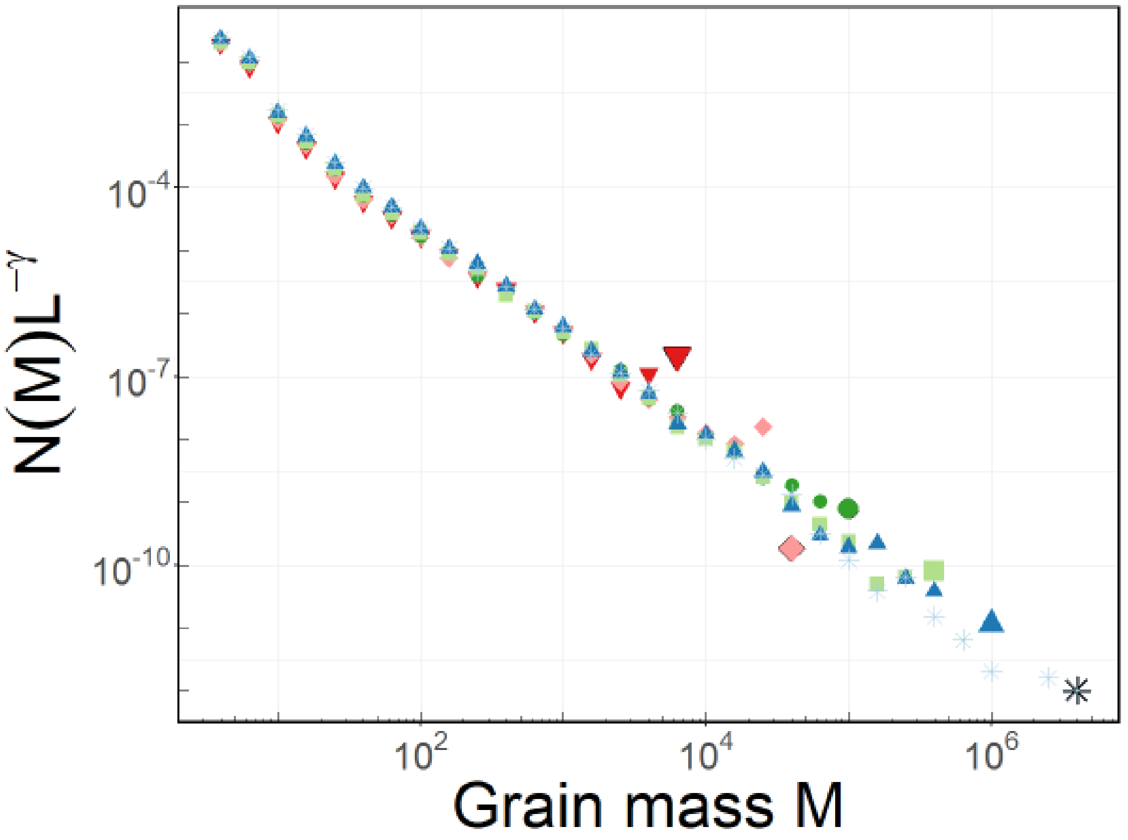
(Note: focus on large-strain limit for remainder of talk)

Finite size effects

Find number of grains scales sub-extensively, goes like $\sim L^{\gamma}$ for $\gamma < 2$

