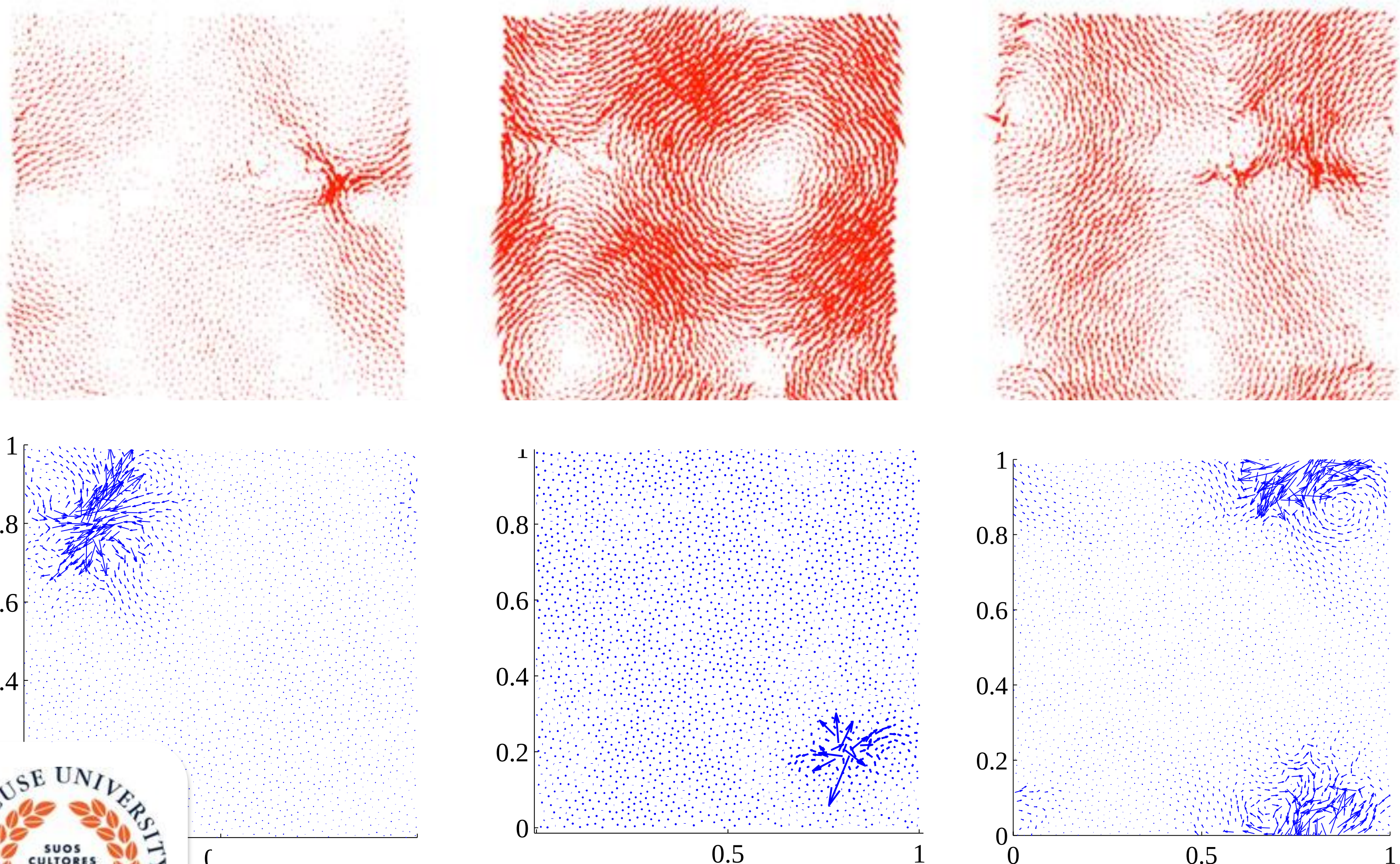
Defects in disordered solids: building blocks for avalanches?

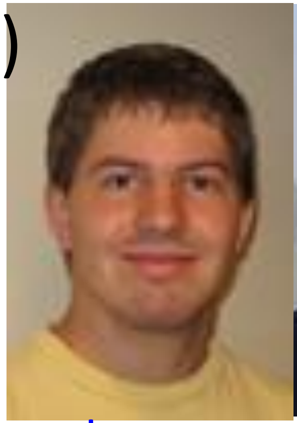


M. Lisa Manning,
Syracuse University

KITP 10/10/2014

Manning group and collaborators

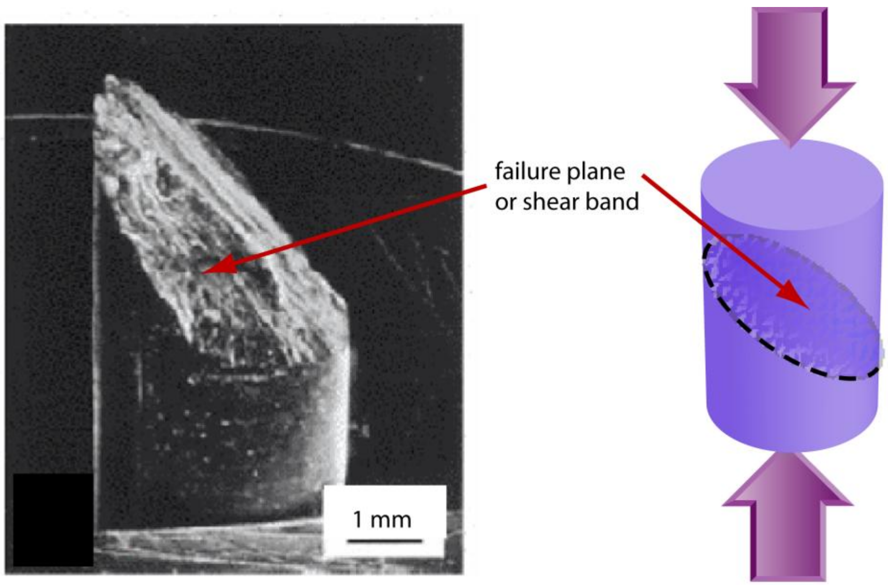
- Manning group (SU)
  - Sven Wijtmans
  - Dapeng “Max” Bi
  - Giuseppe Passucci
  - Craig Fox
  - Contact: mmanning@syr.edu



- Liu Group (UPenn)
  - Andrea Liu
  - Sam Schoenholz
  - Carl Goodrich
- Soft Matter Theory (SU)
  - Jorge Lopez
  - Jennifer Schwartz
  - Cristina Marchetti
  - Xingbo Yang
- Schoetz-Collins lab
  - Eva-Maria Schoetz (UCSD)
  - Marcus Lanio (Princeton)
  - Jared Talbot(Princeton)
  - Ramsey Foty (Princeton)
  - Mal Steinberg(Princeton)
- Henderson Group (SU)
  - Jay Henderson
  - Megan Brasch
  - Richard Baker
- SUNY Upstate Medical
  - Chris Turner
  - Nick Deakin
  - Jeff Amack
  - Guangliang Wang
  - Agnik Dasgupta

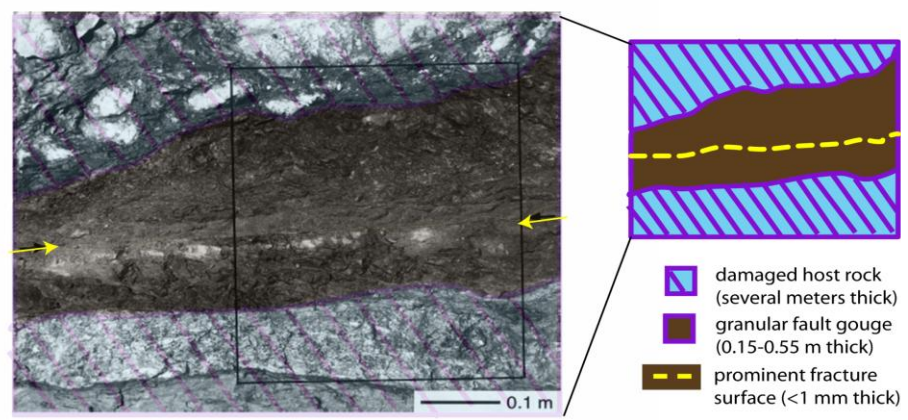
Motivation: what leads to catastrophic failure in disordered solids?

Bulk metallic glasses



W. Johnson Group, Caltech

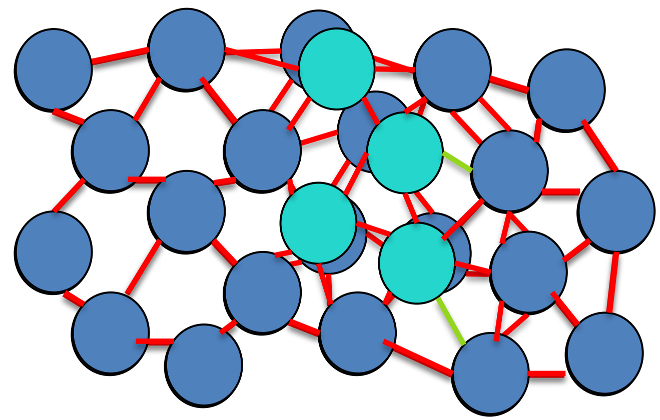
Granular fault gouge



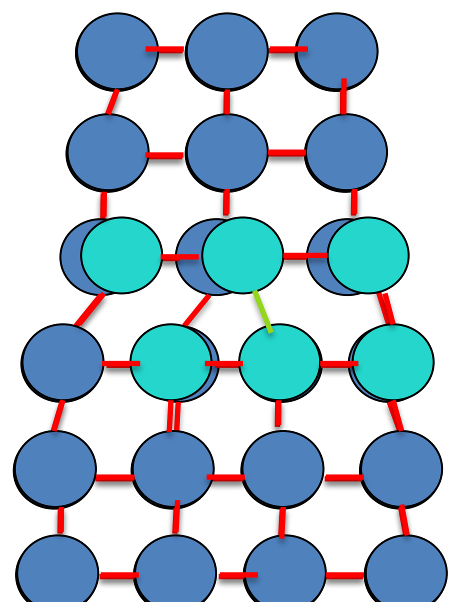
F. M. Chester and J. S. Chester, *Tectonophys.* 295, 1998.

Is there a basic unit of deformation in disordered solids? What is it? How do they interact to form avalanches?

- Liquids: rearrangements can occur anywhere



- Crystalline solids: rearrangements occur at dislocations

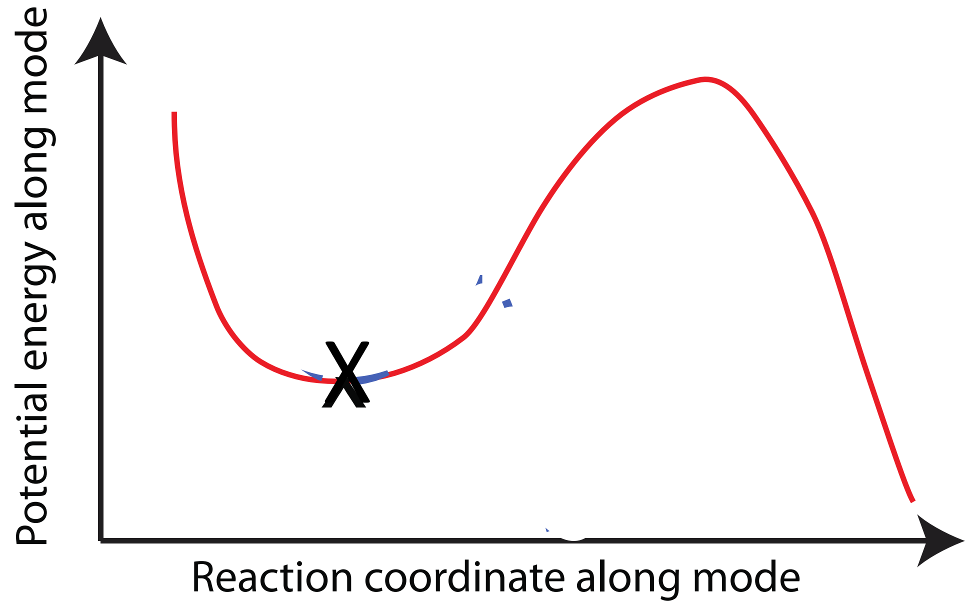


Theoretical framework for solids

- The dynamical matrix describes linear response
  - harmonic approximation for a spring network

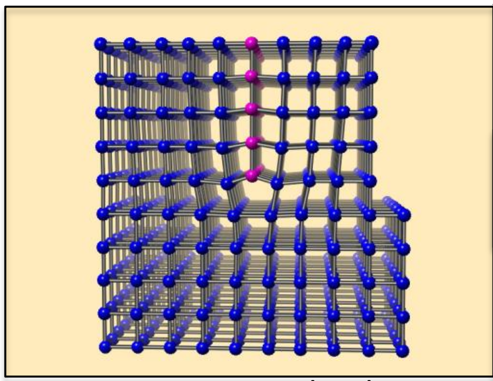
$$m \ddot{u} = M u$$

$$\underset{i \neq j}{M_{iajb}} = \frac{\partial^2 V(|r_i - r_j|)}{\partial r_{ia} \partial r_{jb}}$$

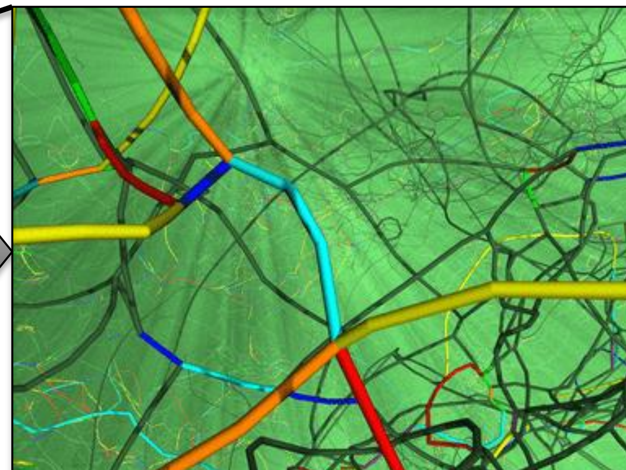


- For an ordered solid, phonons are eigenmodes of the Dynamical Matrix
  - eigenvalues give phonon frequencies
  - matrix is small for crystals (lots of symmetry)

