Identifying soft spots in a sheared amorphous material

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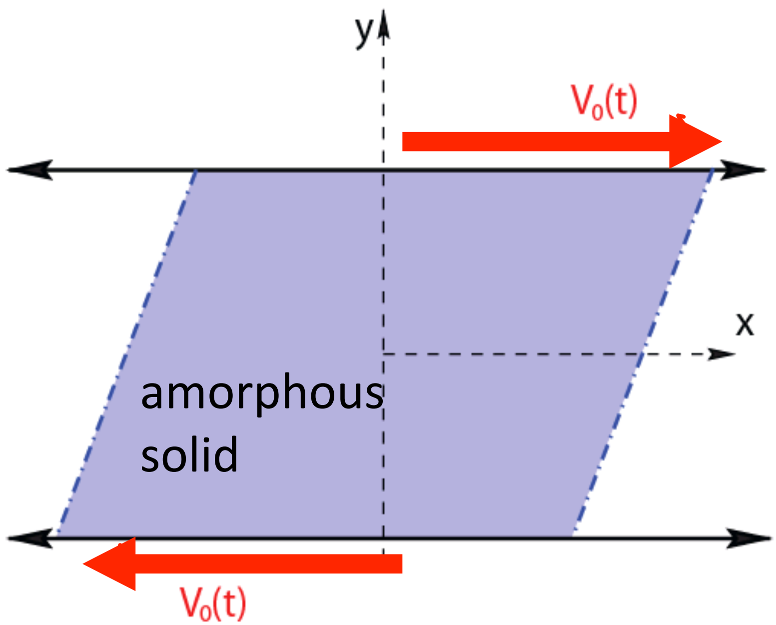
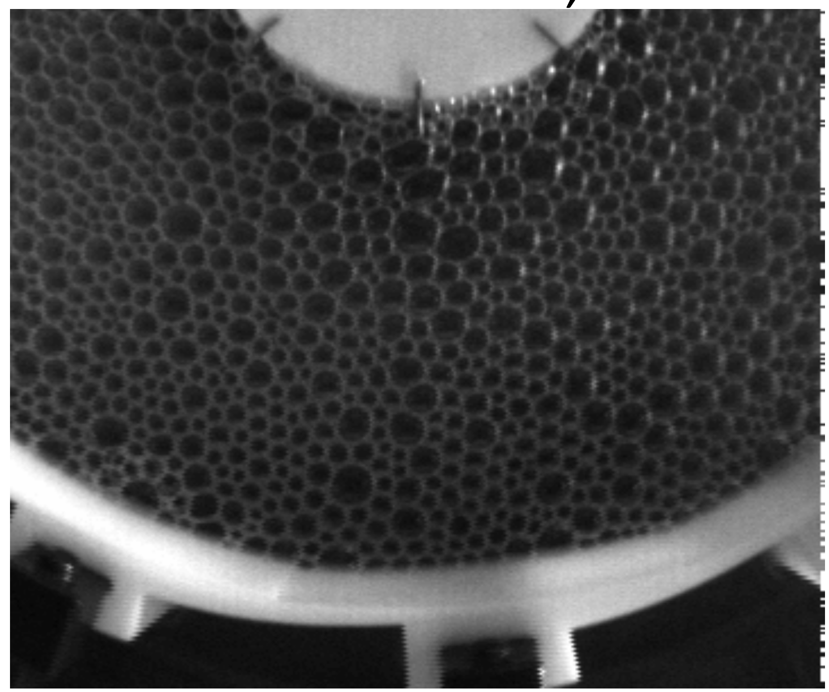
How do amorphous solids deform?



M. Dennin, UCI



- particle packing is disordered (similar to liquids, not crystals)
- possess a yield stress: initial response like an elastic solid

Disorder affects vibrational modes and plastic flow

OUTLINE

1. vibrational properties of jammed solids
2. shear transformation zone (STZ) model for plasticity in amorphous solids
3. using normal modes to identify STZs

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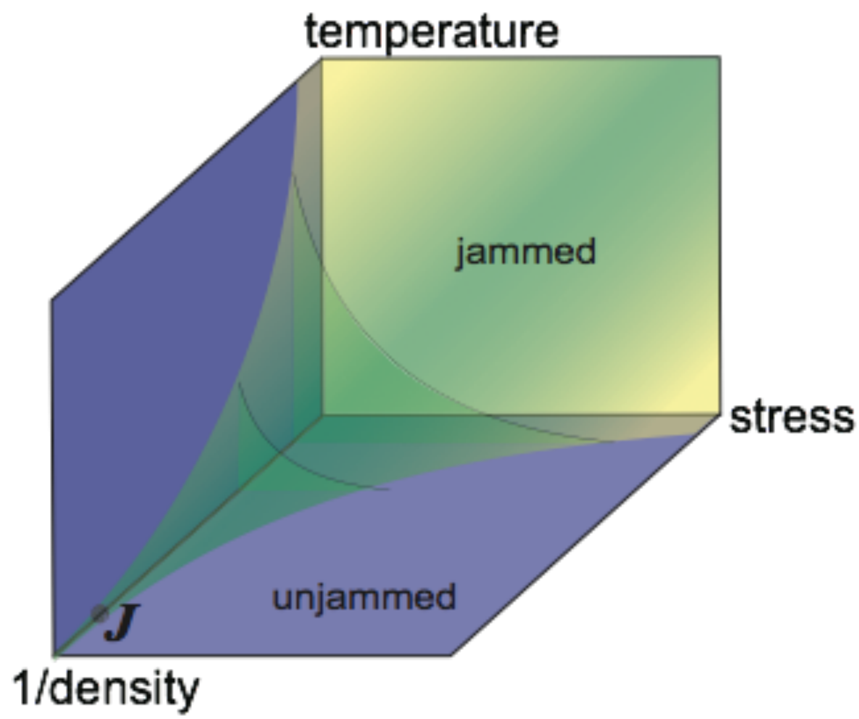
Jamming transition & Point J

- Focus on frictionless, granular packings
- Point J is density where coordination number jumps from zero to isostaticity
- What are the elastic properties near point J?



C. S. O'Hern, S. A. Langer, A. J. Liu and S. R. Nagel, Phys. Rev. Lett. **88**, 075507 (2002).

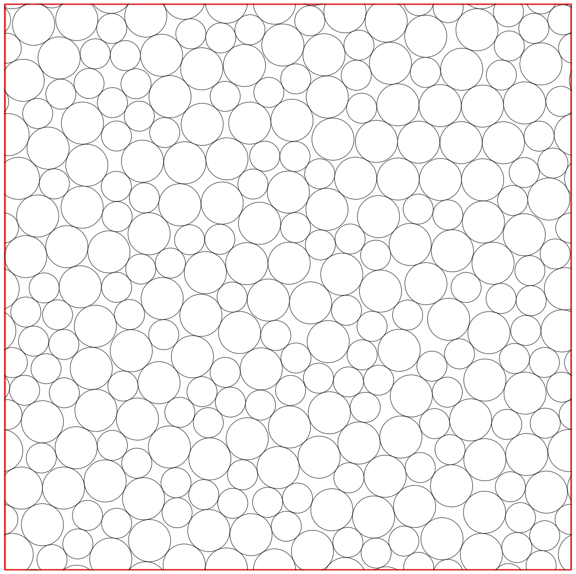
C. S. O'Hern, L. E. Silbert, A. J. Liu, S. R. Nagel, Phys. Rev. E **68**, 011306 (2003).

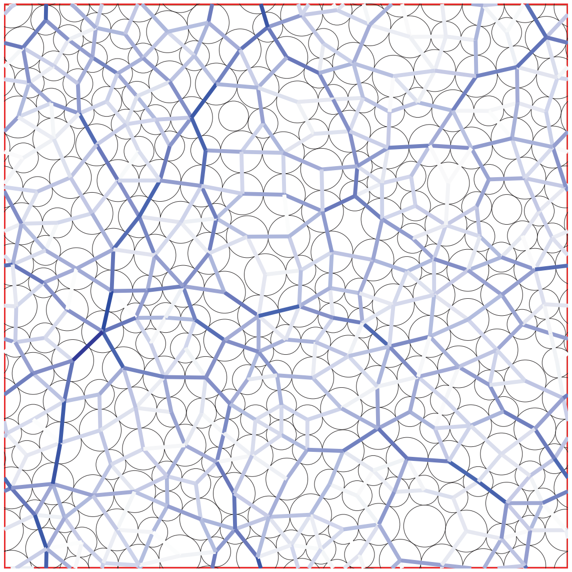
Isostaticity

- What is the minimum number of interparticle contacts needed for mechanical equilibrium?
- No friction, spherical particles, D dimensions
- Match unknowns (number of interparticle normal forces)
- with equations (force balance for mechanical stability)
- Number of unknowns per particle= $Z/2$
- Number of equations per particle = D

$$\rightarrow \quad Z = 2D$$

Just below ϕ_c, no particles overlap





Just above ϕ_c there are Z_c overlapping neighbors per particle

Summary of Point J

- Mixed first order/second order transition
- Number of overlapping neighbors per particle

$$Z = \begin{cases} 0 & \phi < \phi_c \\ Z_c + z_0 (\phi - \phi_c)^{\beta \cong 1/2} & \phi \geq \phi_c \end{cases}$$

- Static shear modulus/bulk modulus

$$G / B \sim (\phi - \phi_c)^{\gamma \cong 1/2}$$

- Two diverging length scales

$$\ell^* \sim (\phi - \phi_c)^{-\nu \cong -1/2}$$

$$\ell^\dagger \sim (\phi - \phi_c)^{-\nu^\dagger \cong -1/4}$$

Recall: calculating vibrational modes for soft repulsive discs

- dynamical matrix $\mathcal{M}$ determines linear response of packing to displacement u away from mechanical equilibrium
- normal modes are eigenvectors of the dynamical matrix
- each normal mode composed of N polarization vectors (or d N components)
- eigenvalue is energy ~ frequency
- Find density of states, etc.