Can, again, vertically collapse distributions to confirm scaling

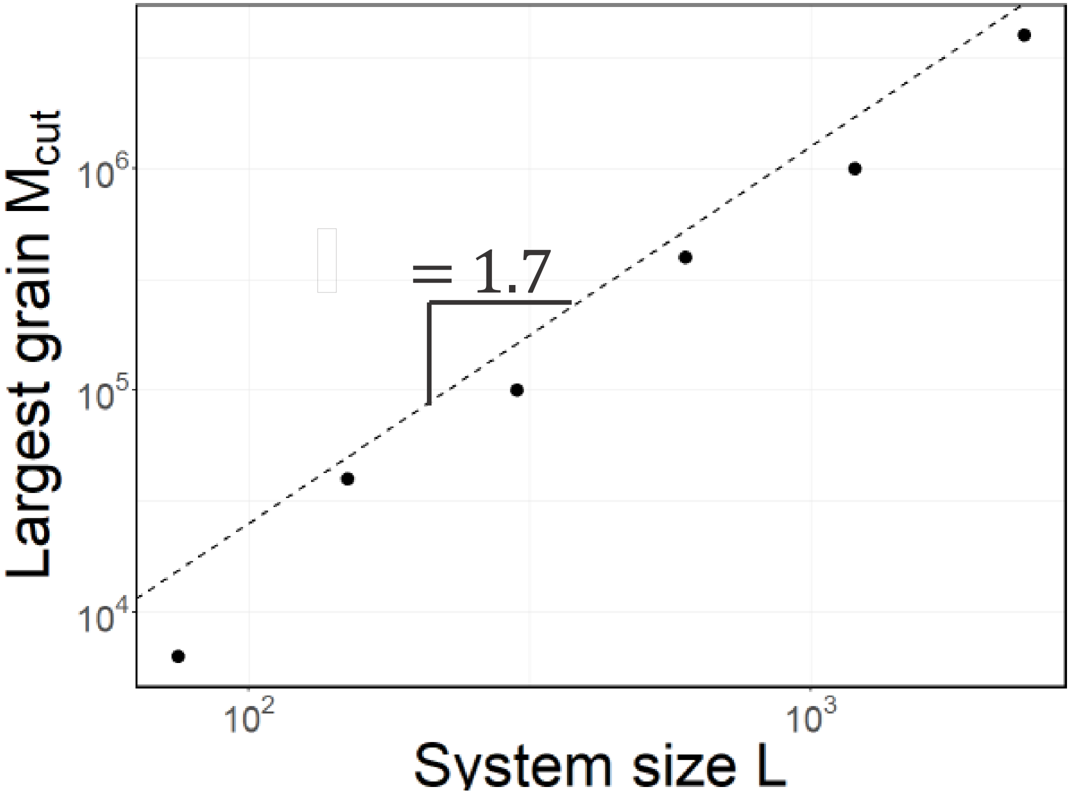


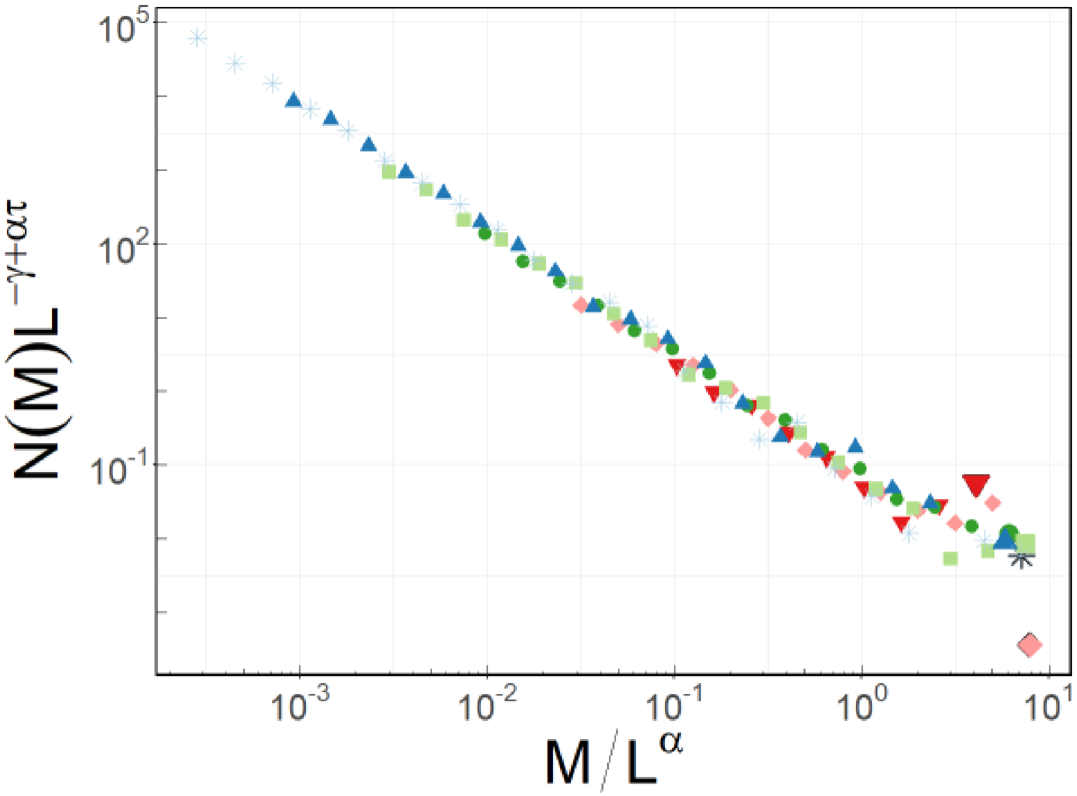


Finite size effects

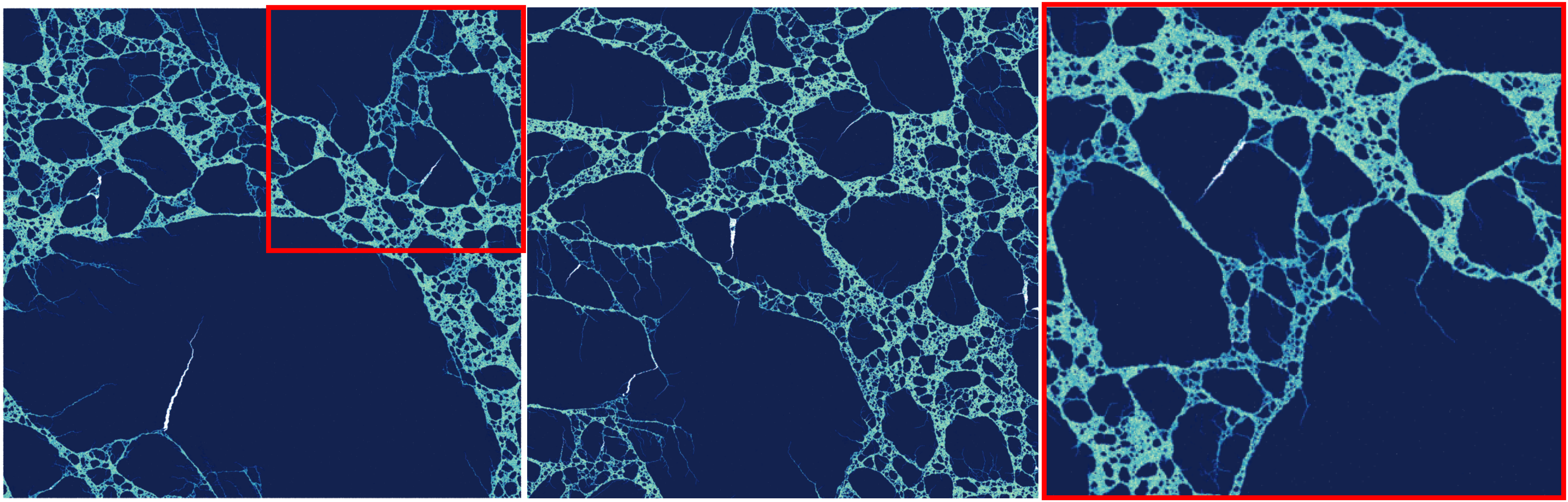
Largest grain also scales sub-extensively as $M_{\text{cut}} \sim L^{\alpha}$ for $\alpha < 2$, fractal behavior

From conservation of mass, can derive and test scaling relation $2 = \gamma + \alpha(2 - \tau)$





Which of the three images is not like the others?