Yes, but we're interested in plasticity – that's a nonlinear response



www.crystalmaker.com



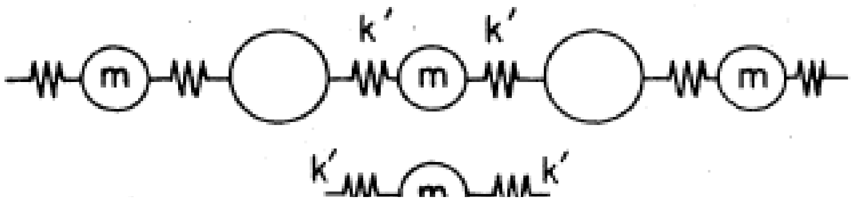
paradis.stanford.edu

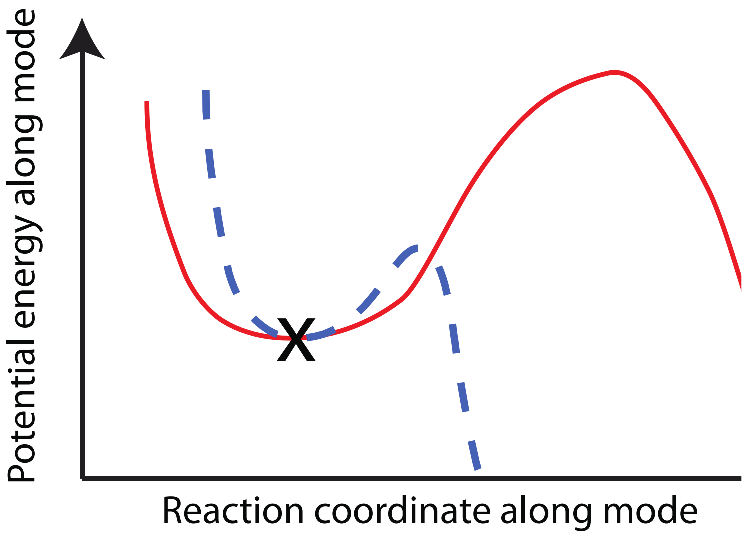
site.uri-geller.com

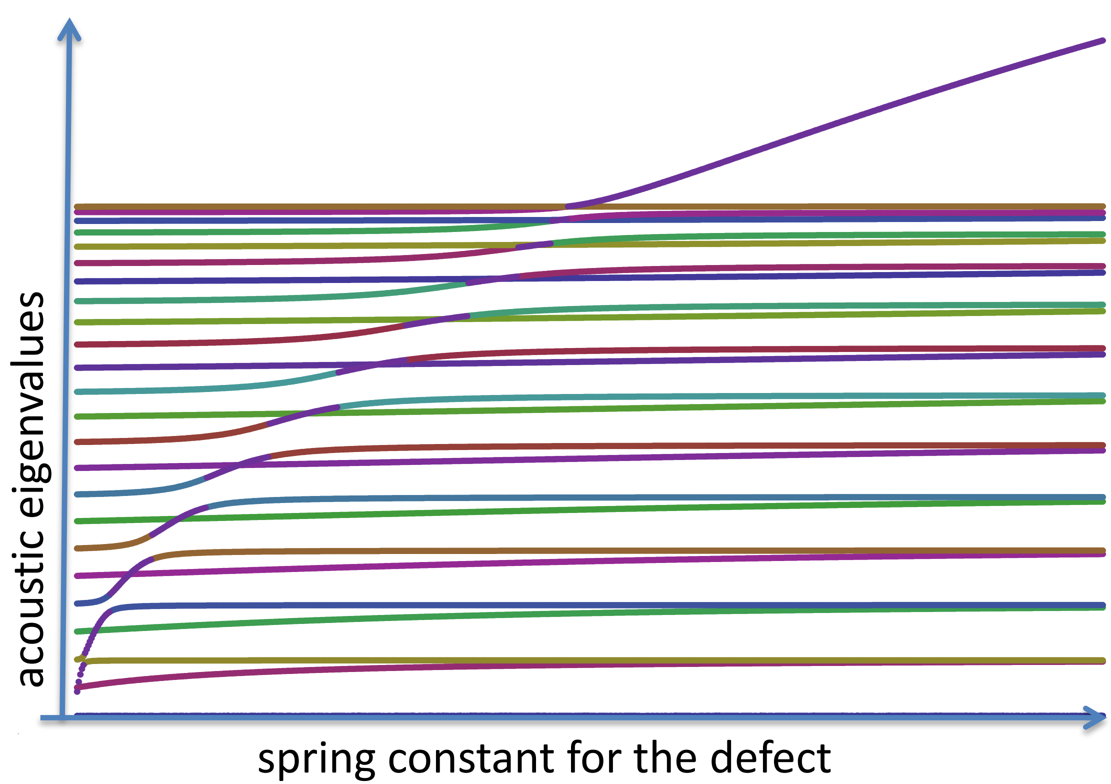
e.g. ordered solids flow via dislocations, locations where geometric order parameter is small.

Linear modes identify defects!

Barker and Sievers, Rev. Mod. Phys. 47 (1975)



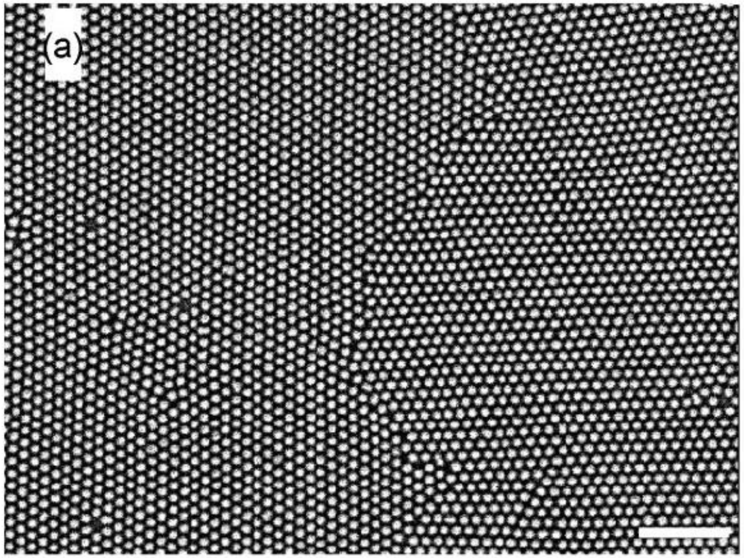


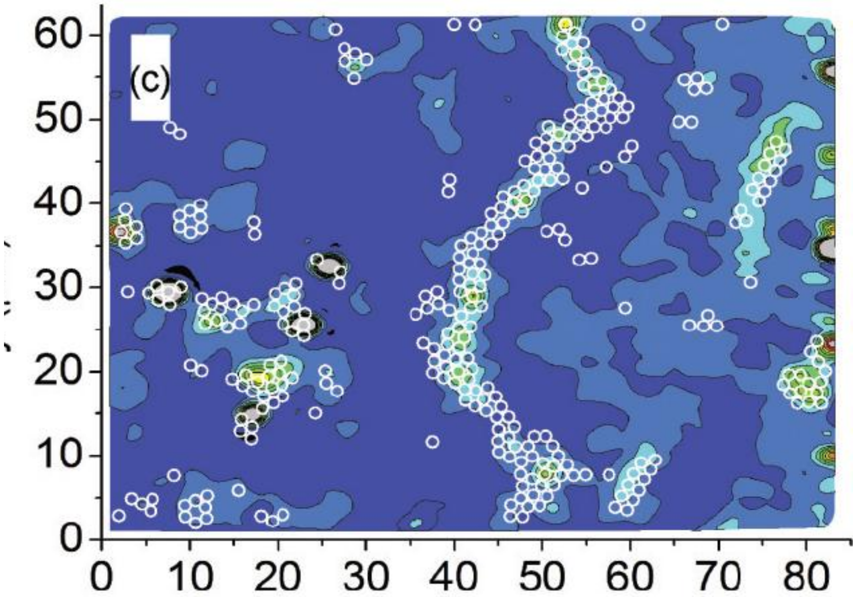


Particle packing | Sum of lowest vibrational modes

experiment

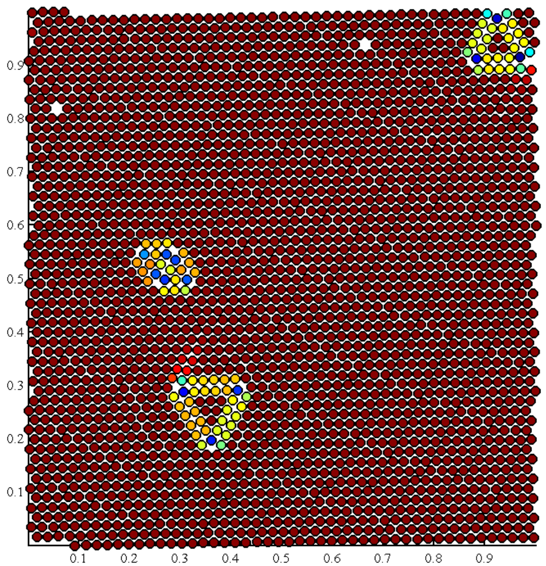
Chen et al, PRE **88, 022315 (2013)**

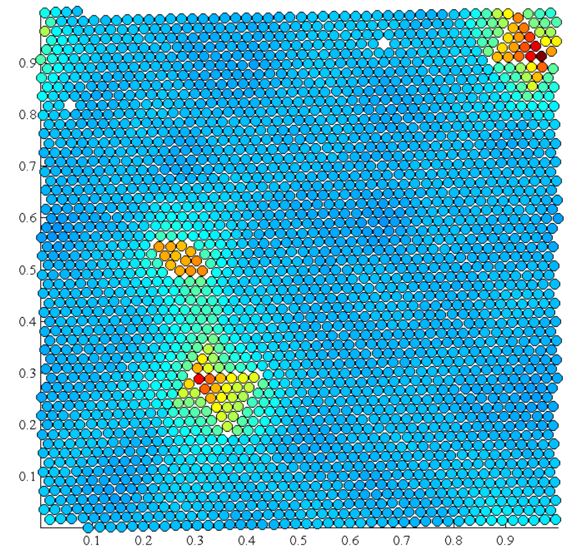




simulations

MLM





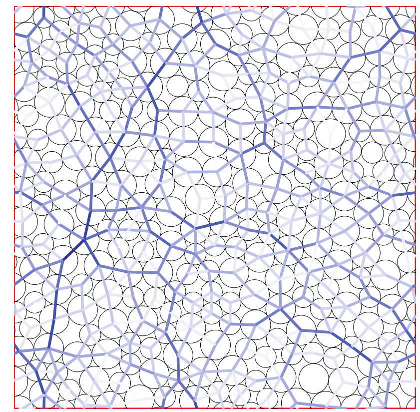
Plan: do the same thing in disordered solids

problem: disordered solids are horrible and messy

Dynamical Matrix for disordered solids

- Simulated frictionless 2D soft repulsive discs

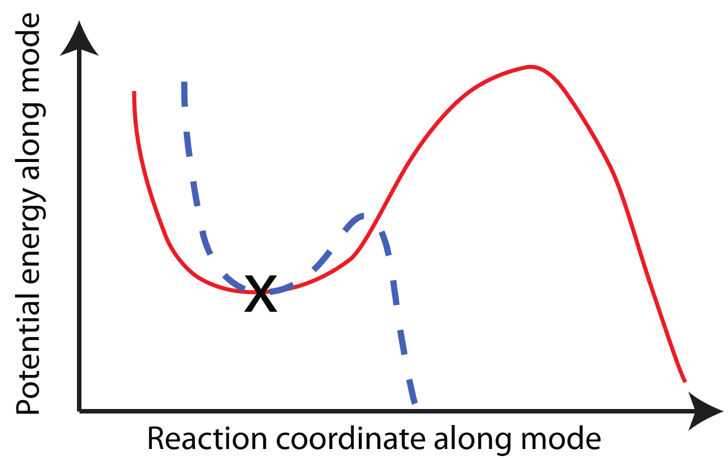
$$V(r) = \begin{cases} \frac{\epsilon}{\alpha}\left(1 - \frac{r}{\sigma}\right)^{\alpha} & r \le \sigma \\ 0 & r > \sigma \end{cases}$$



- Dynamical matrix (DM):
  - Much larger: Nd by Nd
  - ignores changes to nearest neighbor contacts

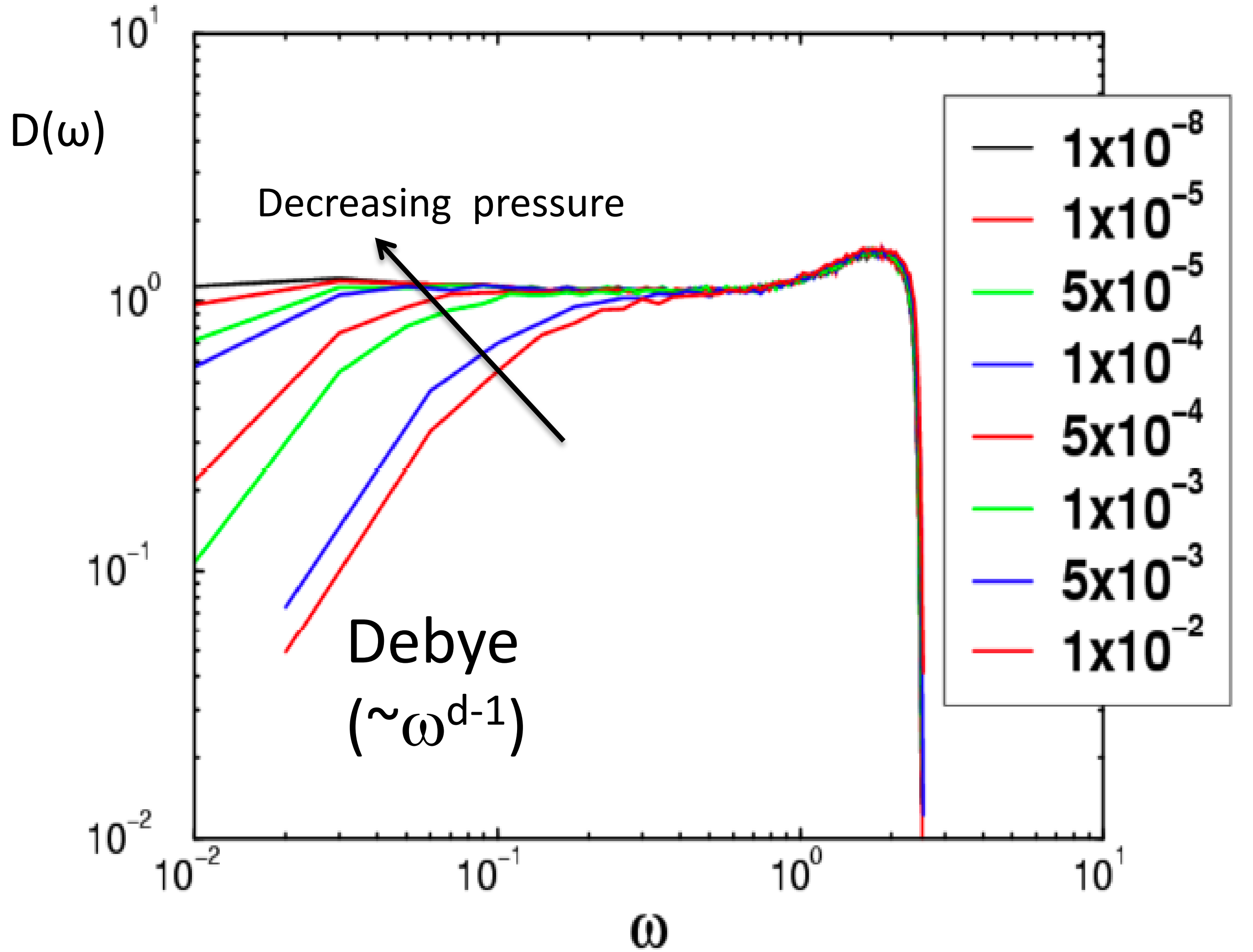
$$m\ddot{u} = Mu$$

$$M_{\substack{i\alpha j\beta \\ i \neq j}} = \frac{\partial^2 V(|r_i - r_j|)}{\partial r_{i\alpha} \partial r_{j\beta}}$$