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

$$r = |r_{ij}| = \sum_{\alpha}\left(r_{i\alpha} - r_{j\alpha}\right)^2$$

$$M_{i\alpha j\beta} = \frac{\partial^2 V}{\partial r_{i\alpha}\partial r_{j\beta}}$$

$$PE = \frac{1}{2}u^T M u$$

Vibrations in Solids at Low ω

- Solids all have density of vibrational states
  $D(\omega) \sim \omega^{d-1}$ in d dimensions (Debye prediction)
- Why?
  Low-frequency excitations are sound modes. At long length scales all solids look elastic

BUT

near Point J, there is a diverging length scale :

$$\ell \approx \frac{1}{Z - Z_c} \approx \left(\phi - \phi_c\right)^{-0.5}$$

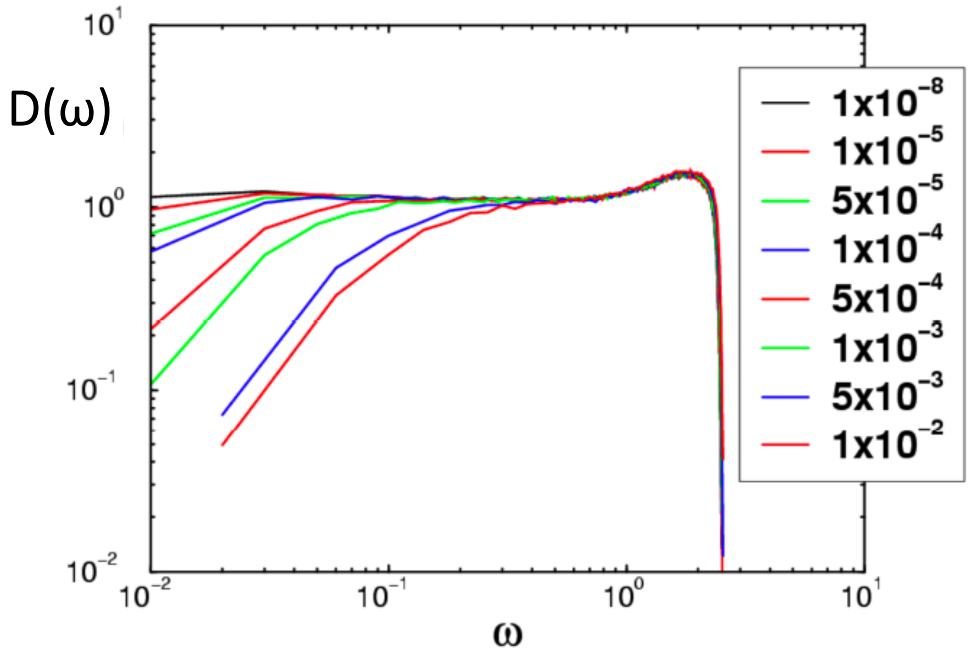
M. Wyart, S.R. Nagel, T.A. Witten, EPL **72**, 486 (05)

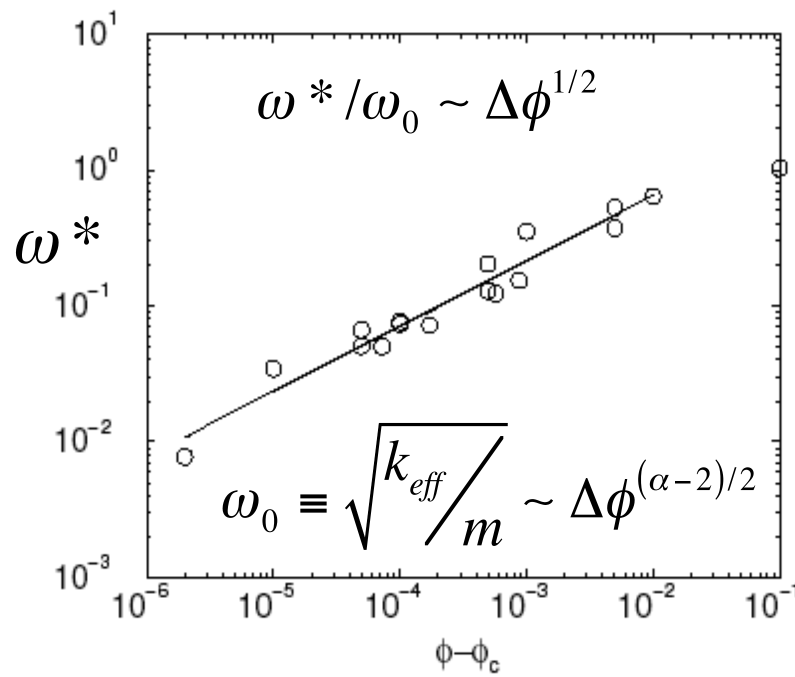
L. E. Silbert, A. J. Liu, S. R. Nagel, PRL **95**, 098301 ('05)

So what happens?

Vibrations in Marginally Jammed Solids

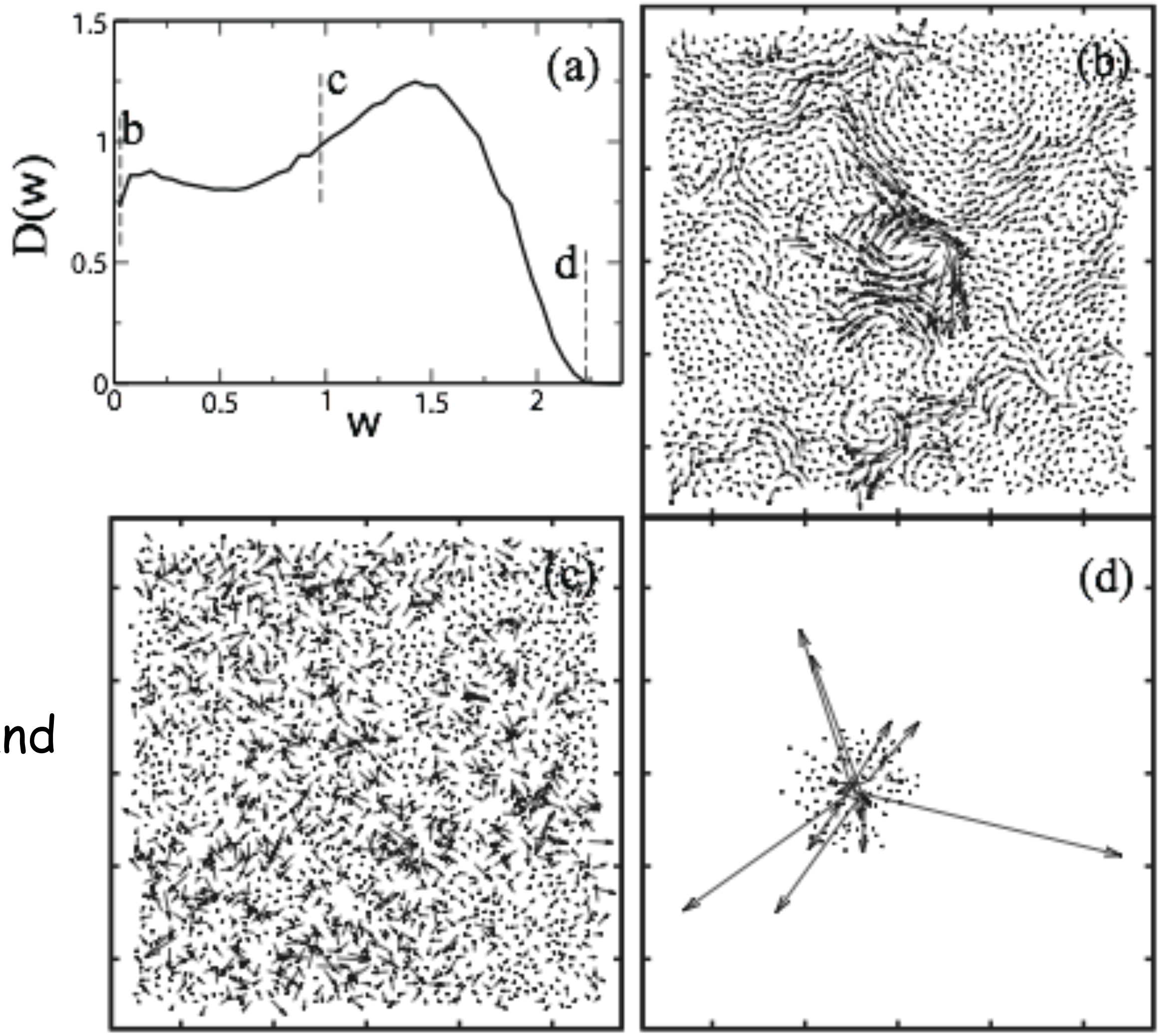
L. E. Silbert, A. J. Liu, S. R. Nagel, PRL **95**, 098301 ('05)





- More and more modes in excess of Debye prediction as $\phi \to \phi_c$
- New class of excitations distinct from sound modes originates from soft modes at Point J M. Wyart, S.R. Nagel, T.A. Witten, EPL **72**, 486 (05)

Nature of Excess Modes



quasilocalized

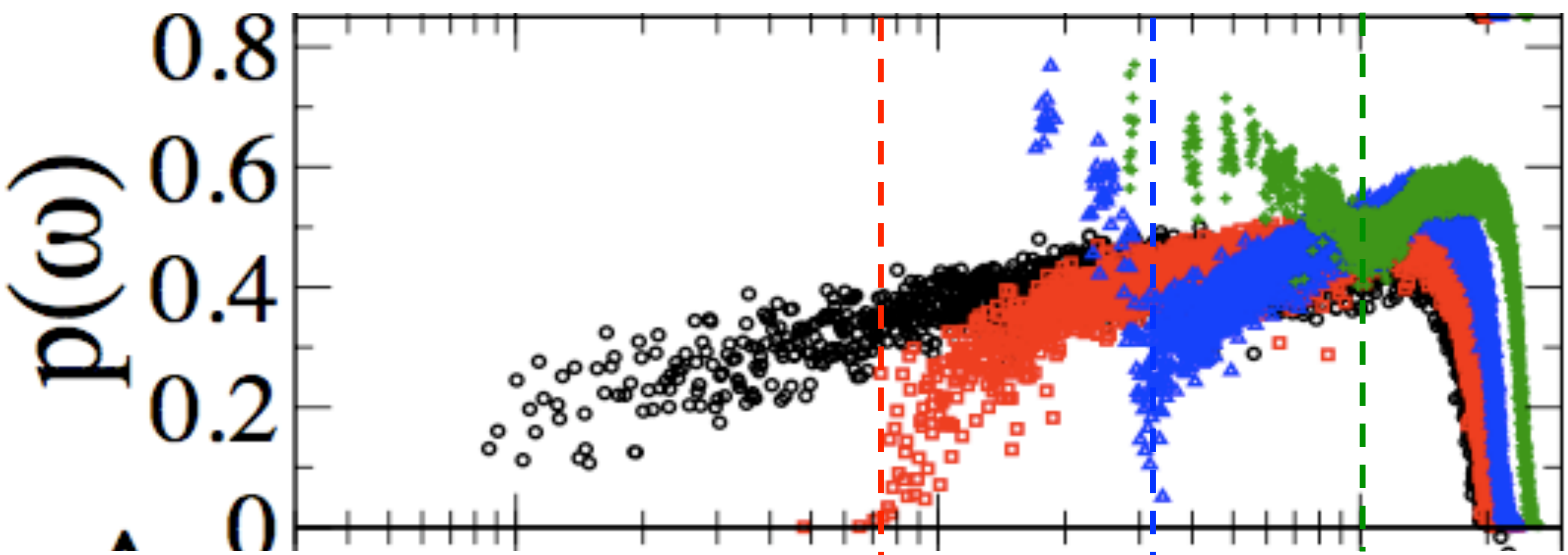
extended and disordered

localized

N. Xu, Vi Vitelli, A. J. Liu, S. R. Nagel, EPL 90 (2010) 56001.

Excess Modes (over Debye prediction)