Scale invariance – critical behavior?

Scale invariance in power laws, zooming in × 2:

$$M \rightarrow 4\,M \quad \Rightarrow \quad N(4M) \sim (4M)^{-\tau} \sim M^{-\tau}$$

Due to scale invariance, it has been postulated that fragmentation is an example of self-organized criticality

(Oddershede 1993, Astrom 1998, Einav 2007)

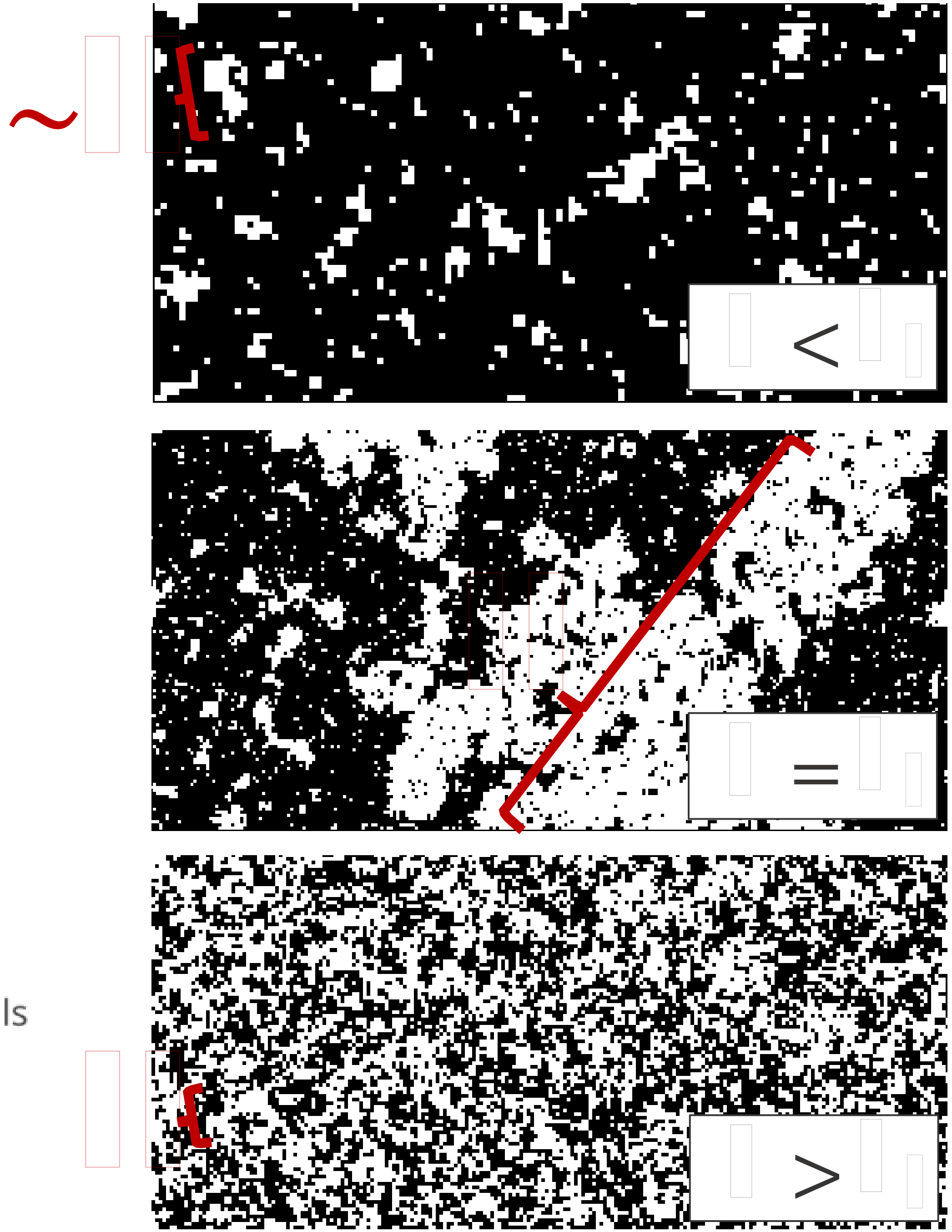
Equilibrium critical points are locations in phase space where systems undergo a continuous phase transition

e.g. paramagnetic/ferromagnetic

Several important properties at T_c

- Diverging correlation length: $\xi \sim (T - T_c)^{-\nu}$
- Scale invariance, power-law scaling
- Universality, exponents depend on symmetries not microscopic details

Is there a diverging correlation length in fragmentation? What universality classes exist? How does $N(M)$ scale?