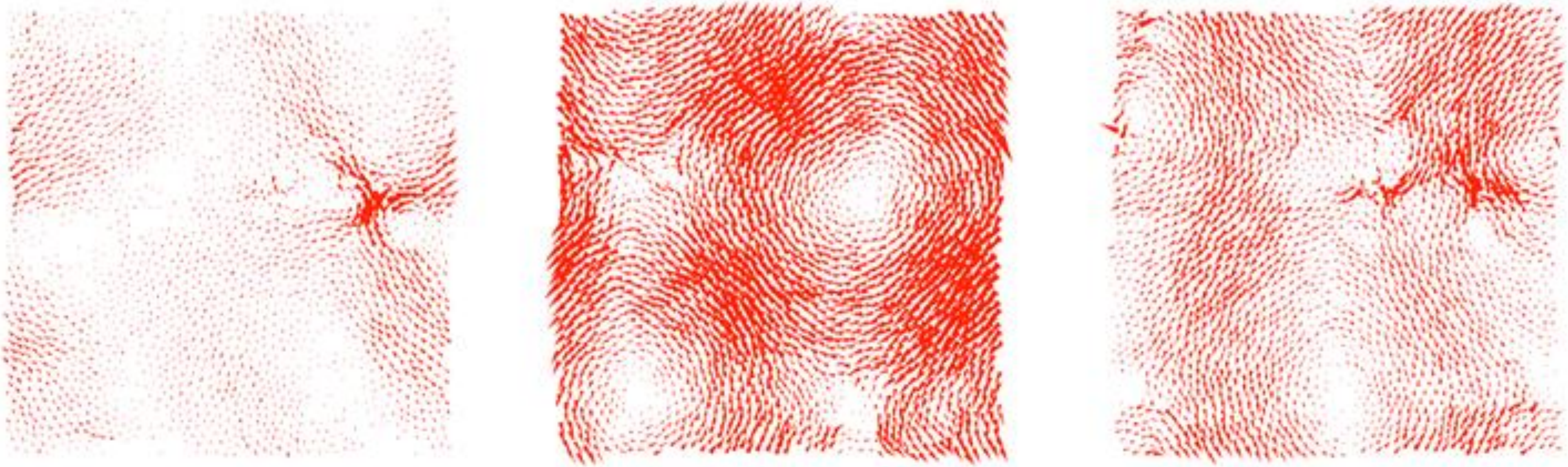


All solids have a Debye regime in their density of states

L. E. Silbert, A. J. Liu, S. R. Nagel, PRL **95**, 098301 ('05



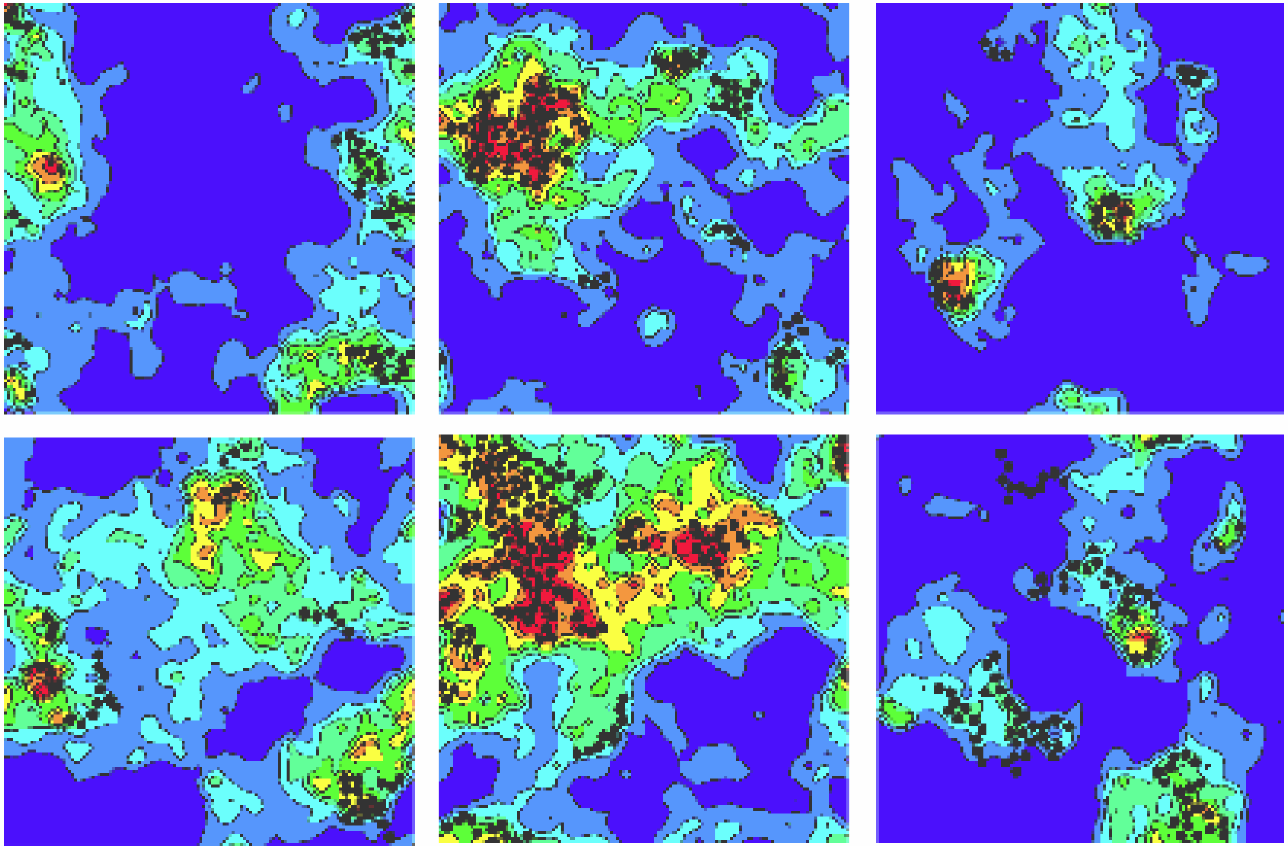
Debye regime



But these aren’t just plane waves!

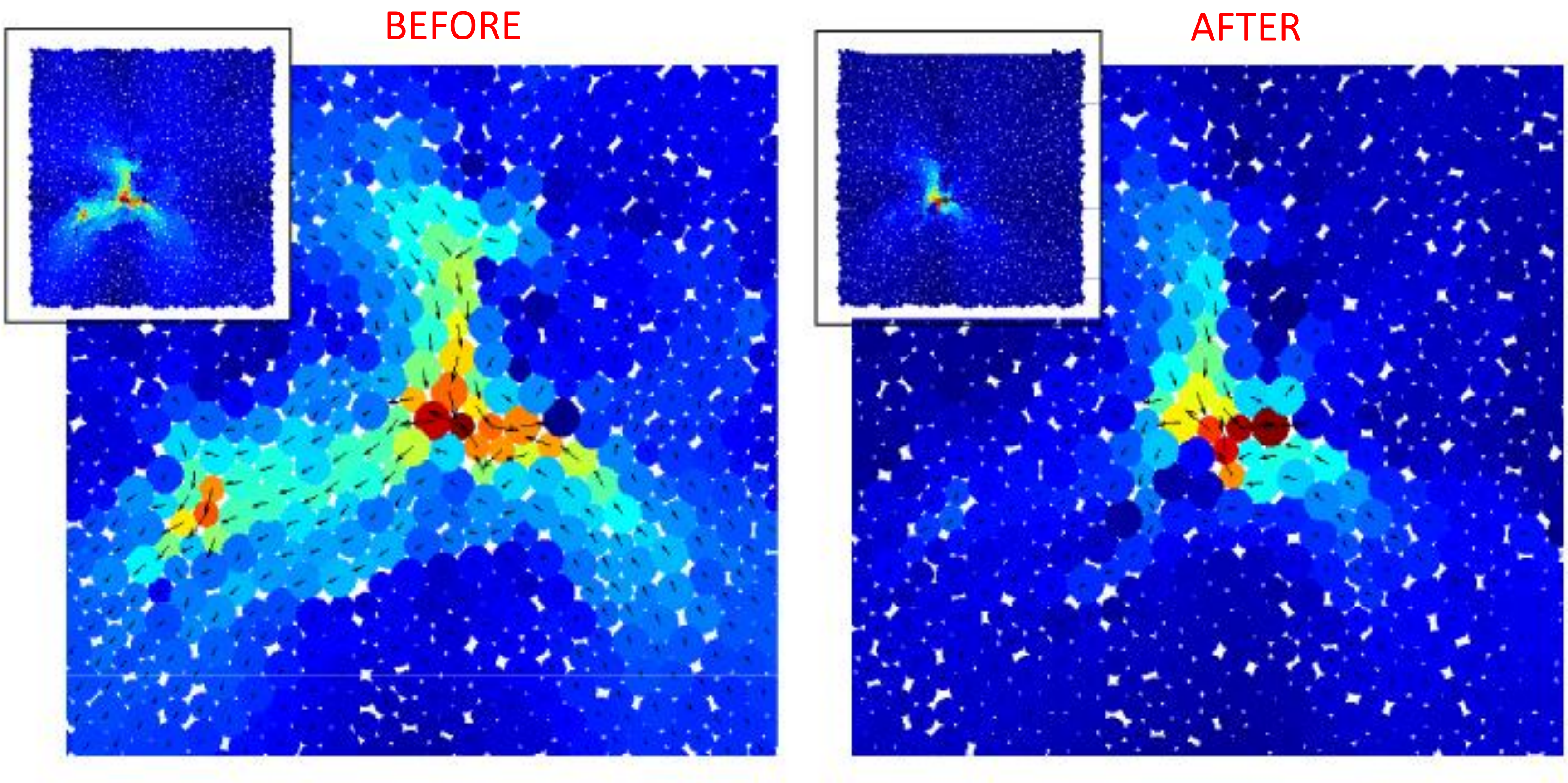
Correlation between short-time vibrations and rearrangements

Widmer-Cooper and Harrowell, PRL 96 185701 (2006)



- Black spots: long time propensity (particle rearrangements)
- colormap: local Debye Waller factor (soft vibrational modes)

Correlation between lowest energy mode and particle rearrangement

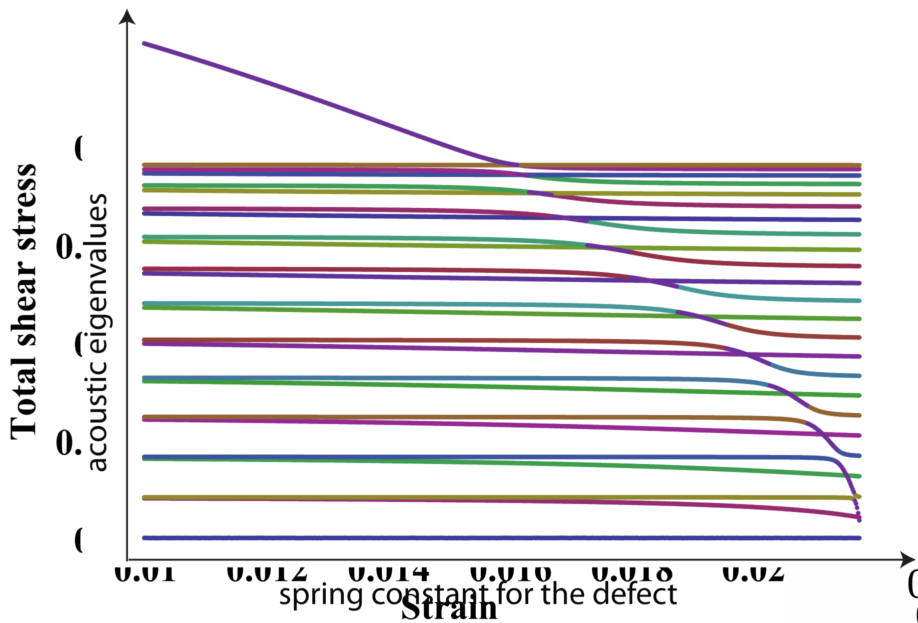


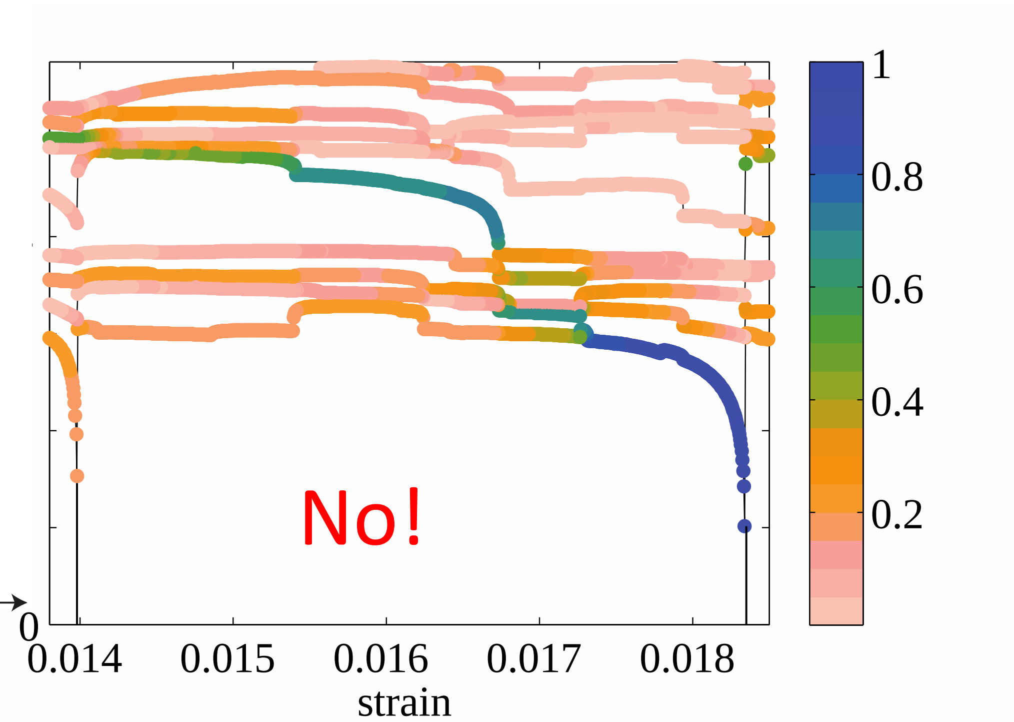
Quasi-localized mode

Rearrangement at higher strain

Normal modes analyzed at 10^{-6} units of strain from plastic rearrangement

Does the lowest energy mode determine the rearrangement?