Modes become quasilocalized near ω*

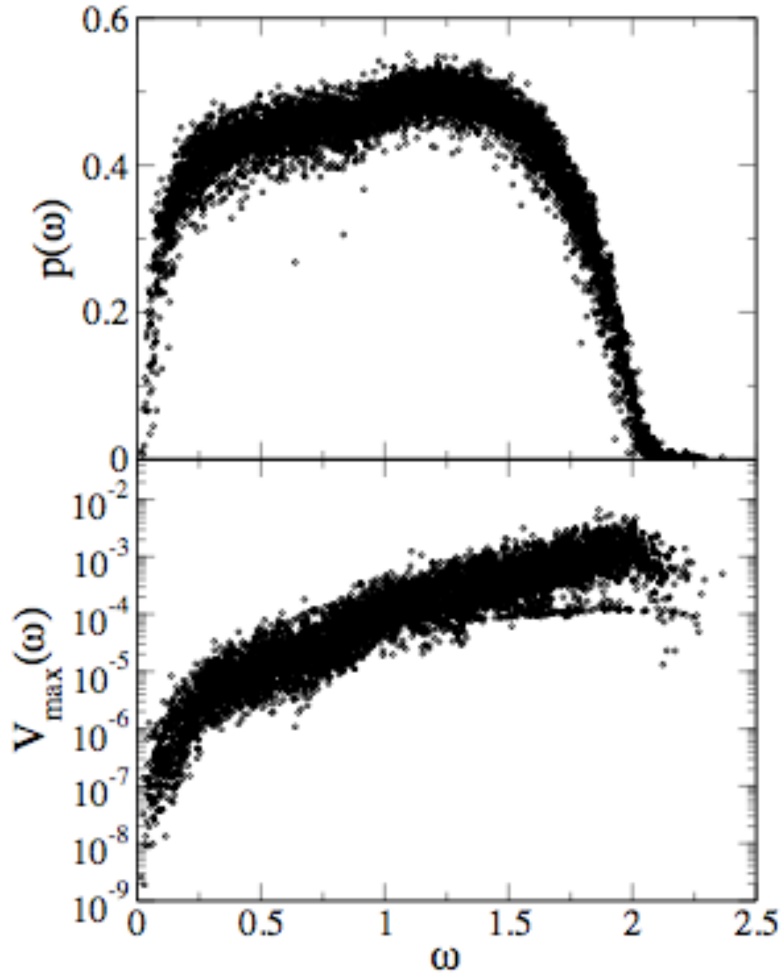


N. Xu, Vi Vitelli, A. J. Liu, S. R. Nagel, EPL 90 (2010) 56001.

Some excess modes very anharmonic

N. Xu, Vi Vitelli, A. J. Liu, S. R. Nagel, EPL 90 (2010) 56001.

- Low-frequency quasi-localized modes have the lowest energy barriers to rearrangement
- These modes are the most likely to go unstable due to temperature or mechanical load



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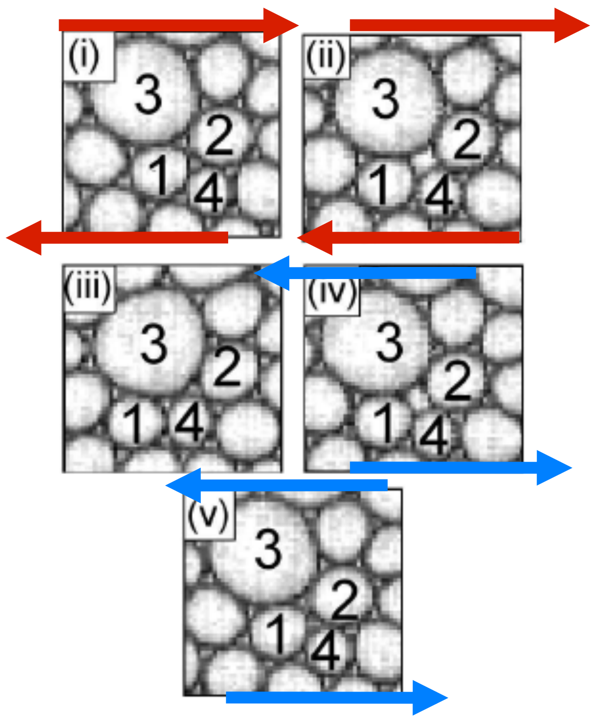
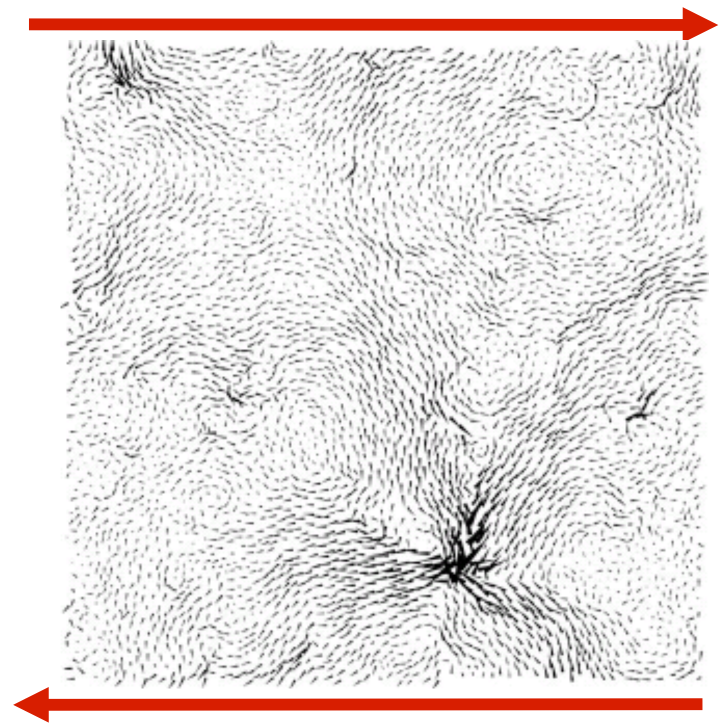
Observation of plastic deformation

Experimental Foams (Lundberg *et al, 2007*)



Images for reversible plastic events in a foam

Simulated granular materials (Maloney PRE **74** 1 2006)



Instantaneous nonaffine displacement field

Apparently:

deformation accommodated in localized regions

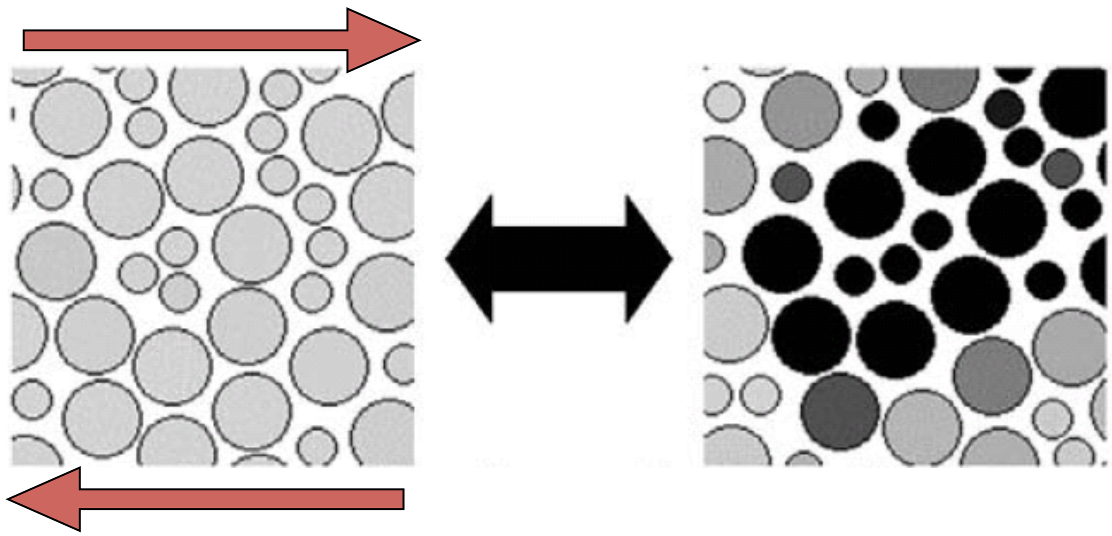
where are they located?

what sets the attempt rate?

how do these regions interact?

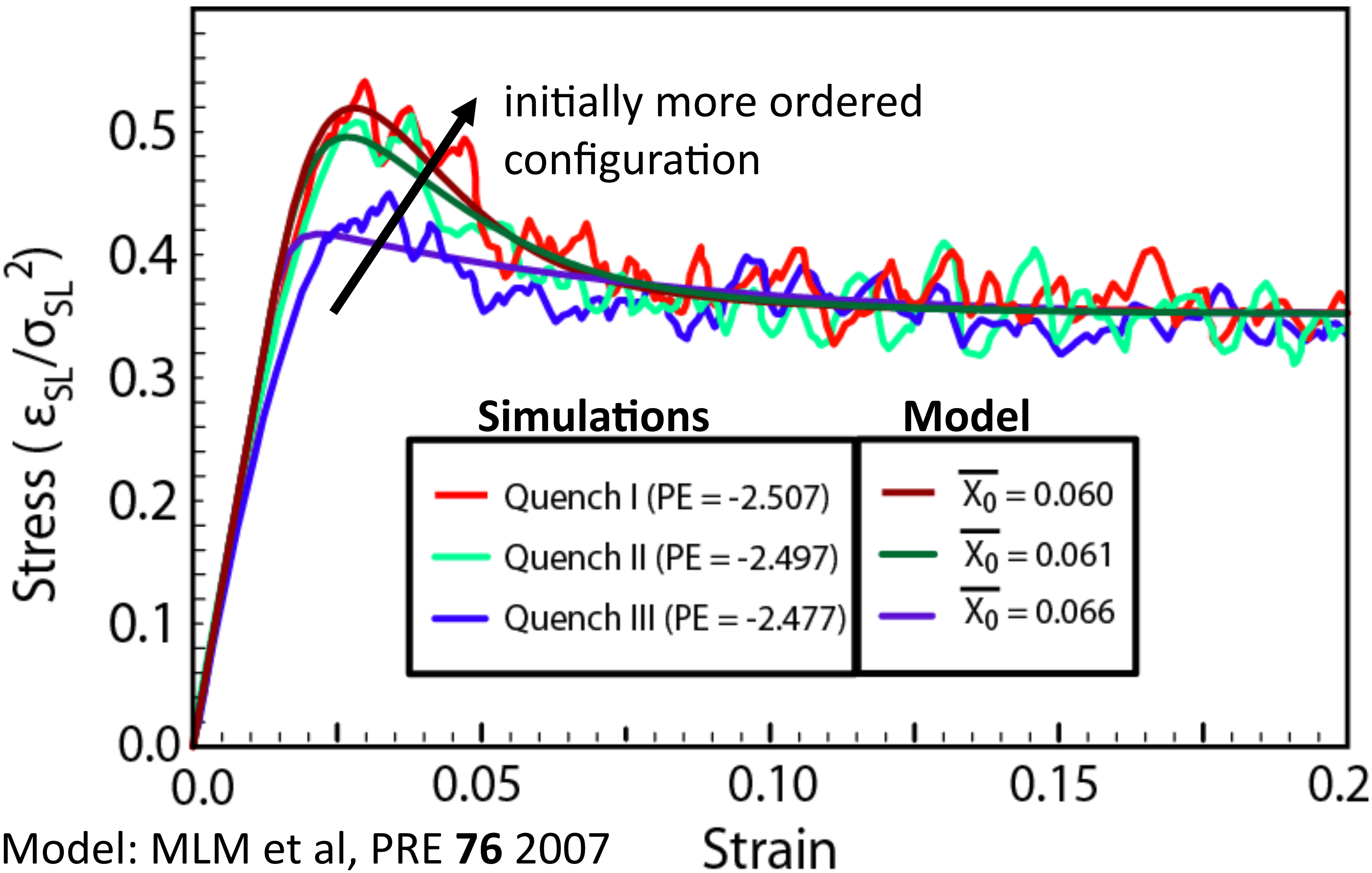
One model: Shear Transformation Zones

- continuum model for disordered solids
- postulates equations for density and orientation of susceptible regions: STZs