https://mattbierbaum.github.io/ising.js/

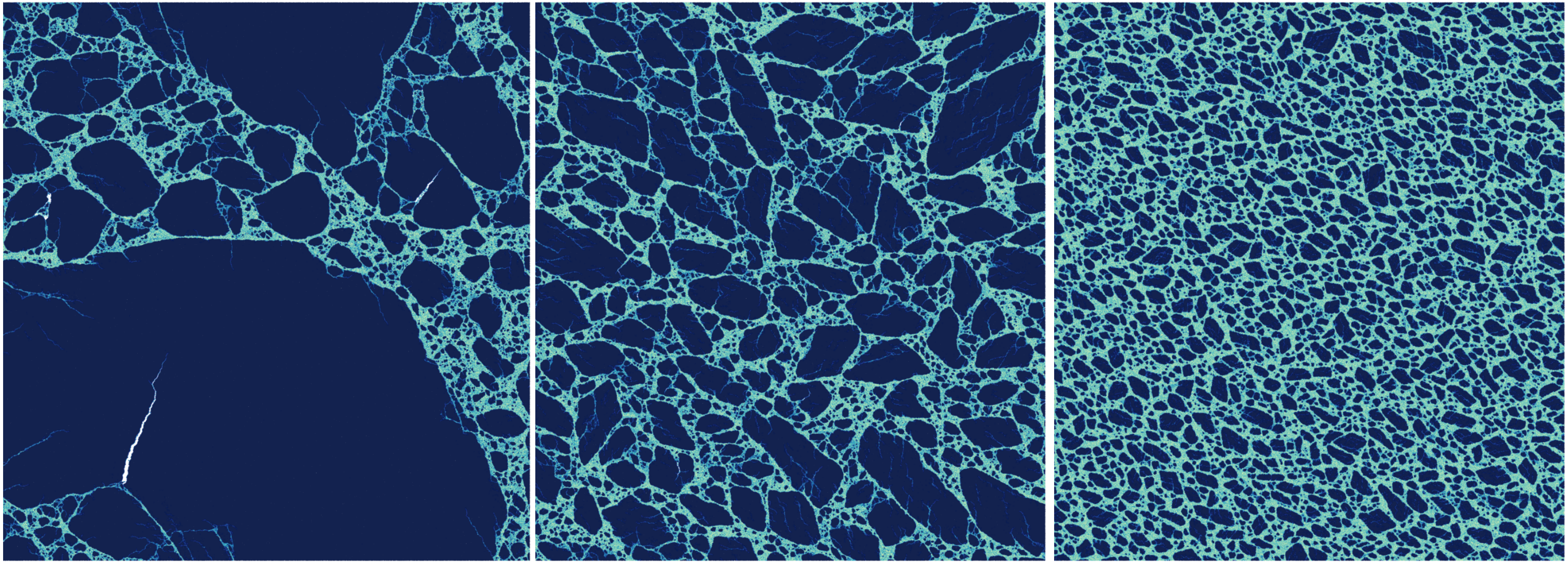
Factors affecting the number of grains

1. ~~The strength of the mug~~
2. ~~The number of times you dropped it~~
3. ~~The size of the mug~~
4. The impact velocity

Finite strain rate effects

As one would expect, increasing the strain rate leads to smaller fragments

(Grady 1985, Lankford 1996, Wittel 2008, Cereceda 2017)



Increasing strain rate by 3 orders of magnitude

Finite strain rate effects

As strain rate increases, see two effects:

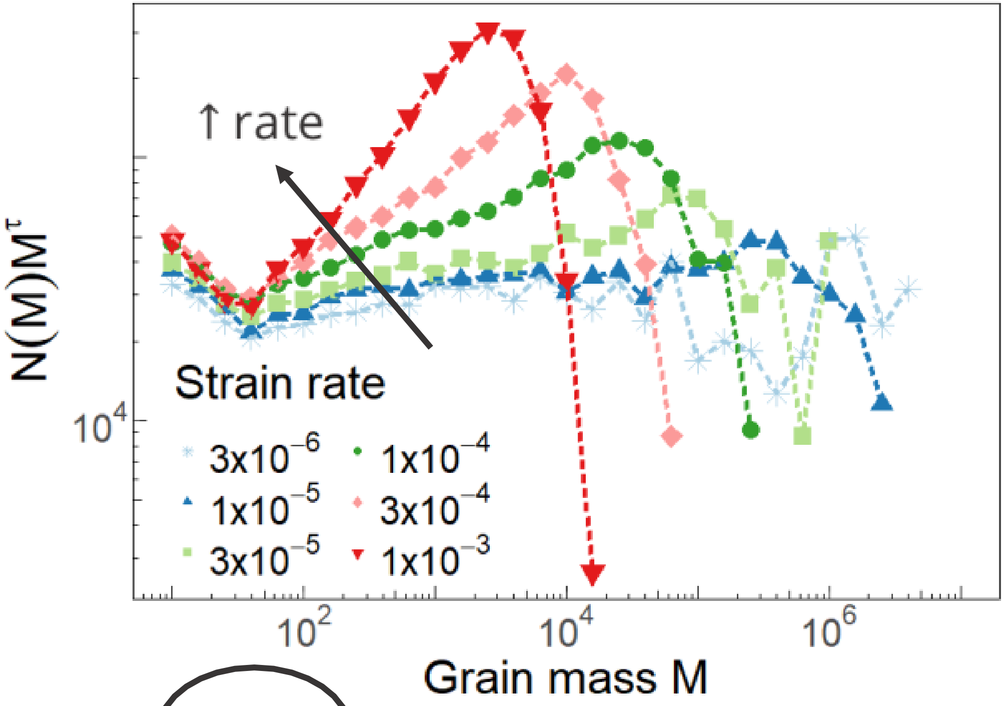
1. Reduction in max size M_{cut}
2. Larger power-law exponent – unexpected
   May explain some variation in measured τ?