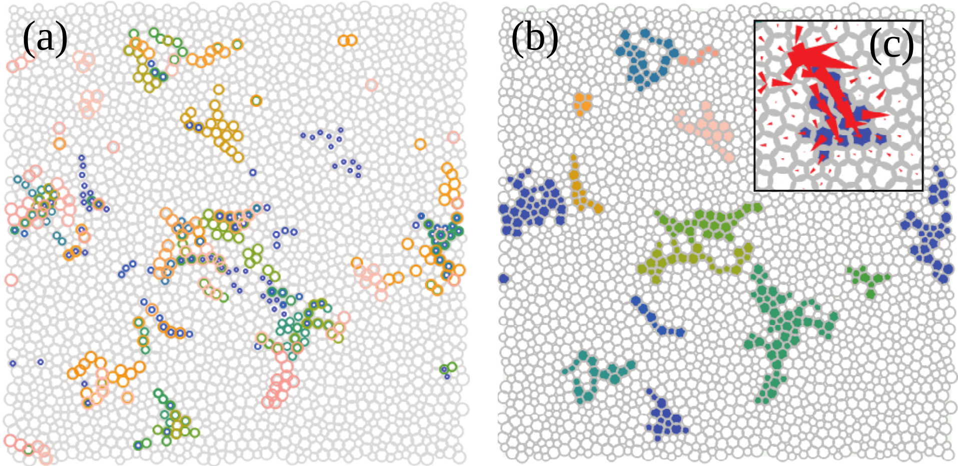




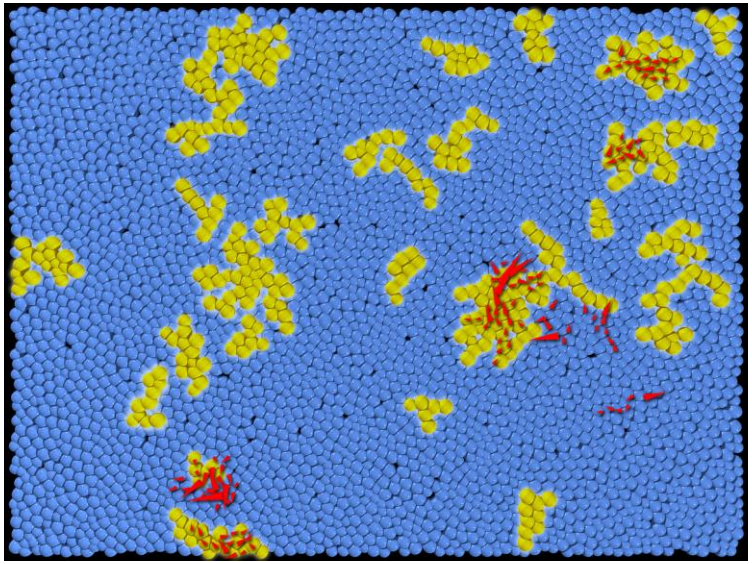
Initial particle rearrangement is only the same as lowest mode close to rearrangement

Original soft spot algorithm:

- Identify clusters of **localized excitations** inside **Debye regime**
  - characteristic length scale and energy scale
  - matches rearrangement locations
  - also works in 2D experimental colloidal systems
- Cons:
  - does not identify directions of displacements
  - does not allow energy barrier calculations
  - systematic errors at low packing fractions



MLM and A. J. Liu PRL **107** 108302 (2011)



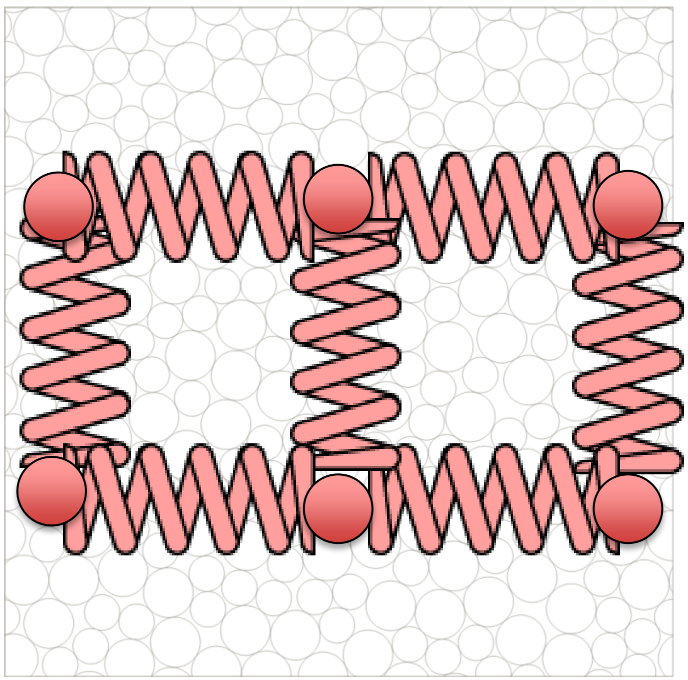
K. Chen, MLM, P. J. Yunker, W. G. Ellenbroek, Z. Zhang, A. J. Liu, and A. G. Yodh. *PRL* **107** 108301 (2011)

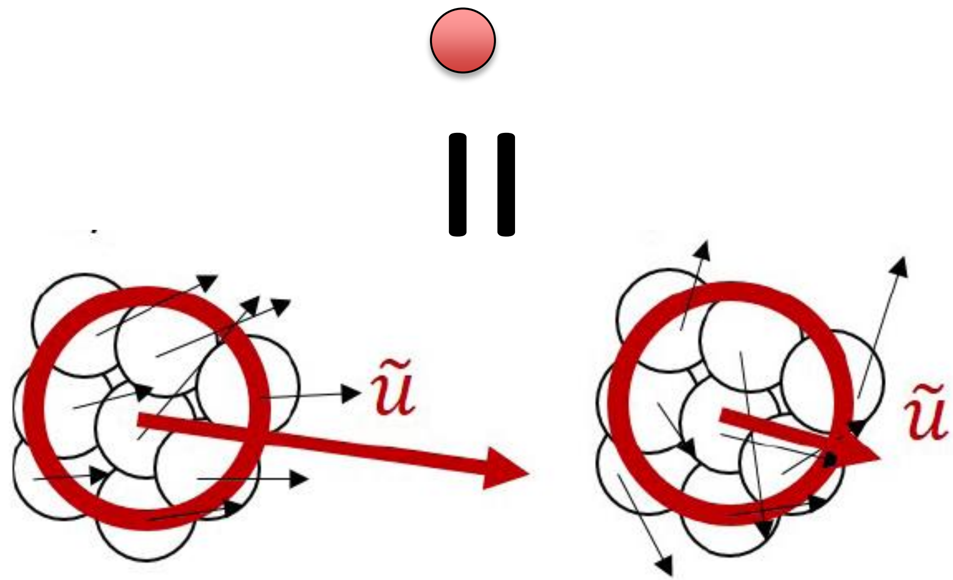
Problem:

extended modes are messy, so it is difficult to filter them

long range elastic tails “pollute” our basic units of deformation

Idea: Add an artificial term to the energy that acts as a high pass filter:





$$\tilde{V} = u^T \tilde{M} u$$

Particles no longer at a minimum of this new energy functional, but can still calculate eigenvectors of this new (symmetric, real) matrix

New method: Change the dynamical matrix by adding a mechanical high pass filter

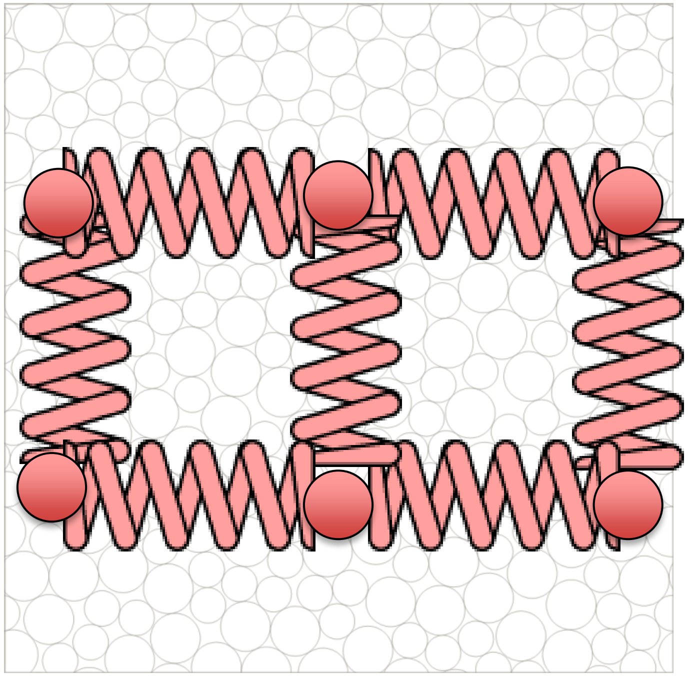
$$\tilde{V} = u_i M_{ij} u_j + \underline{K_{lk}(\tilde{u_l} - \tilde{u_k})^2}$$

$$\tilde{u}_k = \sum_i^N u(x_i) e^{-(x_i - ka)^2/\sigma^2}$$

$$\tilde{V} = u_i \tilde{M}_{ij} u_j$$

$$\tilde{M}_{ij} = M_{ij} + \underline{\tilde{K}_{ij}}$$

"Augmented Matrix (AM)"

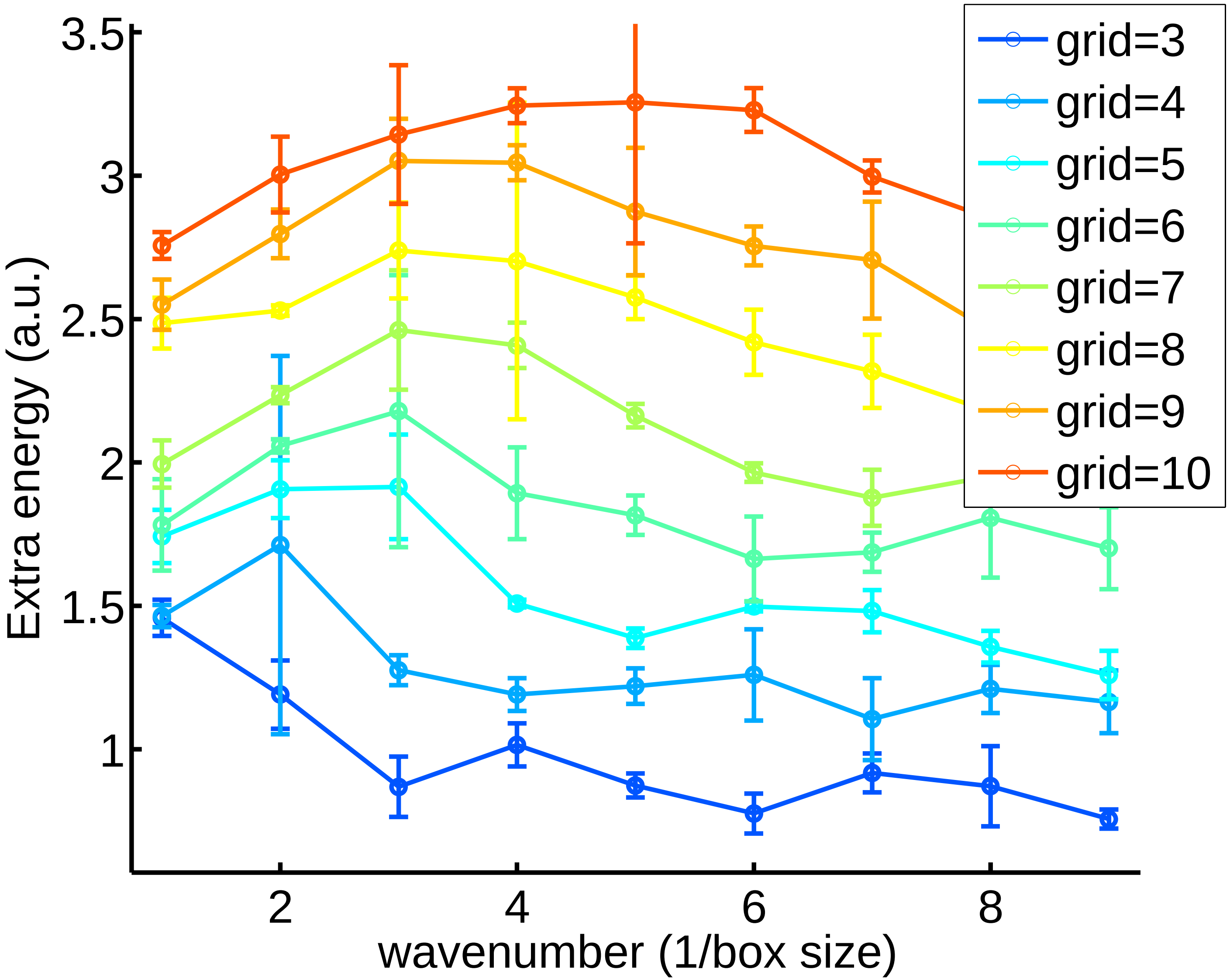


$$\tilde{K_{ij}} = K_{lk}\left(e^{-(x_i-la)^2/\sigma^2} e^{-(x_j-la)^2/\sigma^2} - 2e^{-(x_i-la)^2/\sigma^2} e^{-(x_j-ka)^2/\sigma^2} + e^{-(x_i-ka)^2/\sigma^2} e^{-(x_j-ka)^2/\sigma^2}\right)$$