Spaepen (1977), Argon (1979), Falk and Langer (1998)

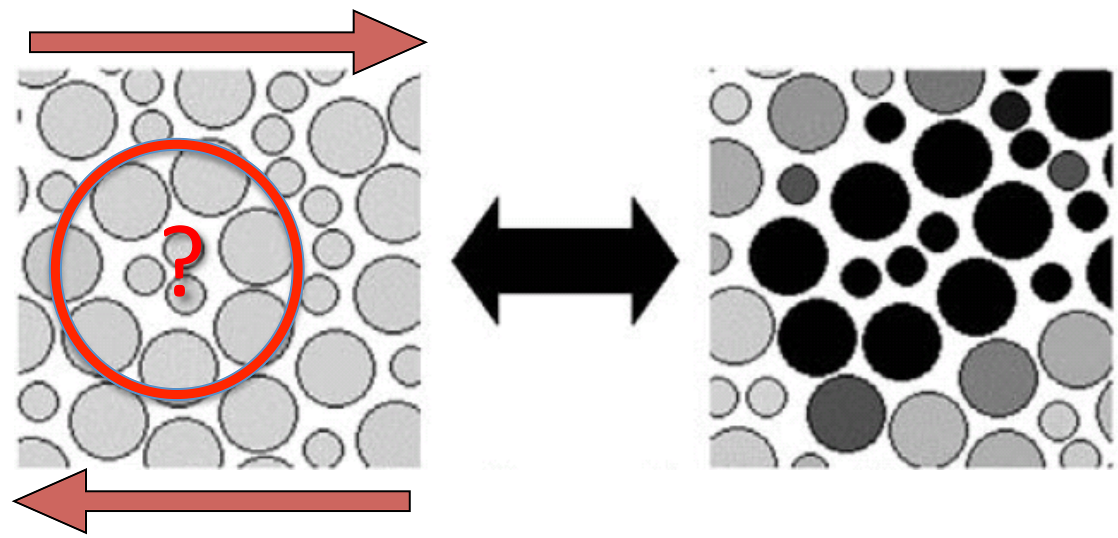
STZ model fits simulation data



Model: MLM et al, PRE **76** 2007
Simulations: Shi et al, PRL **98** 2007

but where are the STZs?

want to identify region susceptible to deformation before a plastic rearrangement



then we can ask:

how many STZs? How does the population change with strain? How do they interact?

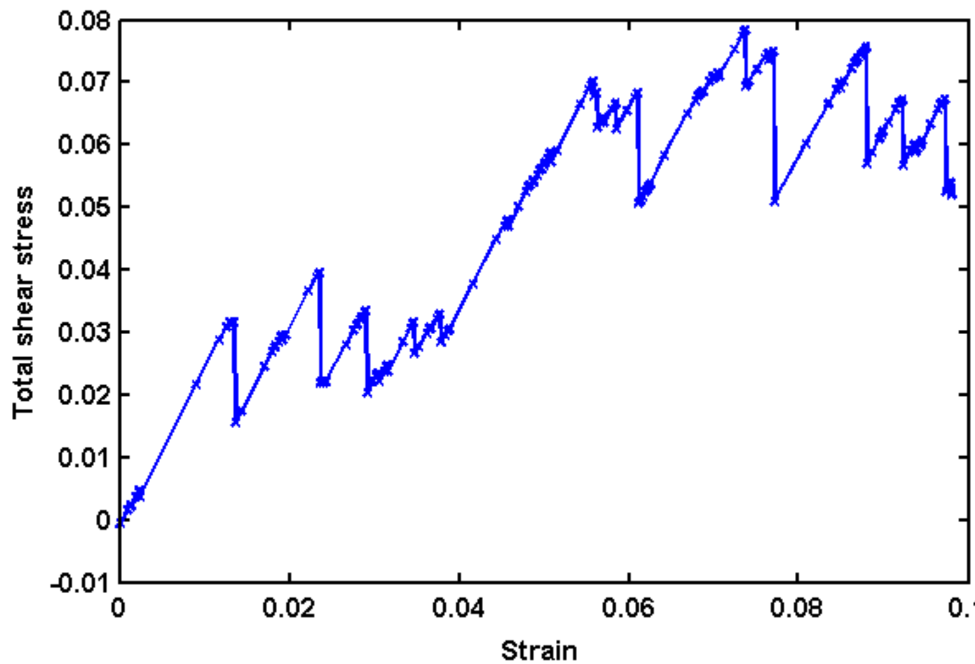
Can vibrational modes be used to predict plastic rearrangements?

idea: use normal modes to identify soft spots in sheared amorphous solids

Model system: harmonic discs under quasi-static shear

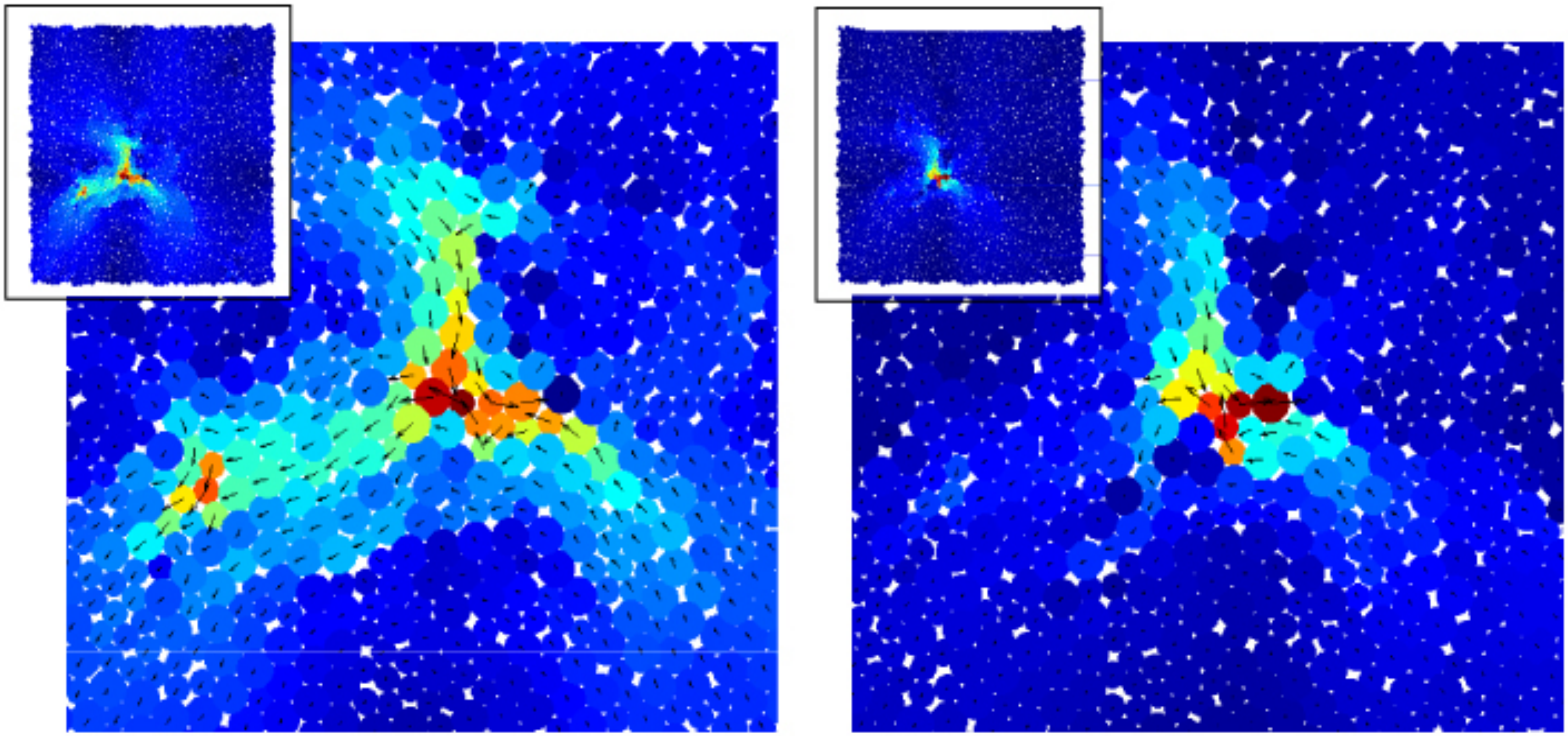
$$V(r) = \begin{cases} \dfrac{\varepsilon}{\alpha}\left(1 - \dfrac{r}{\sigma}\right)^{\alpha} & r \le \sigma \\ 0 & r > \sigma \end{cases}$$

High packing fraction: 0.99



- At T=0, rearrangements (stress drops) occur when a vibrational mode goes unstable (reaches ω=0)
- So lowest-ω quasilocalized mode is most likely culprit