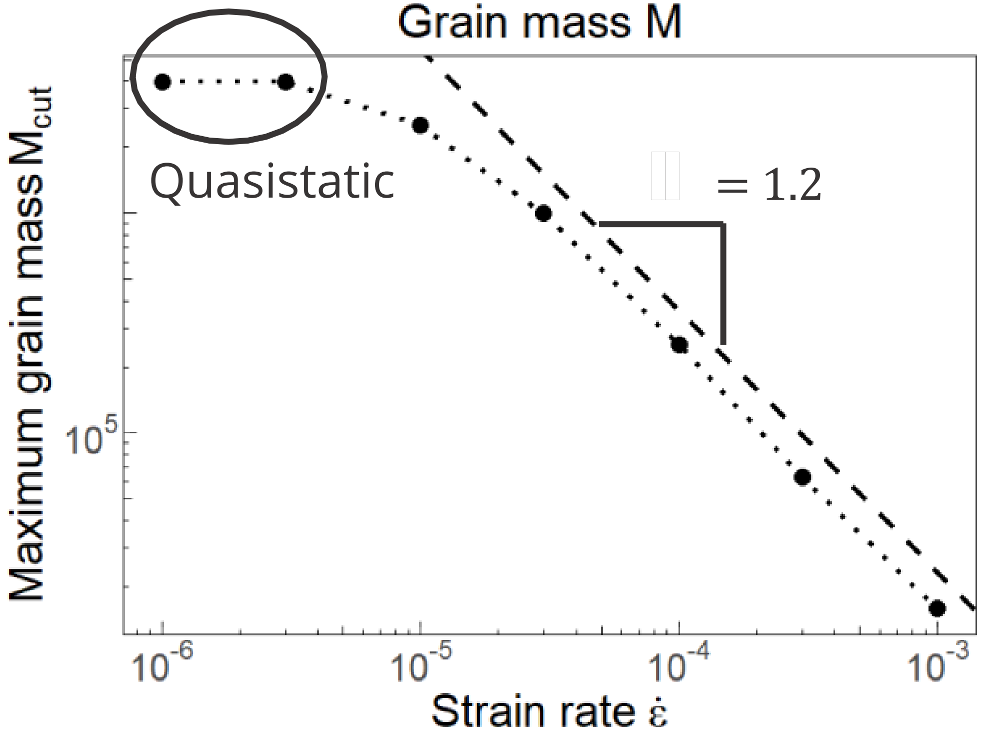
Largest grows as a power of decreasing rate:

$$M_{\text{cut}} \sim \xi^{\alpha} \sim \dot{\epsilon}^{-\alpha\nu}$$

This gives us our diverging correlation length:

$$\xi \sim \dot{\epsilon}^{-\nu}$$





Factors affecting the number of grains

1. ~~The strength of the mug~~
2. ~~The number of times you dropped it~~
3. ~~The size of the mug~~
4. ~~The impact velocity~~

Extra mathematical details, transitioning to the quasistatic limit

Can define crossover to quasistatic limit by relating L to ξ:

- If $\xi > L$, then system size determines scaling and the system is in the quasistatic limit
- If $L > \xi$, then strain rate determines scaling and the system is in the finite-rate limit

Given some assumptions*, can construct scaling relations for $N(M)$ in the two regimes:

- $N_{QS}(M, L) \sim L^{\gamma-\alpha\tau} f(M/L^{\alpha})$
- $N_{FR}(M, \dot{\epsilon}) \sim L^2 \dot{\epsilon}^{\nu(2-\gamma+\alpha\tau)} \not{f}(M\dot{\epsilon}^{\nu\alpha})$

Then derive distribution moments

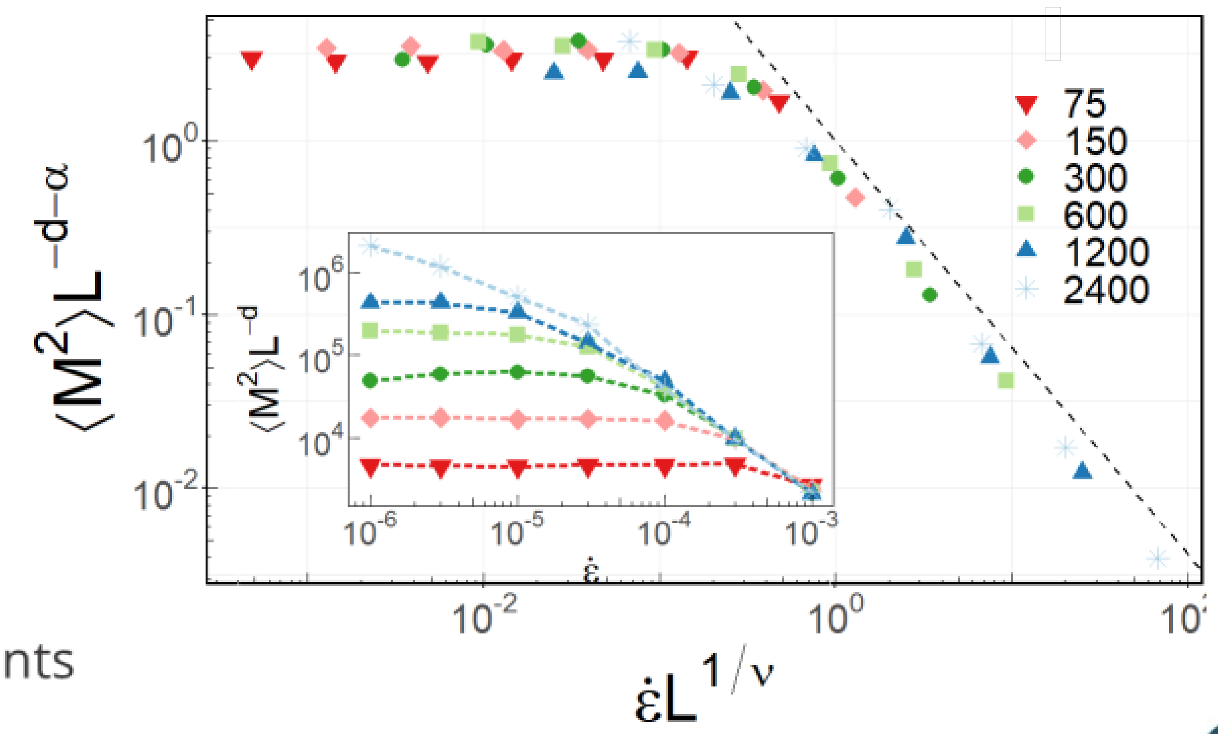
$$\langle M^n \rangle = \int M^n N(M) dM$$