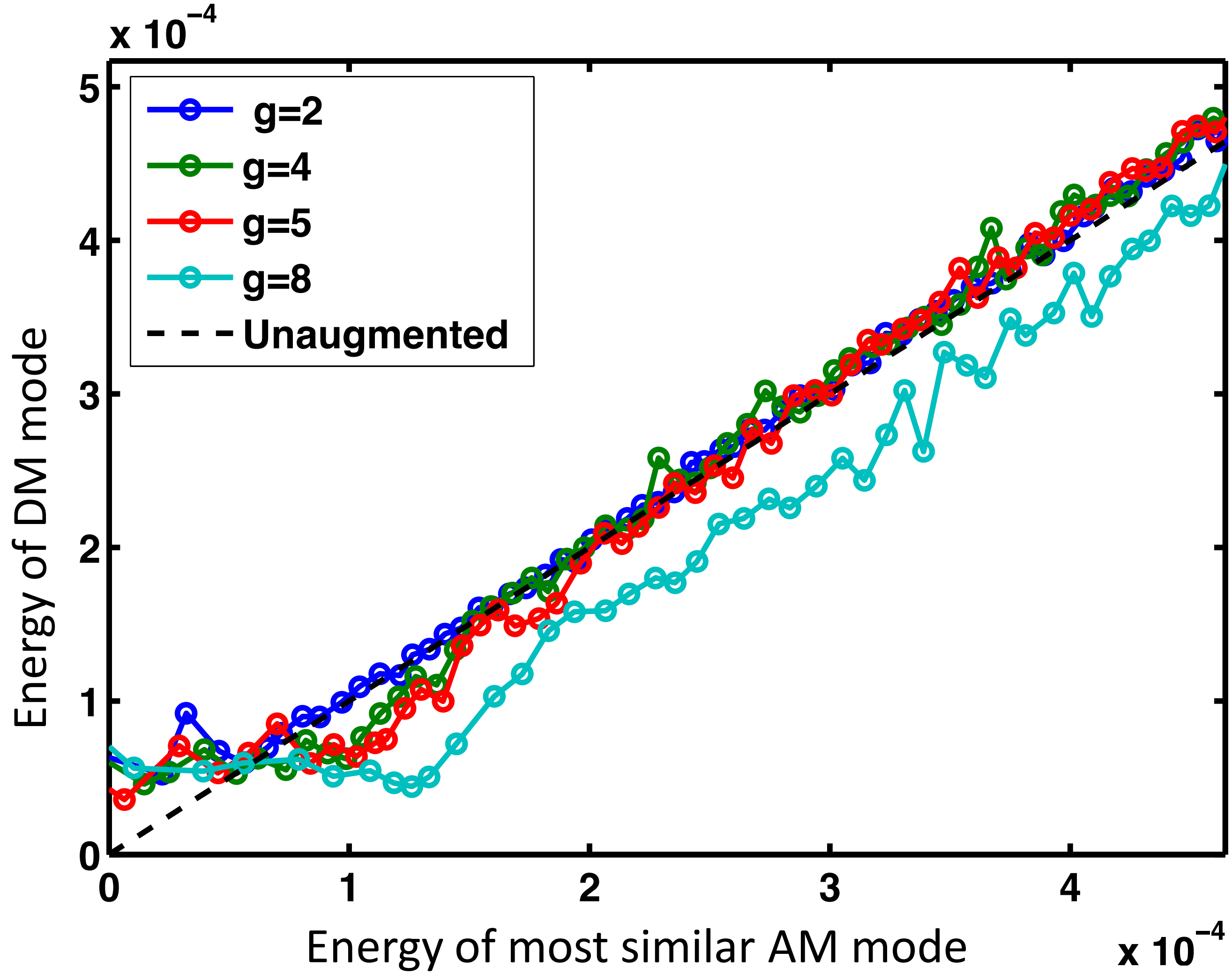
Data shown for 2500-particle systems at packing fraction of 0.90 generated by infinite temperature quenches

Is it acting as a high-pass filter? Test on "pure" plane waves

Yes, though not perfect. We choose g=5 for the rest of the simulations shown here.



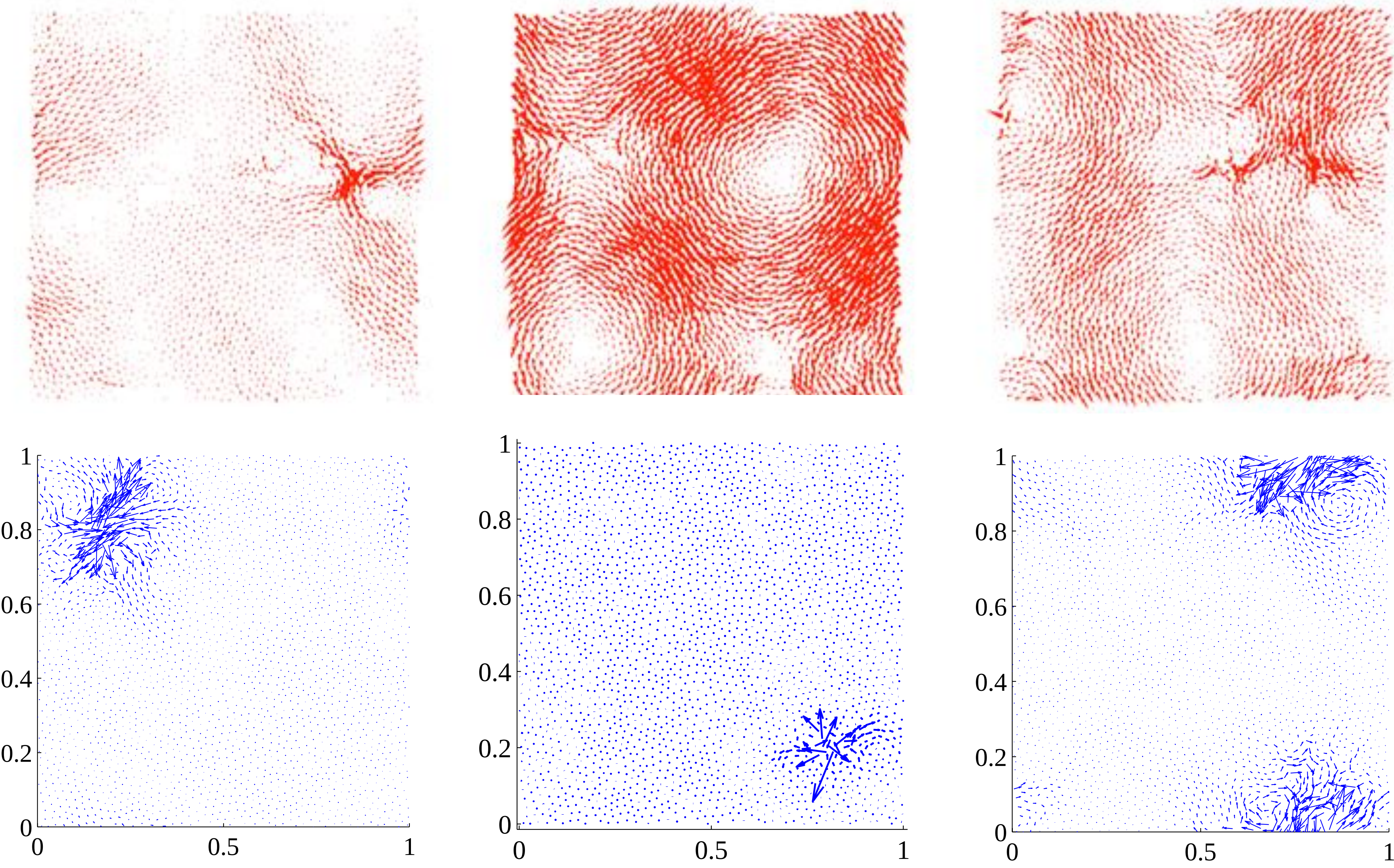
Is it acting as a high-pass filter?
In real jammed packings



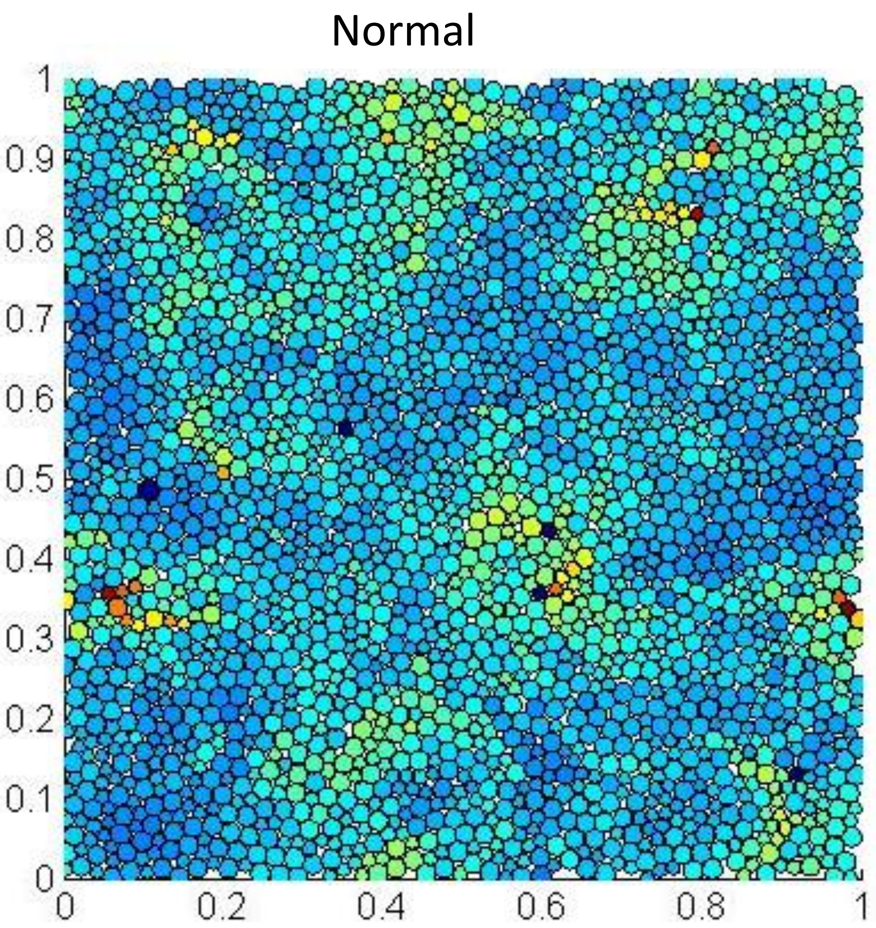
Yes, low frequency plane waves are shifted to higher frequencies

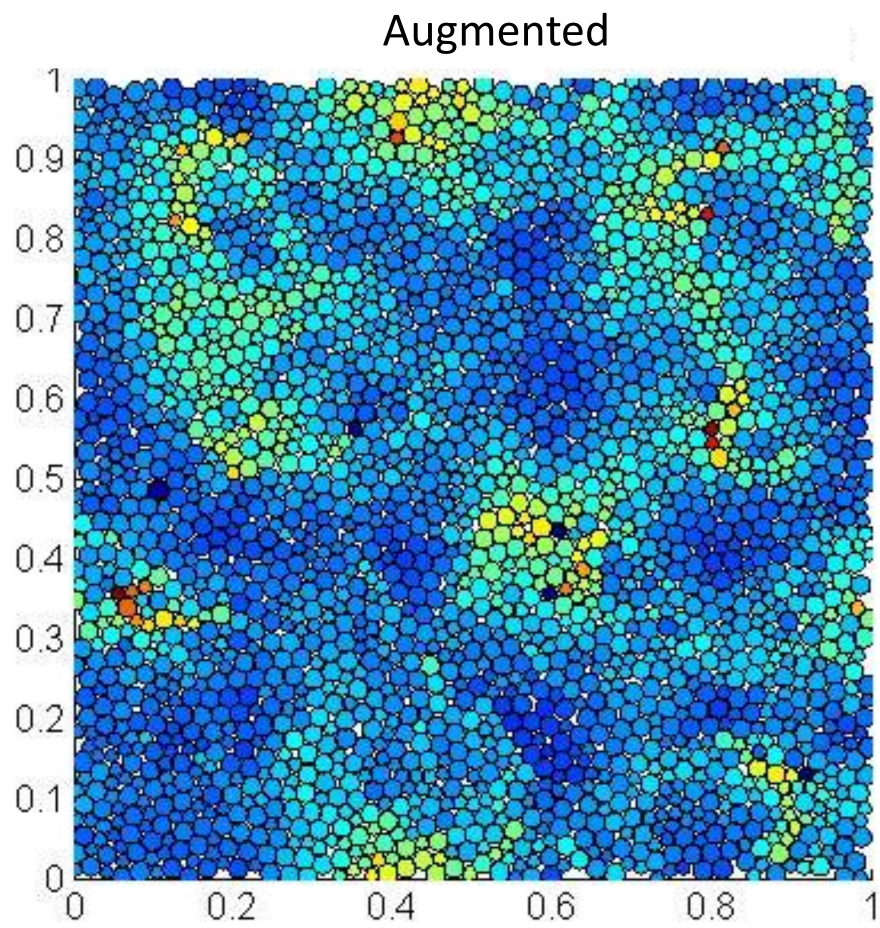
It works!