Lowest energy mode and plastic displacement

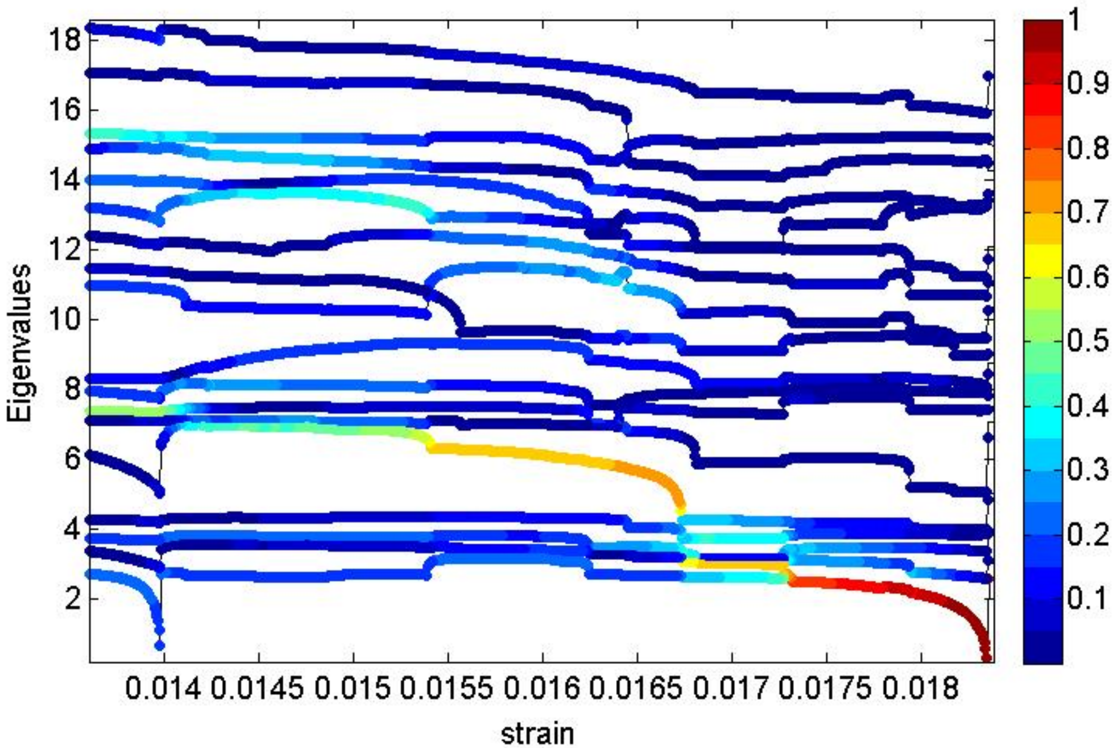


Quasi-localized mode　　Rearrangement at higher strain

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

Predicting Rearrangements

- Lowest-ω quasilocalized mode most likely to go unstable NO!



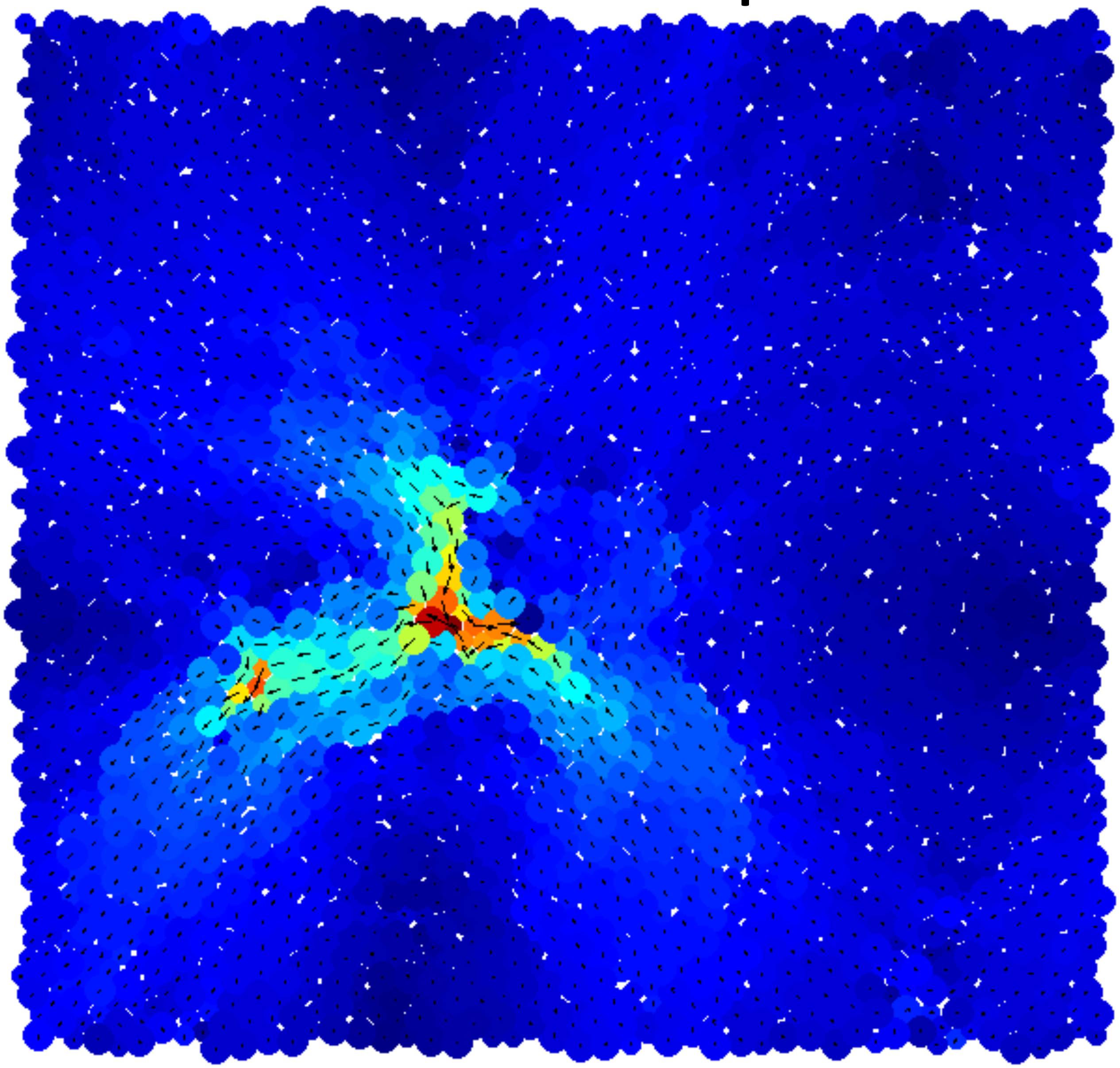
In a large system, lowest mode is the one that goes unstable only very close to the instability!

Can we find spatial regions susceptible to rearrangement well before the instability?

Identifying Soft Spots

- unlike Anderson-localized modes, the low energy quasi-localized modes are in same energy band as plane waves and modes can mix
- idea: analyze all lowest energy modes and identify subsets of the mode which are special
  - tool: variance in the polarization vector distribution
- combine subsets together to identify soft spots
- quantify similarity between soft spots and plastic rearrangements
  - tool: binary overlap

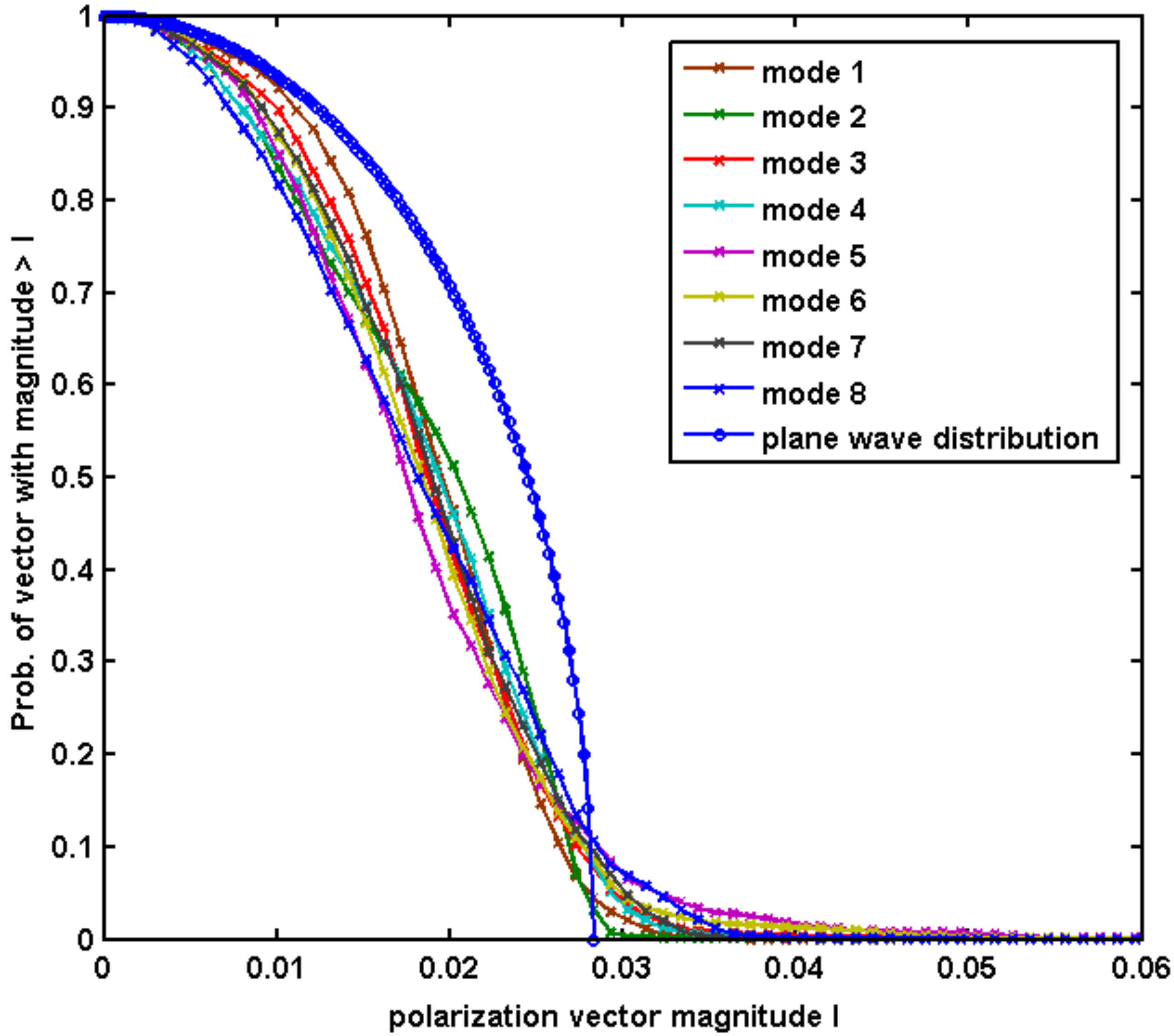
Which subsets of polarization vectors are special?



obviously want high displacement regions . . .

where should the threshold be?