and construct a finite-size scaling relation

$$\langle M^2 \rangle \sim L^{2+\alpha} g(\dot{\epsilon} L^{1/\nu})$$

to collapse $\langle M^2 \rangle$ as a function of L and $\dot{\epsilon}$

⇒ Can characterize the crossover between QS and FR limits and improve estimates of exponents



*Must be close enough to critical point, e.g. no change in power-law exponent or extra size effects

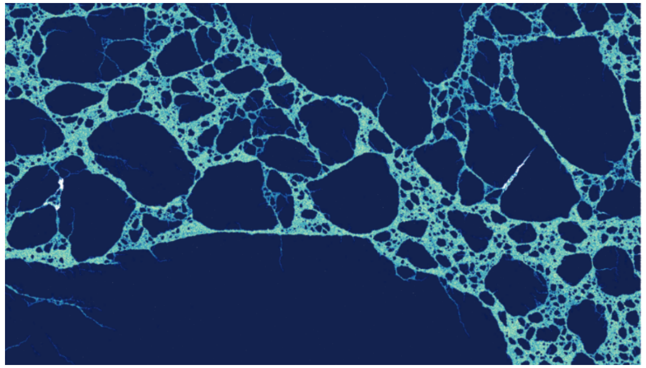
Why does this matter? Granular rheology

Fundamentally interesting to know how grains are produced and how distributions scale:
Can we tailor fragmentation to get a desired $N(M)$?

$N(M)$ also affects granular rheology

During fragmentation, see unusual ~log decay in stress ratio with increasing inertial number