Eigenvectors (DM) vs. defects (AM)

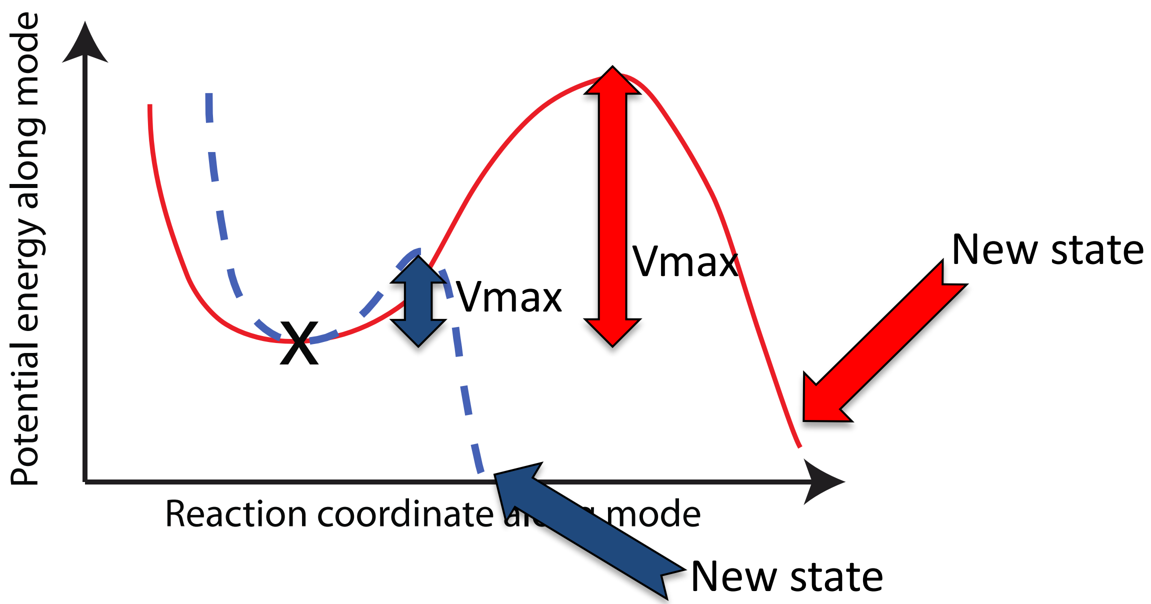


Unweighted sum of lowest 30 modes

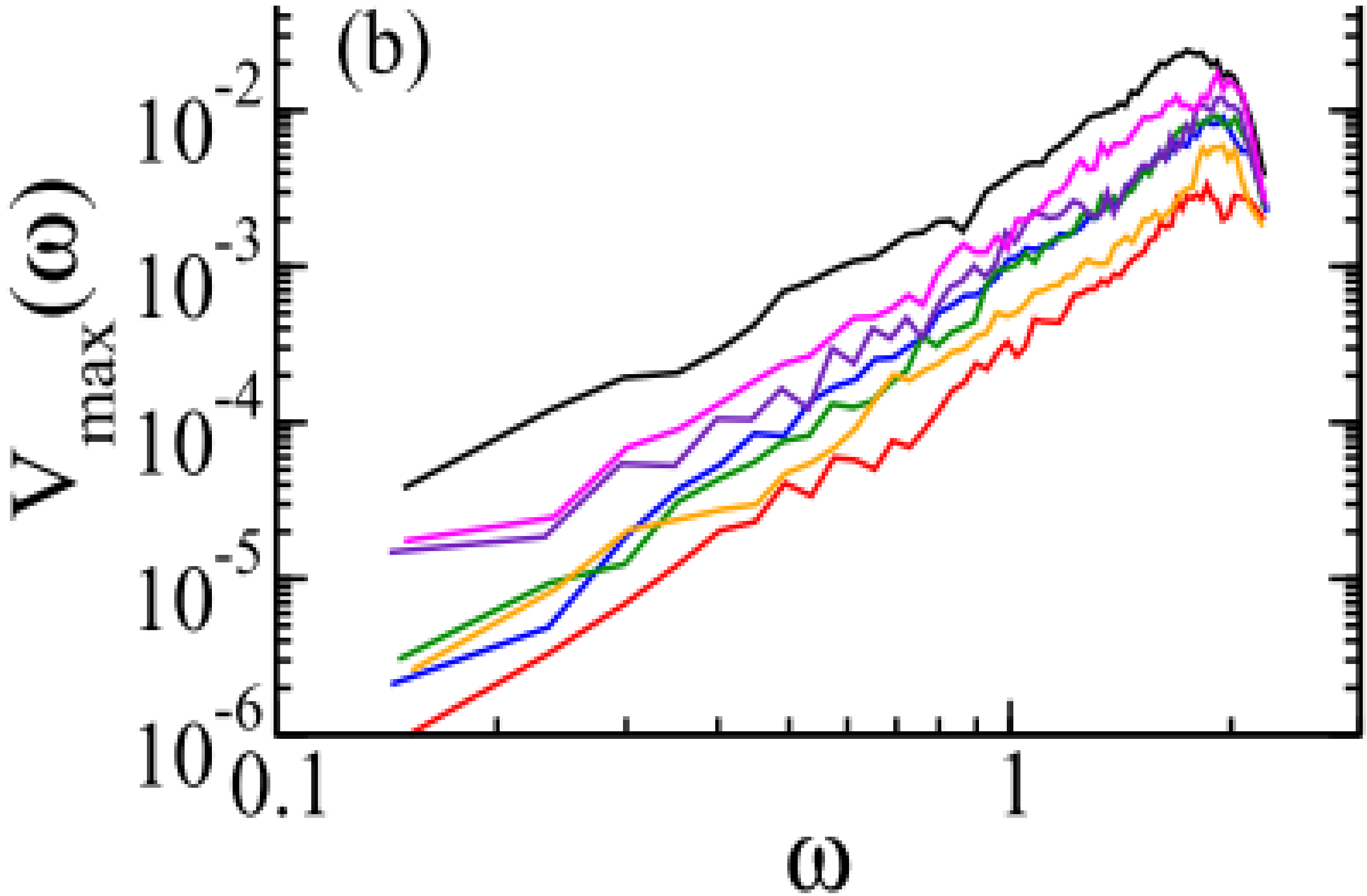




"Great, now all we have to do is show that the AM modes have lower energy barriers than the DM modes, and we're done!"



Energy Barriers



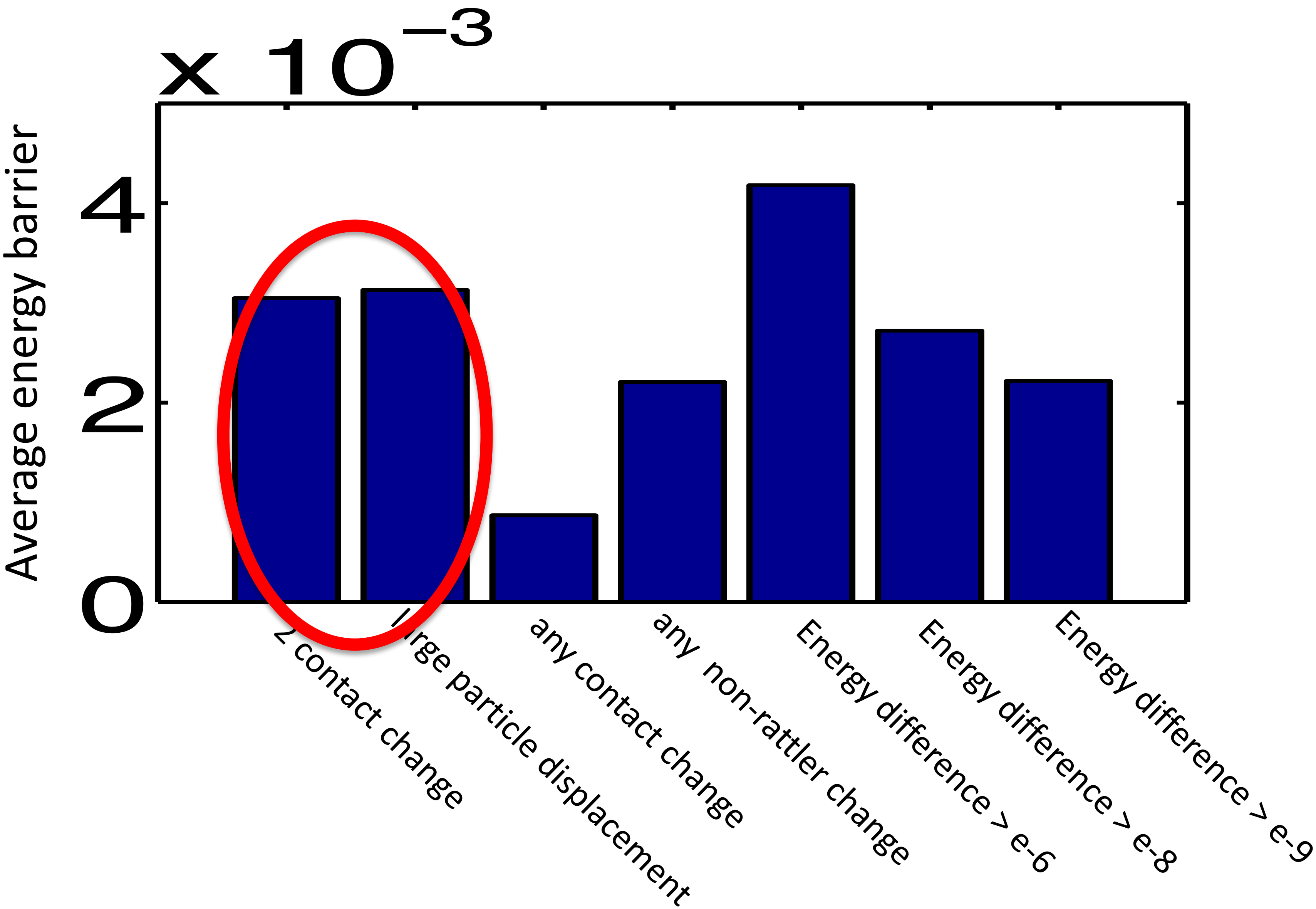
New state = new contact network

Xu, N., Vitelli, V., Liu, A. J., & Nagel, S. R. (2009).

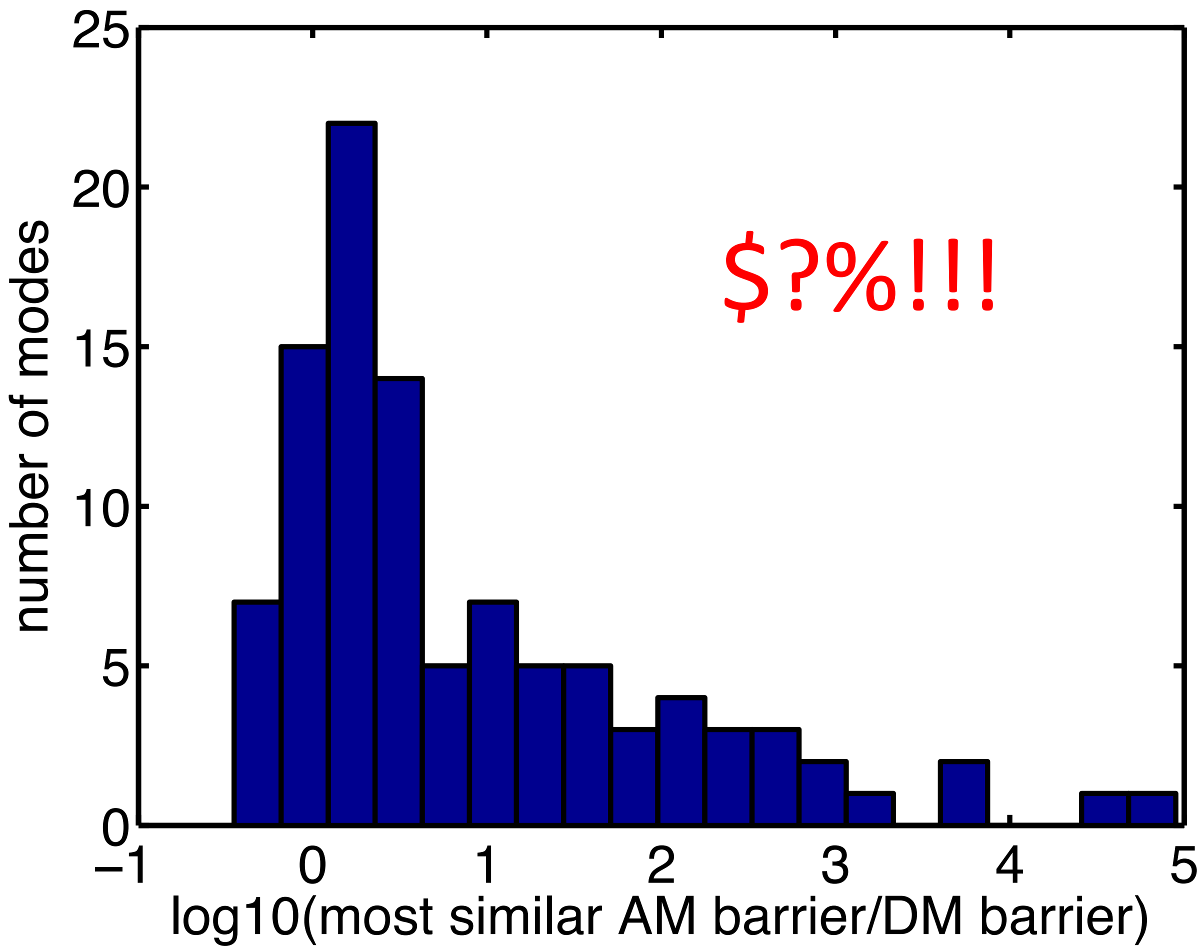
Definitions for a “new state”

- Different contact network (Xu et al)
- Different contact network (rattlers excluded)
- More than two particles with new contacts
- Cutoff on largest (average) particle displacement between old state and new state
- Cutoff on difference in energy between old state and new state
- Mark Robbins (with inertia – kinetic energy increases rapidly)

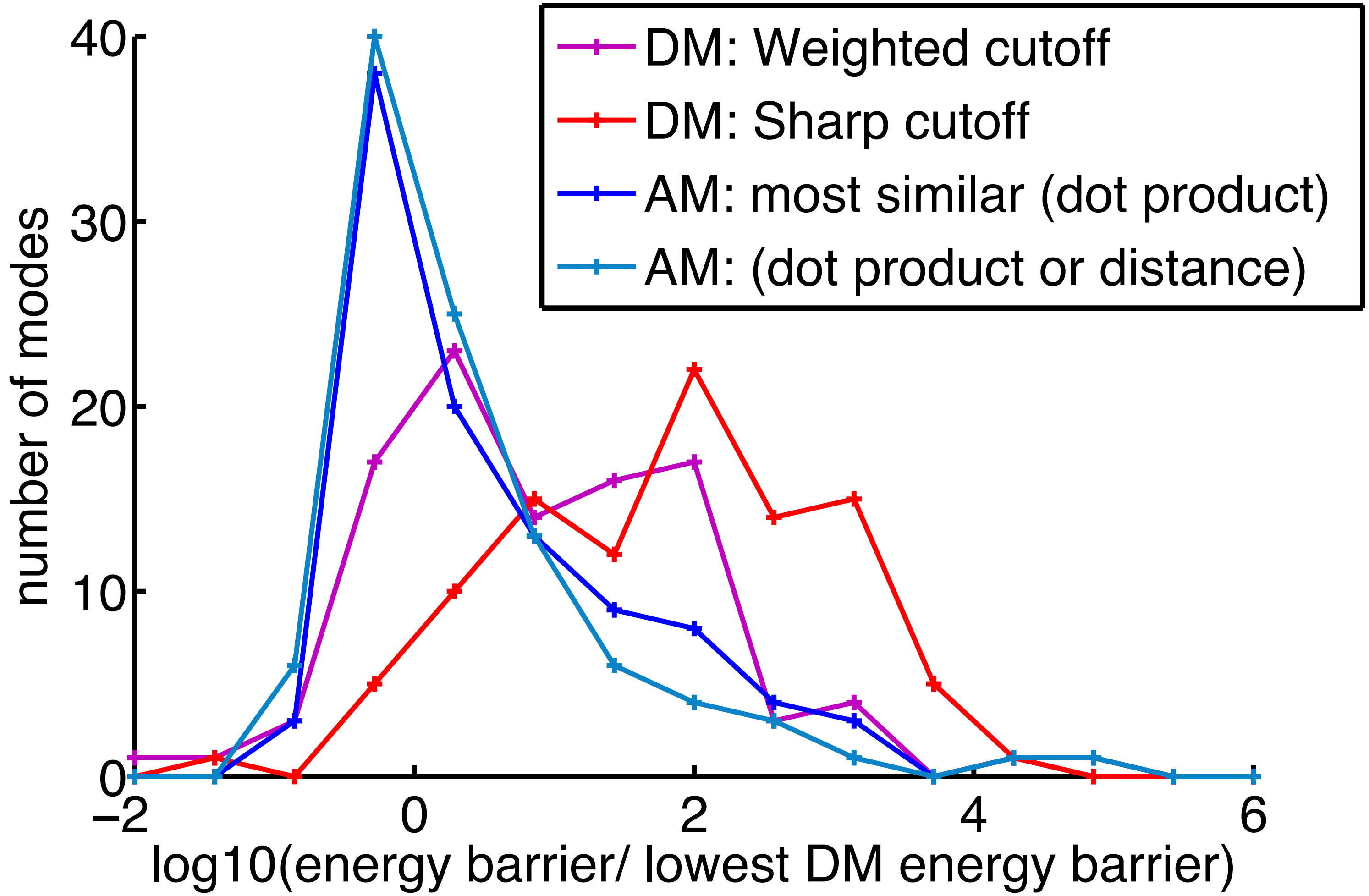
Definitions for a “new state”