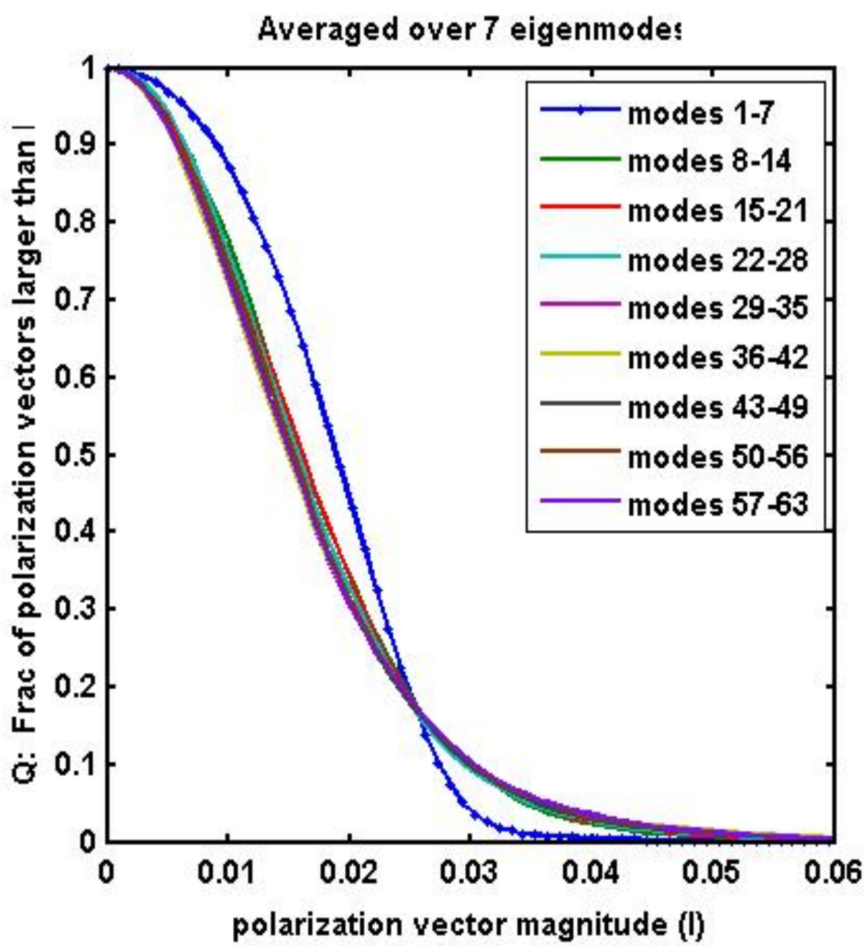
Polarization vector distributions

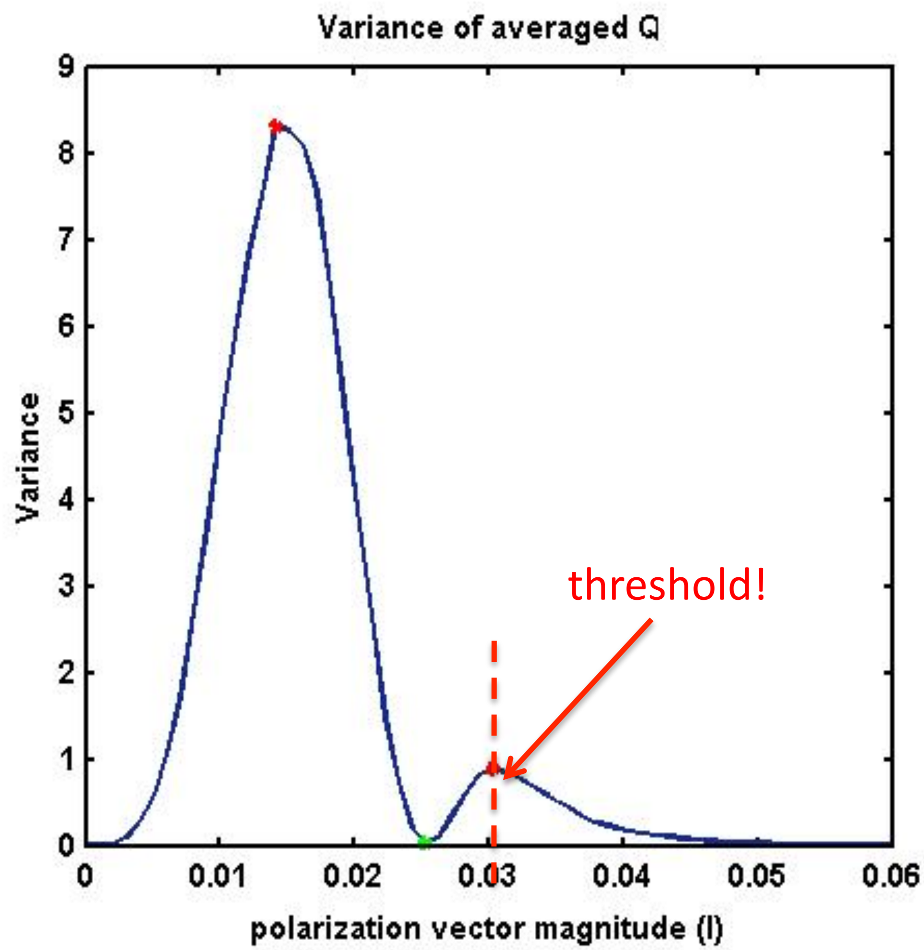


the participation ratio is a scalar measure often used to quantify this distribution.

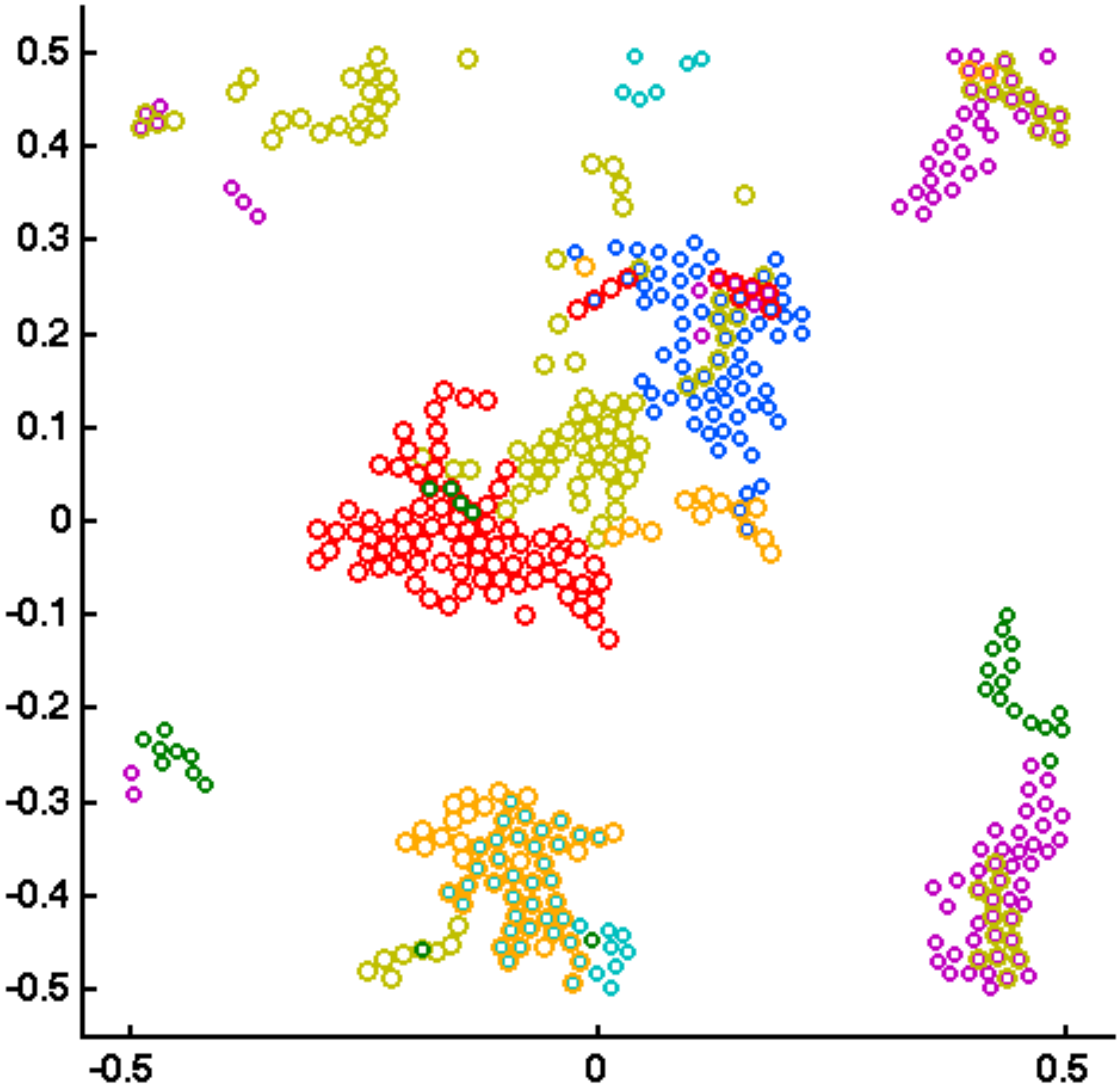
But there's a lot more information here!