Grains are finer at higher rates, so it is easier to flow



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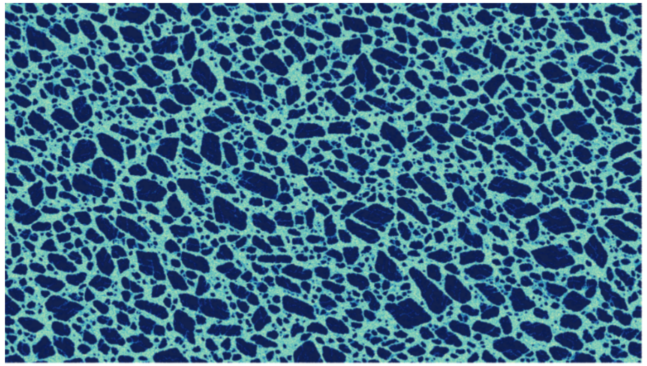
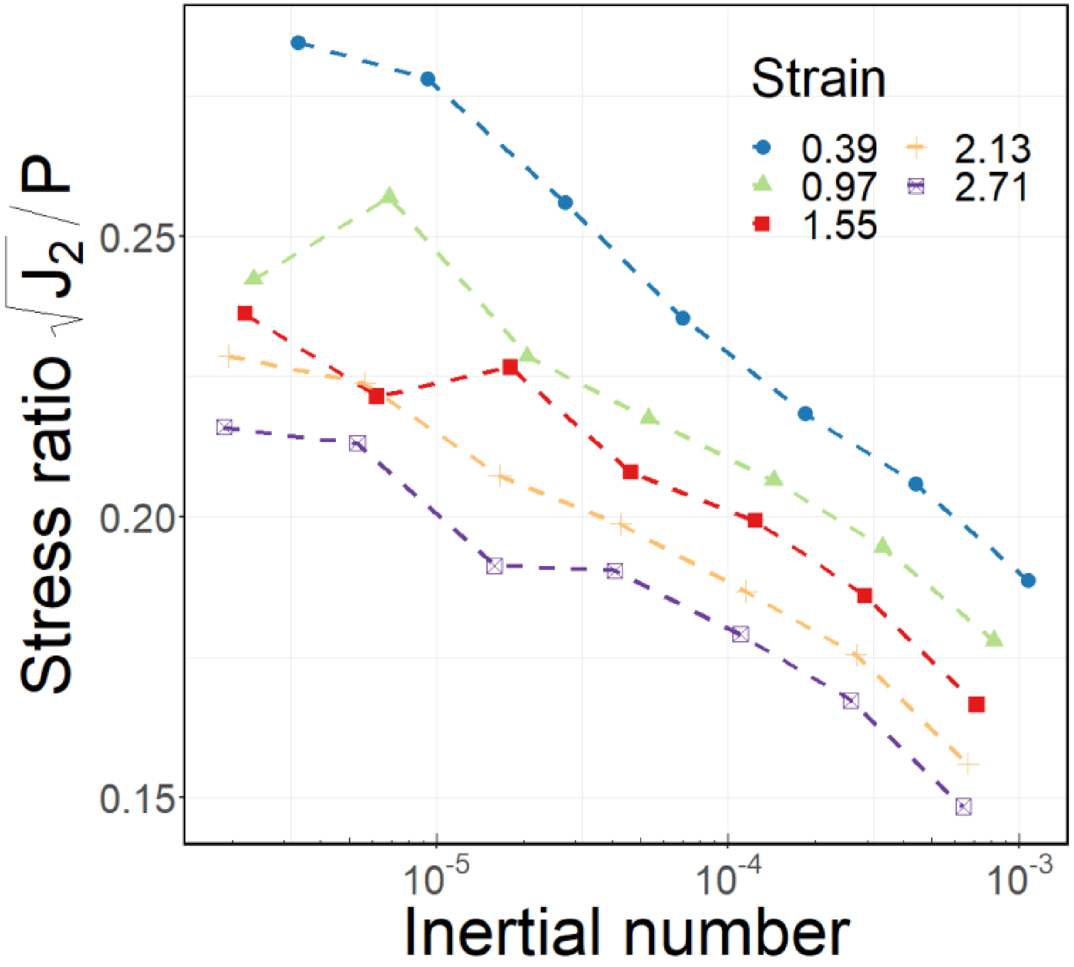
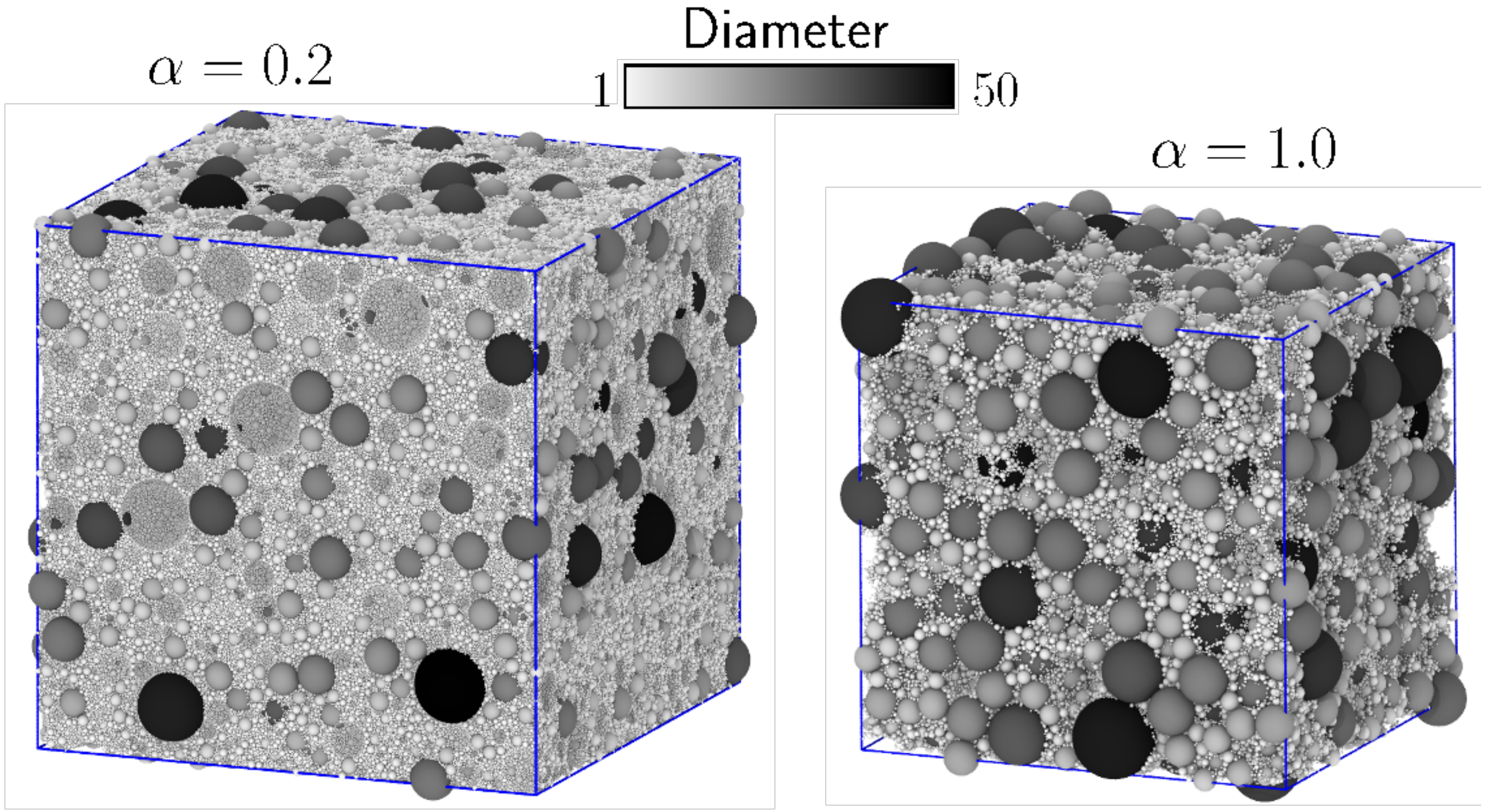