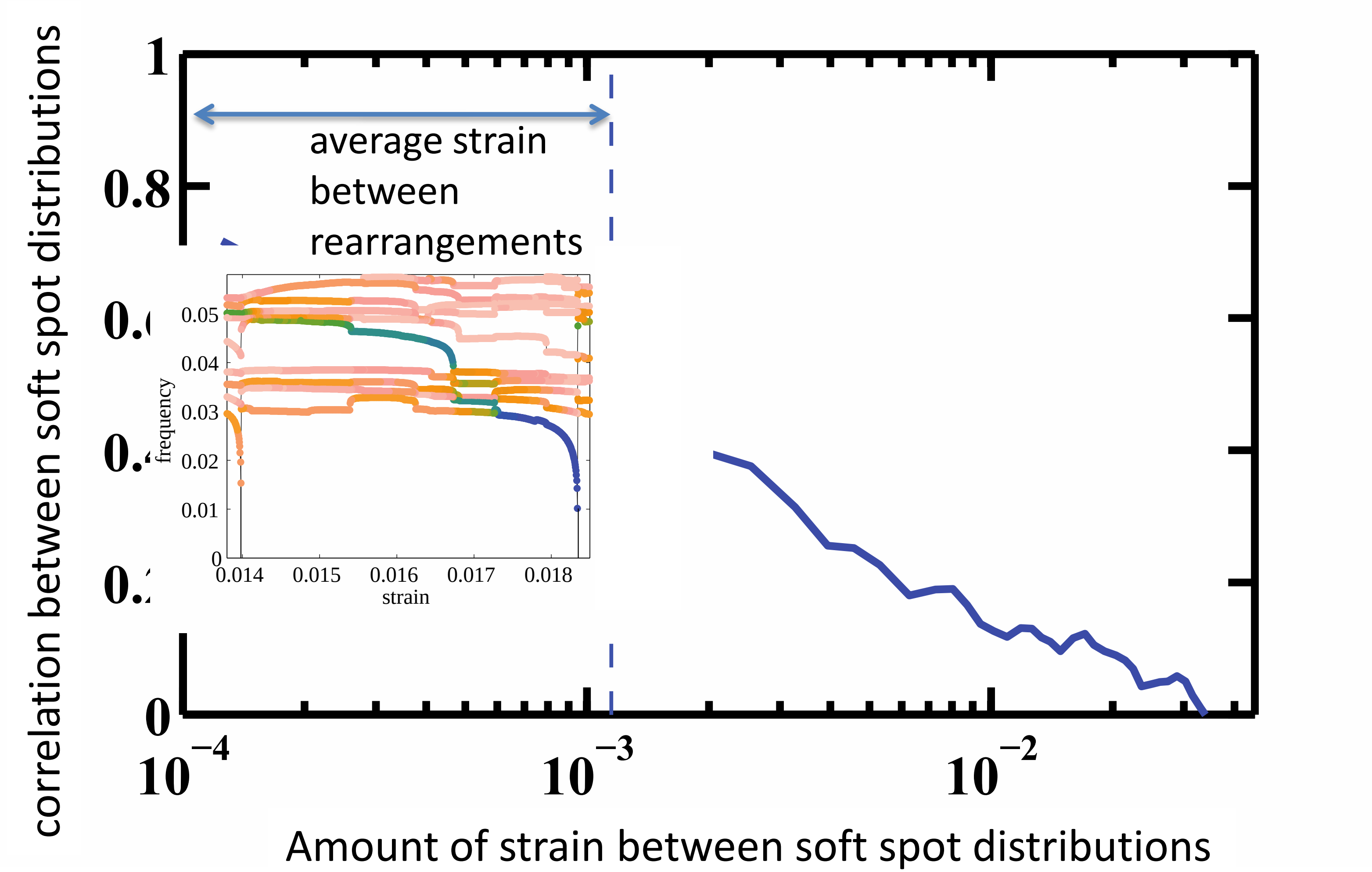
Finally, AM vs. DM energy barrier



Localized modes generically cost more energy



One slide (sort of) about avalanches



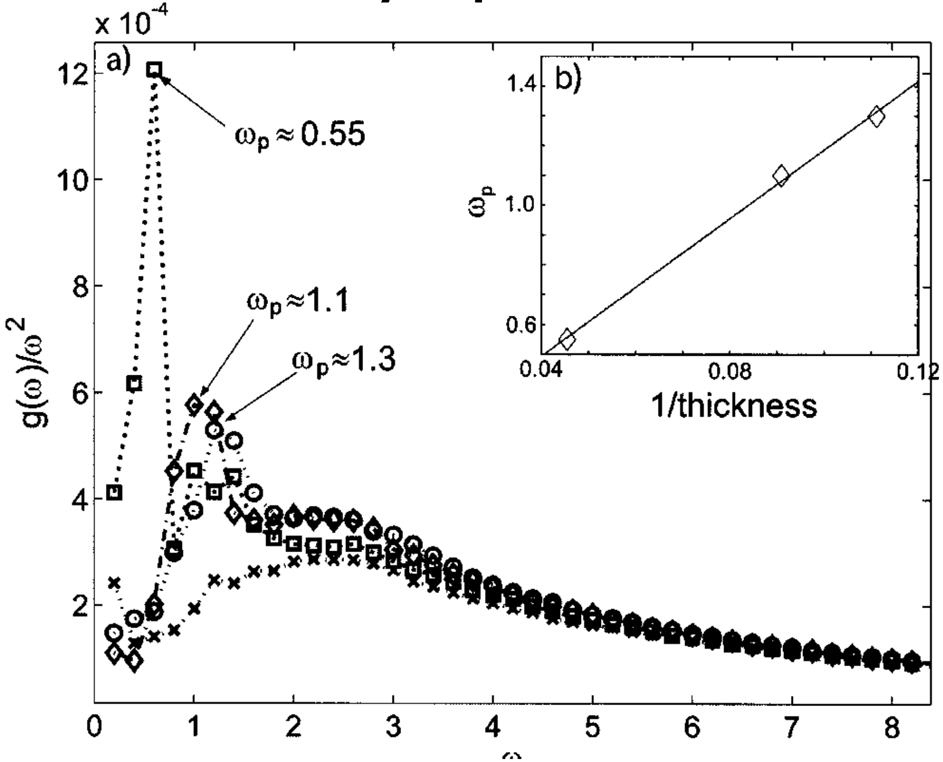
Conclusions:

- Our mechanical high-pass filter:
  - generates truly localized modes (in same places as soft spots)
  - first method to isolate mode frequencies, directions, energy barriers for structural defects
- Strongly supports hypothesis that localized structural defects hybridize with phonon-like modes in disordered solids
- Energy barriers are higher for localized excitations compared to quasi-localized excitations
  - long-range quadrupolar tails lower energy barriers
  - somewhat artificial reaction coordinate (different from nudged rubber band, etc.)
- Still open: what is the best way to think about this?
  - elastically interacting localized defects OR
  - extended defects

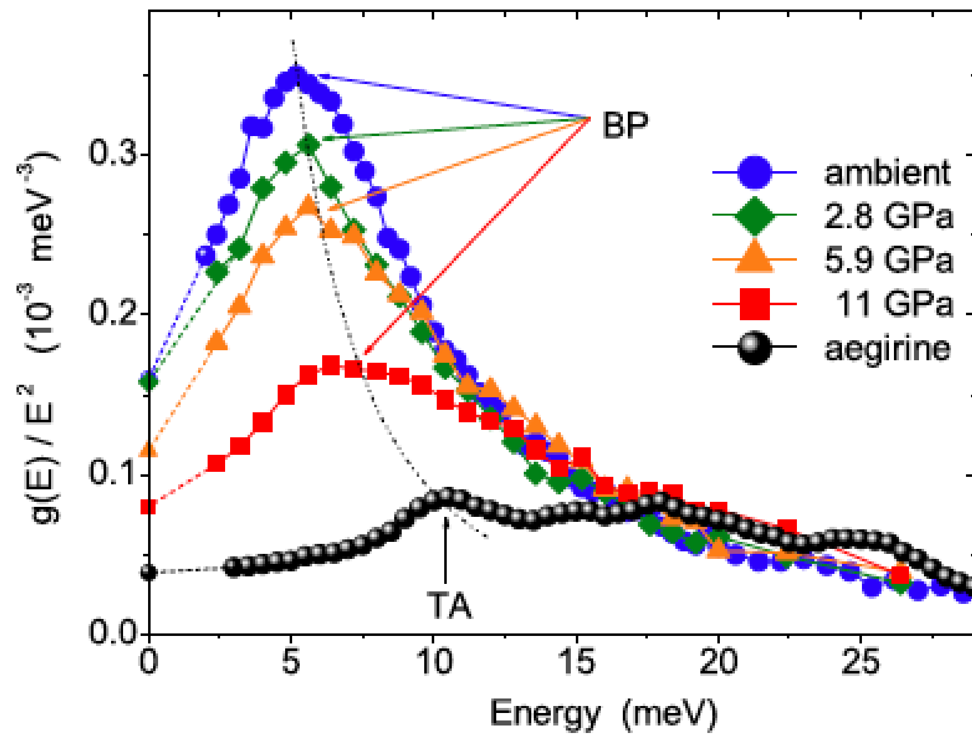
five minutes about the boson peak

What sets the "edge" of the Debye regime? The Boson Peak

Sometimes defined as "an excess of modes above the Debye prediction" in the density of states:

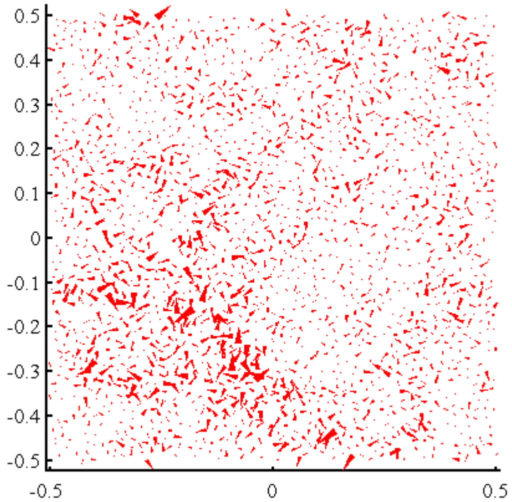


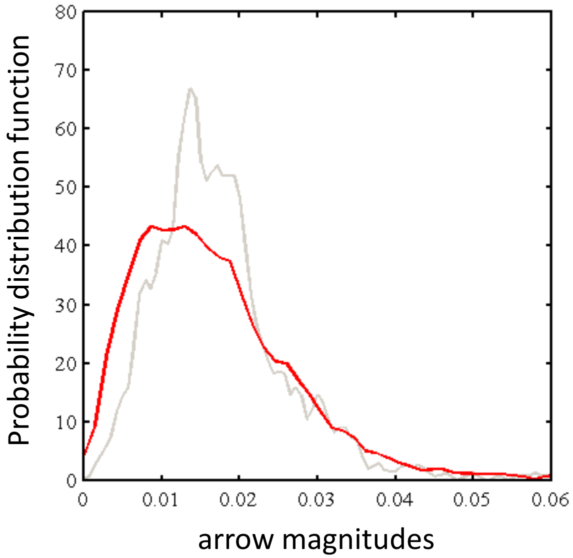
Polymers (Jain & Pablo JCP 2004)

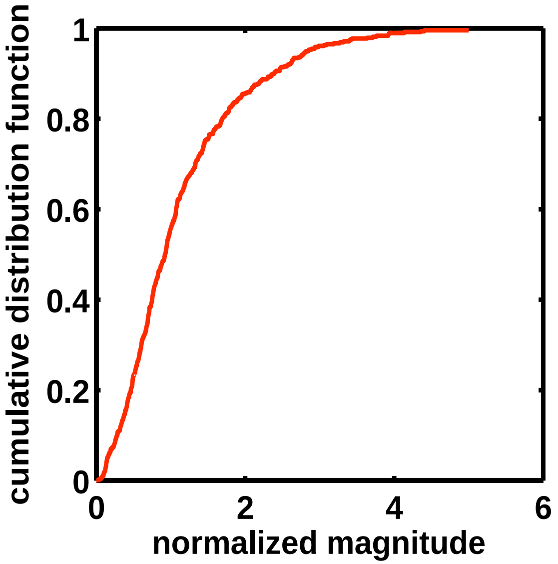


Sodium silicate glass (Chumakov et al PRL 2011)