Variance in the polarization vector distribution





Threshold l* is VERY robust: $l^{*} \approx 1.1\sqrt{\frac{2}{N}}$

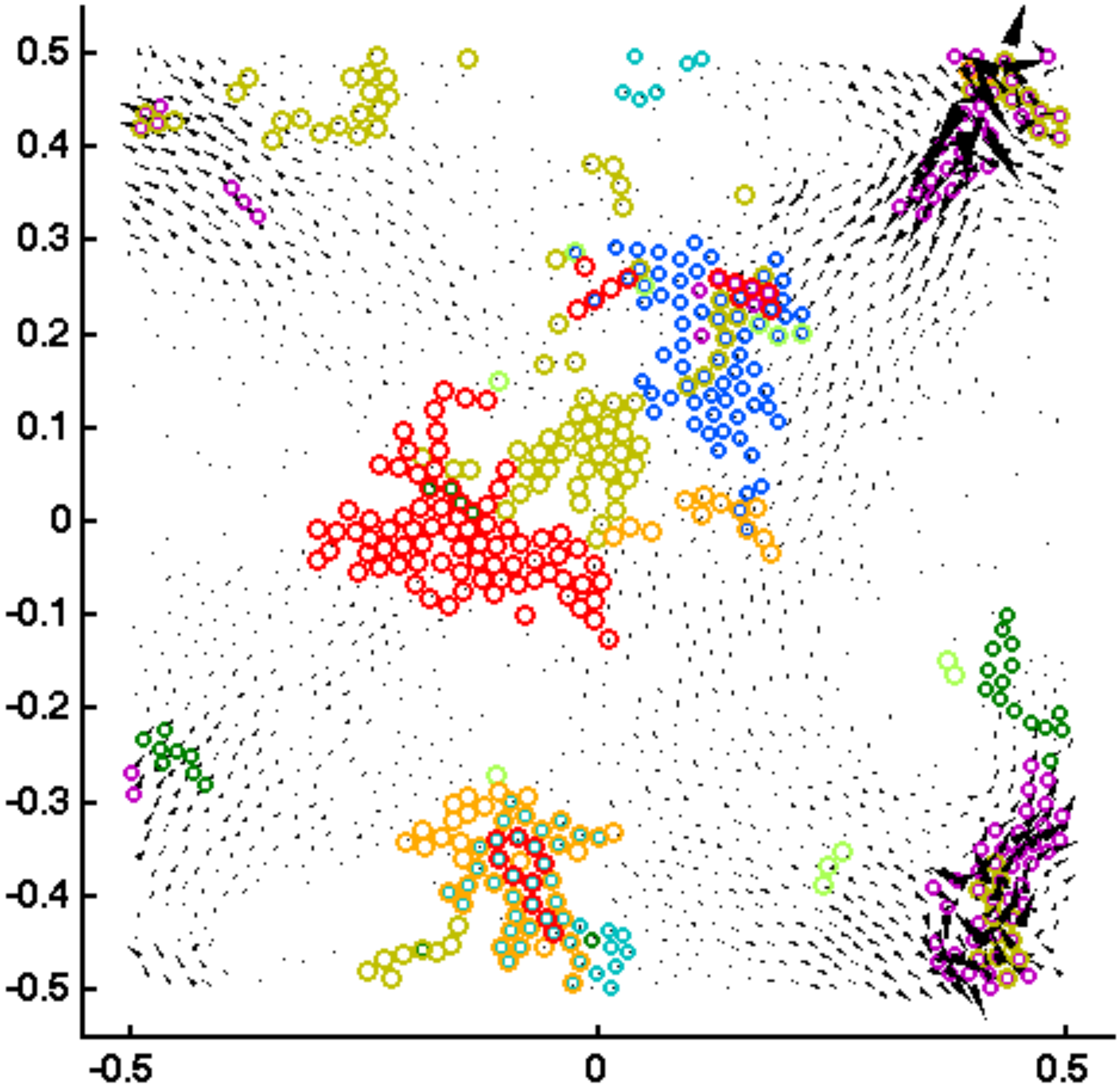


Identifying Soft Spots

Each color corresponds to the large displacement region of a particular normal mode

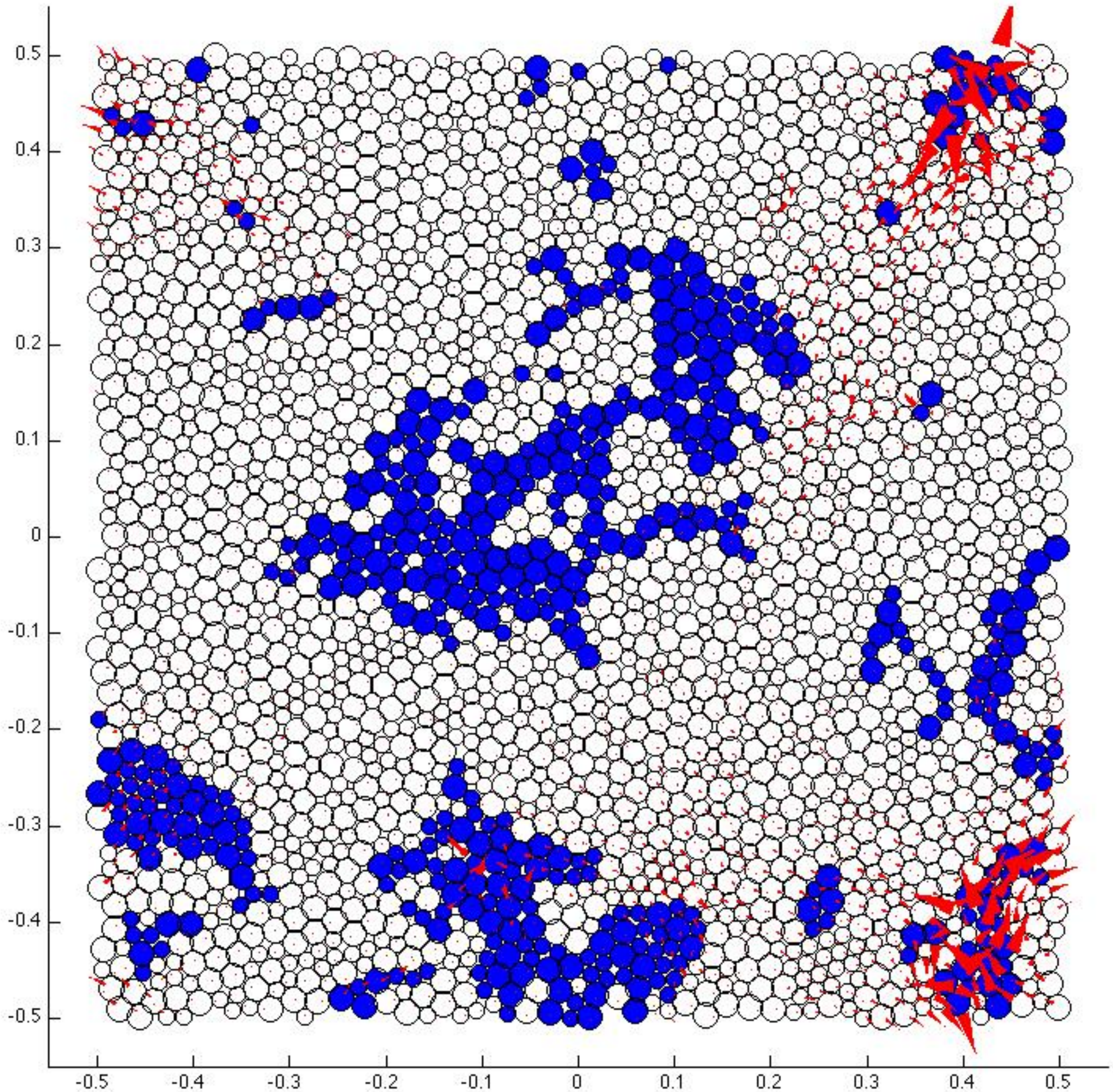
Regions often overlap

Regions are clustered (not very string-y)



Identifying Soft Spots

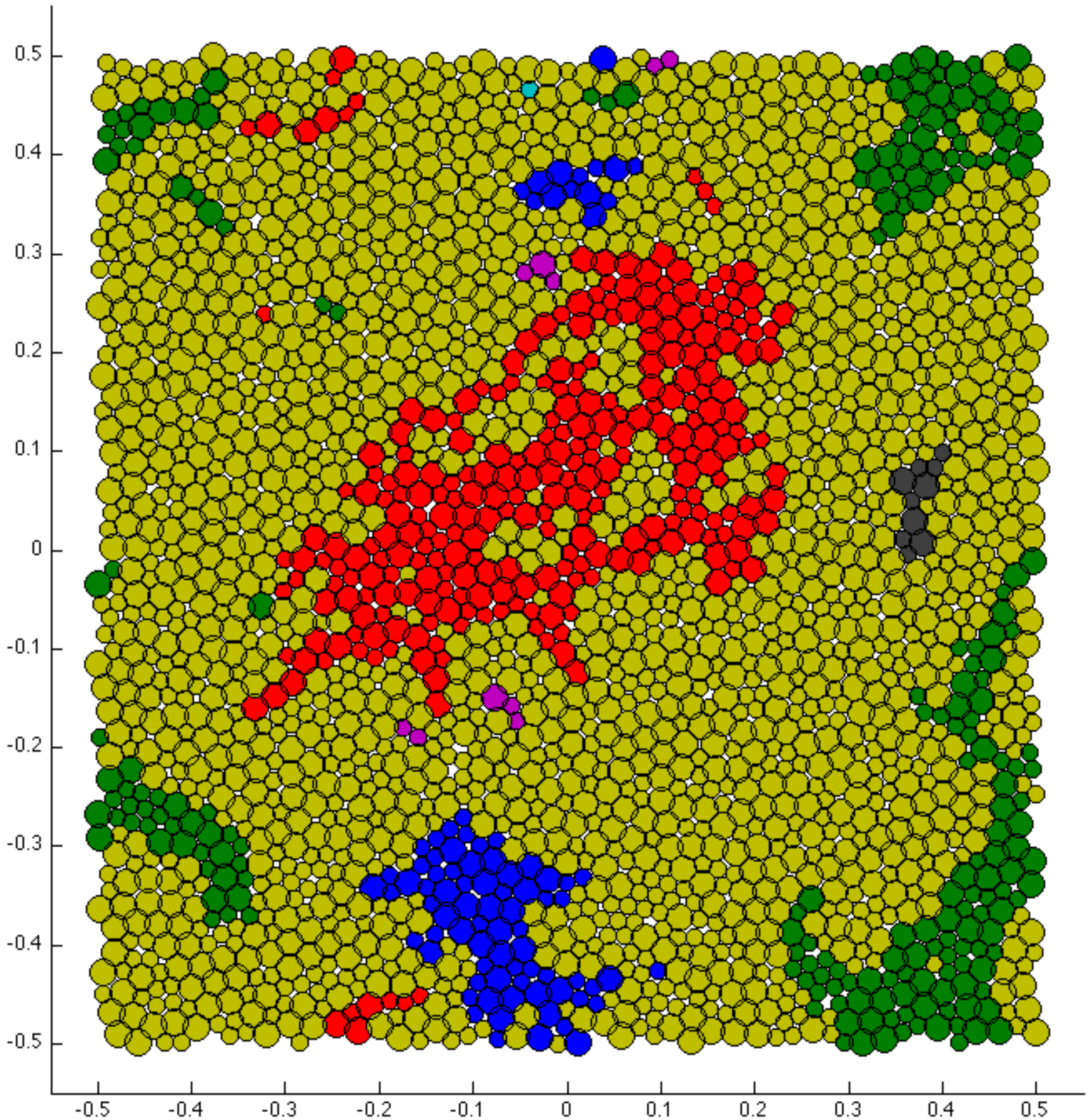
Purple/gold modes have good overlap with next rearrangement