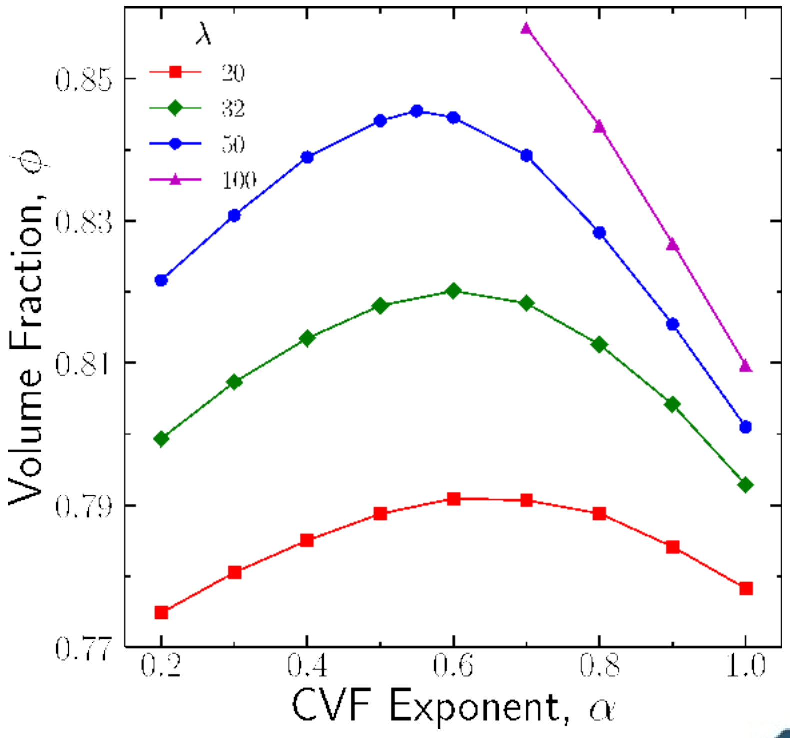


Why does this matter? Granular packing

$N(M)$ also has a dramatic effect on granular packing and the statistics of contacts

Recently Joe Monti has characterized 3D power law packings with large size ratios





Summary

Using bonded particle models, we can explore such complex granular problems that emerge at large stresses

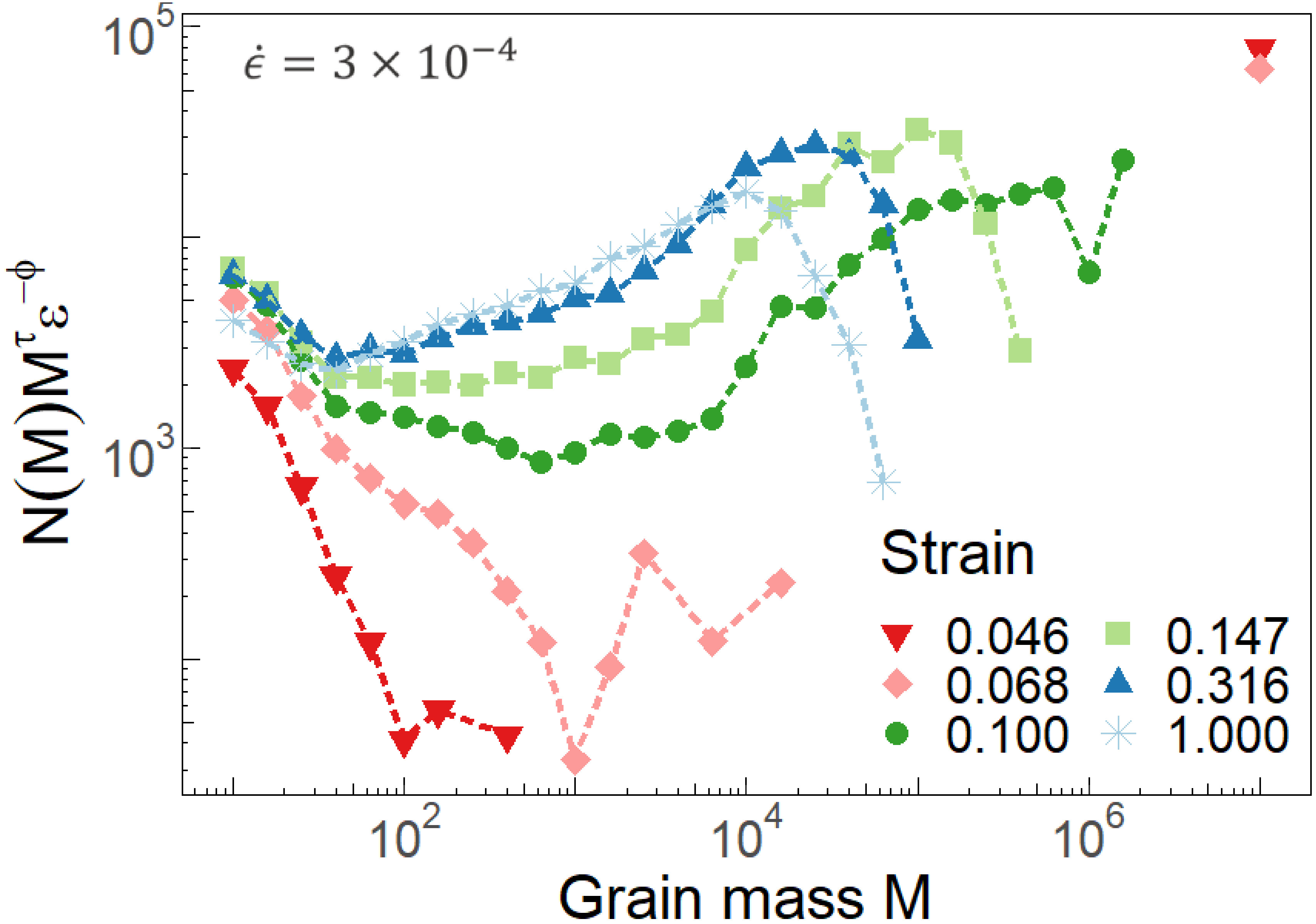
There is a lot of rich behavior behind the production of granular matter during fragmentation, see evidence of critical behavior

Many more frontiers to explore:

- Material properties
- Loading geometry
- Three dimensions
- Other high-pressure granular systems

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	$M_{\text{cut}} \sim L^{\alpha}$
ν	0.70 ± 0.08	$\xi \sim \dot{\epsilon}^{-\nu}$

Strain dependence at high rates



Kraynik-Reinelt boundary conditions

(Kraynick, Reinelt 1992)