Boson peak modes are extended and disordered

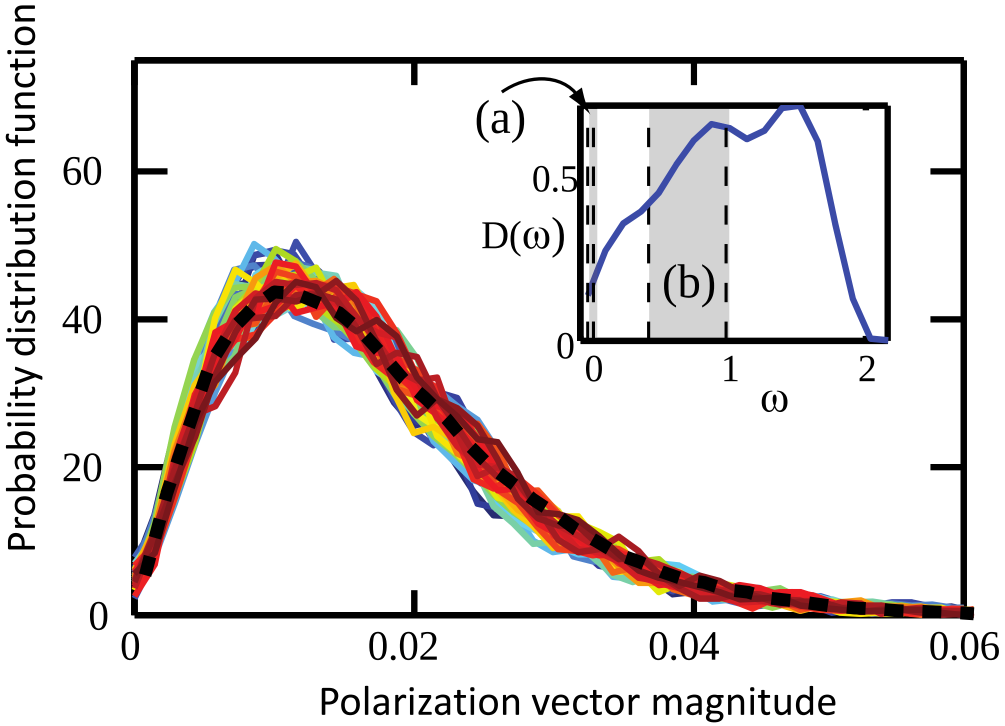


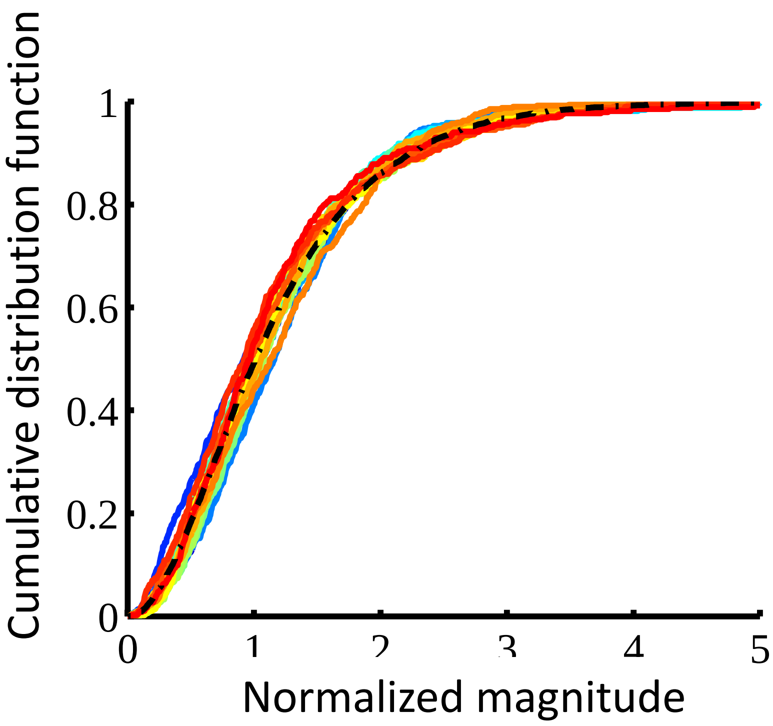




Surprise!

- Boson peak modes look almost identical

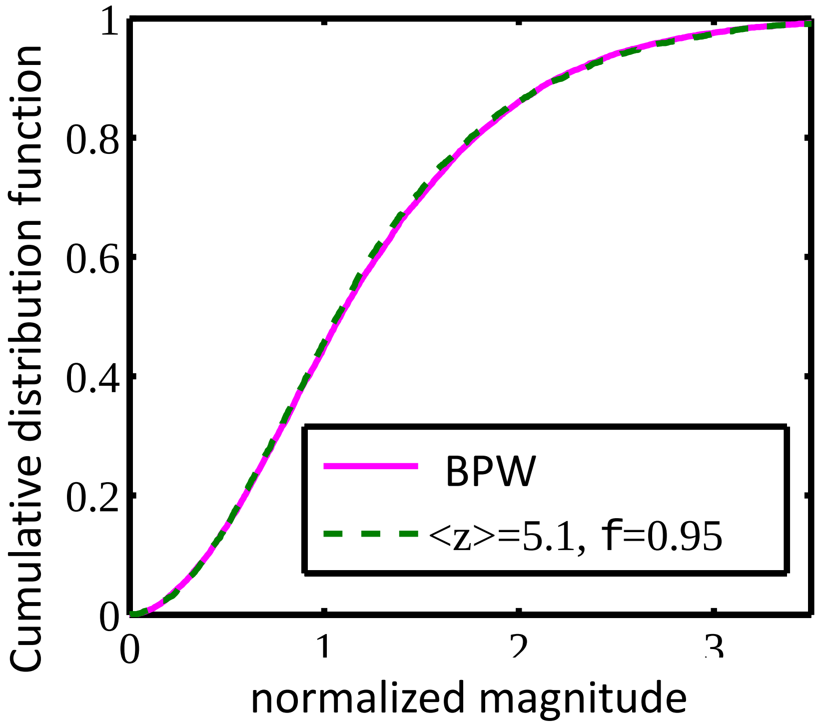




MLM and A. J. Liu PRL **107** 108302 (2011)

Introduce Boson Peak Wigner Matrix: (BPW)

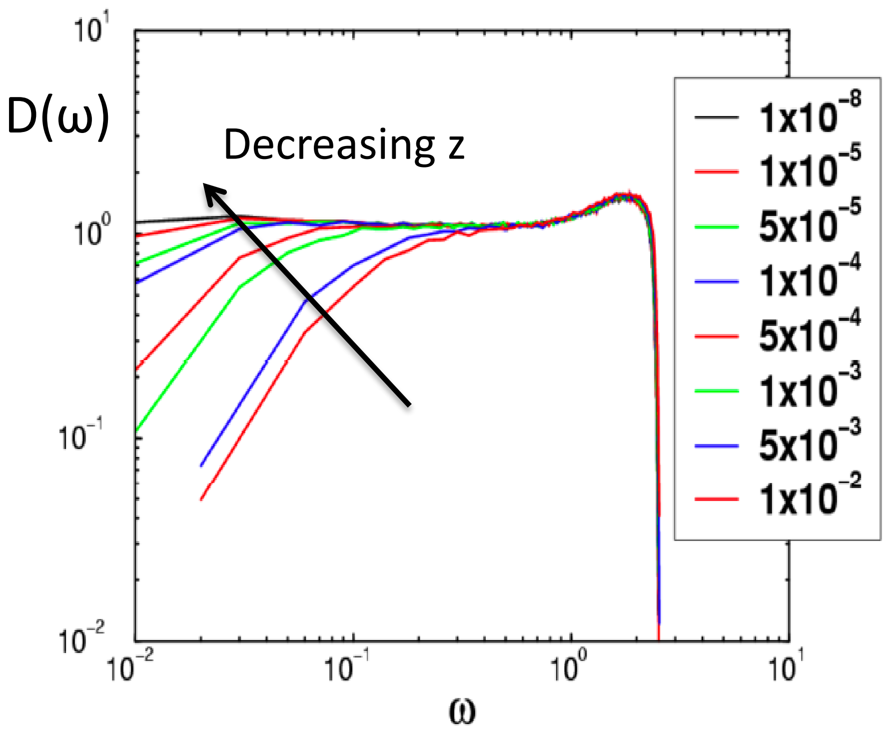
- Symmetric
- Off-diagonal elements: mean μ and variance σ^2
- On-diagonal elements: mean -Nμ and variance $N\sigma^2$



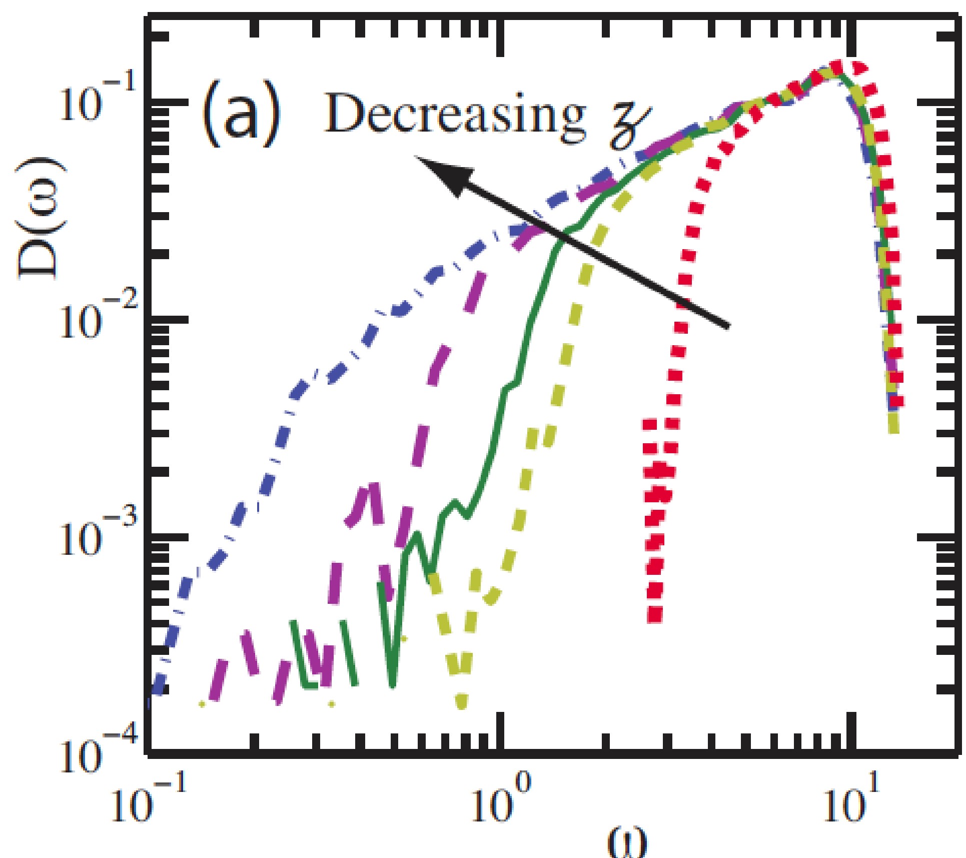
THIS matches the boson peak!!

What happens for sparse matrices with coordination number z?

L. E. Silbert, A. J. Liu, S. R. Nagel, PRL **95**, 098301 ('05



Jammed packings



sparse positive definite random matrices

http://arxiv.org/abs/1307.5904

Conclusions

- We propose a new random matrix definition of the Boson Peak, defined by eigenvector statistics
  - new Boson Peak Wigner Matrix (BPW) universality class
  - this also explains the dependence of boson peak location on pressure/packing fraction

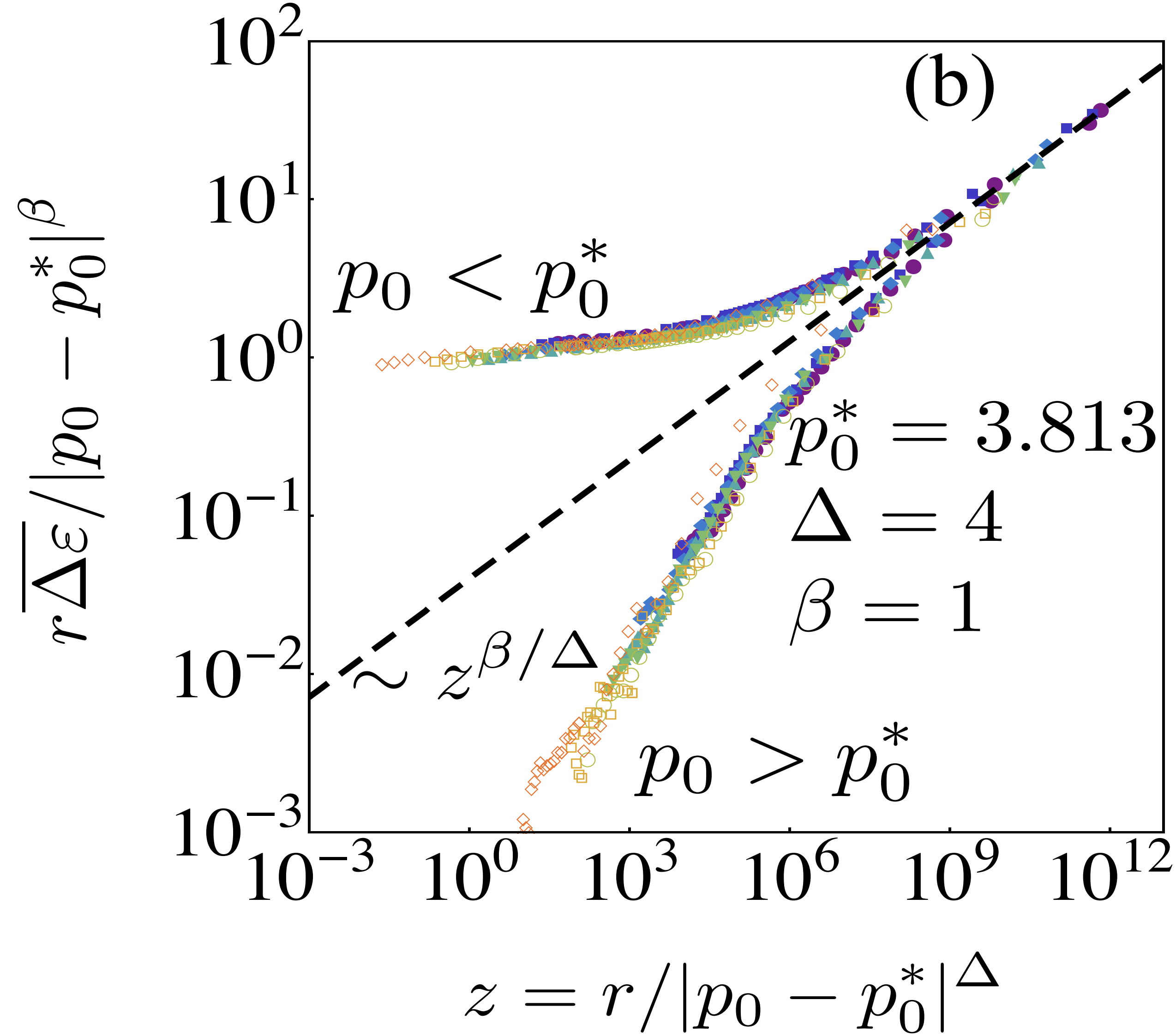
http://arxiv.org/abs/1307.5904

One slide about biological tissues

CHEAT SHEET:
Average energy barrier height ~ yield stress

inverse perimeter modulus r ~ strain rate

preferred perimeter p_0 ~ density



Bi, Lopez, Schwarz, MLM submitted(2014)

Funding and Thanks

- Thanks for your attention!

Collaborators:

- Sven Wijtmans
- Andrea Liu (UPenn)
- Max Dapeng Bi

Funding:

- NSF BMMB CMMI-1334611
- NSF DMR CMMT-1352184
- Alfred P. Sloan Foundation
- Soft Interfaces IGERT (DGE-1068780)

http://www.phy.syr.edu/~mmanning/