Identifying Soft Spots

Blue regions are the "soft" regions identified by our algorithm,

red arrows are the next plastic rearrangement



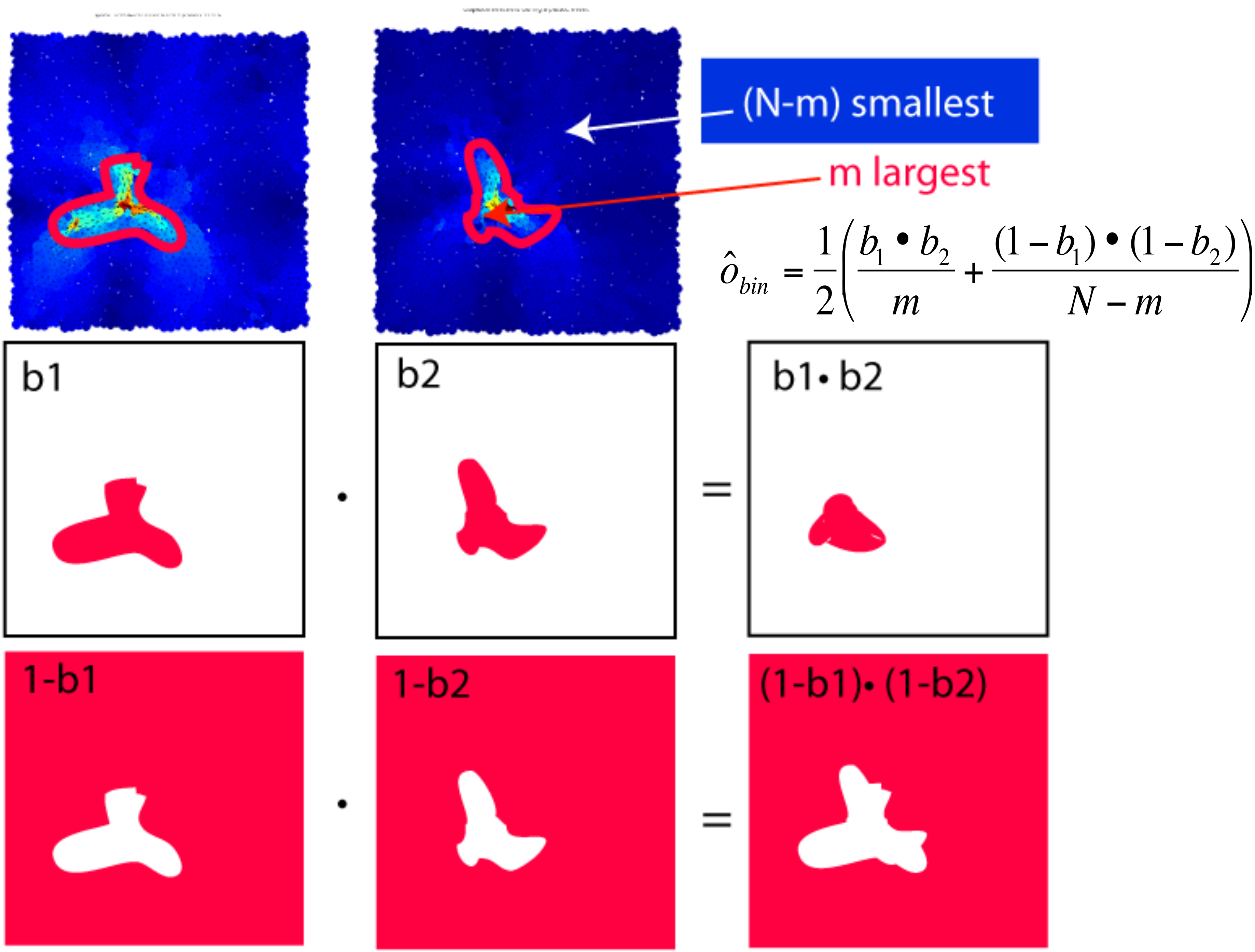
Identifying Soft Spots

The soft regions form clusters, which we identify with a simple percolation clustering algorithm

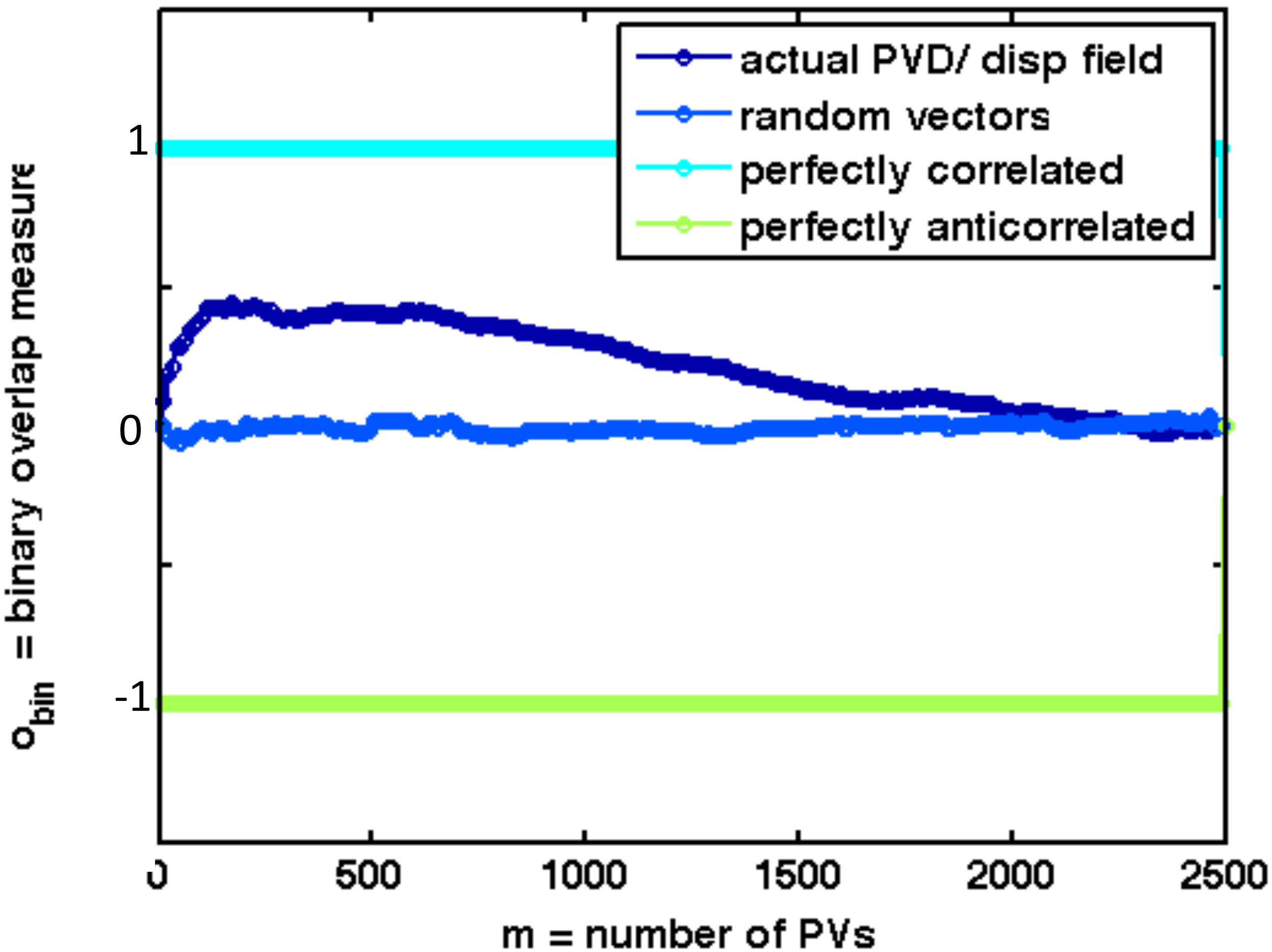
Why clusters? The plastic rearrangements usually only overlay a single spot, not all of the spots.

Identifying soft spots

- Need to quantify the similarity between one a "soft spot" and the plastic displacement field
- Want a metric that
  - does not depend on size of the soft spot
  - equals zero for two random vector fields
  - equals one if the two vector fields are perfectly correllated
- New tool: binary overlap


(N-m) smallest
m largest
$$\hat{o}_{bin} = \frac{1}{2}\left(\frac{b_1 \bullet b_2}{m} + \frac{(1-b_1)\bullet(1-b_2)}{N-m}\right)$$
b1
b2
b1• b2
1-b1
1-b2
(1-b1)• (1-b2)

Identifying soft spots

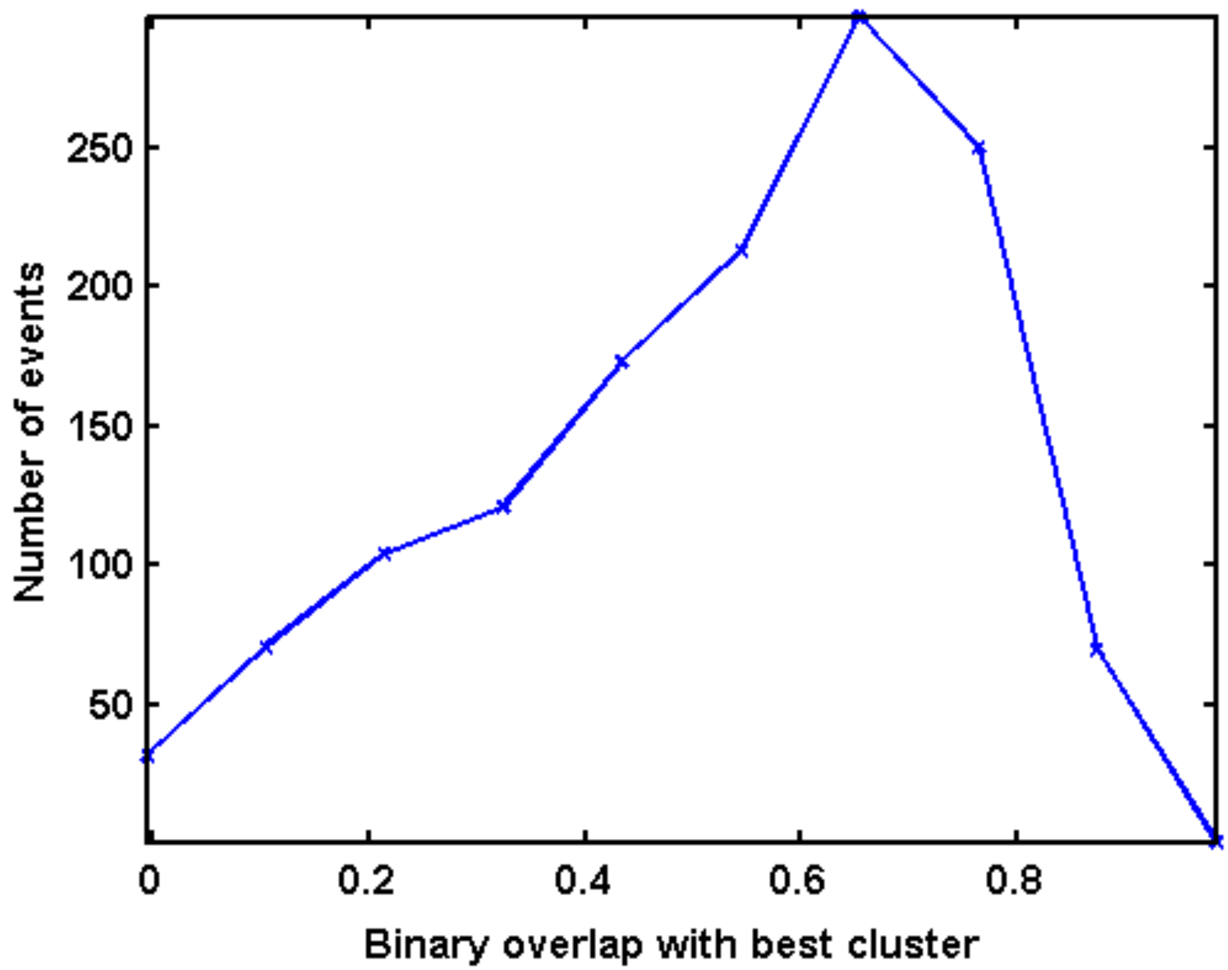


This works!

(with additional term for anticorrelated vectors)

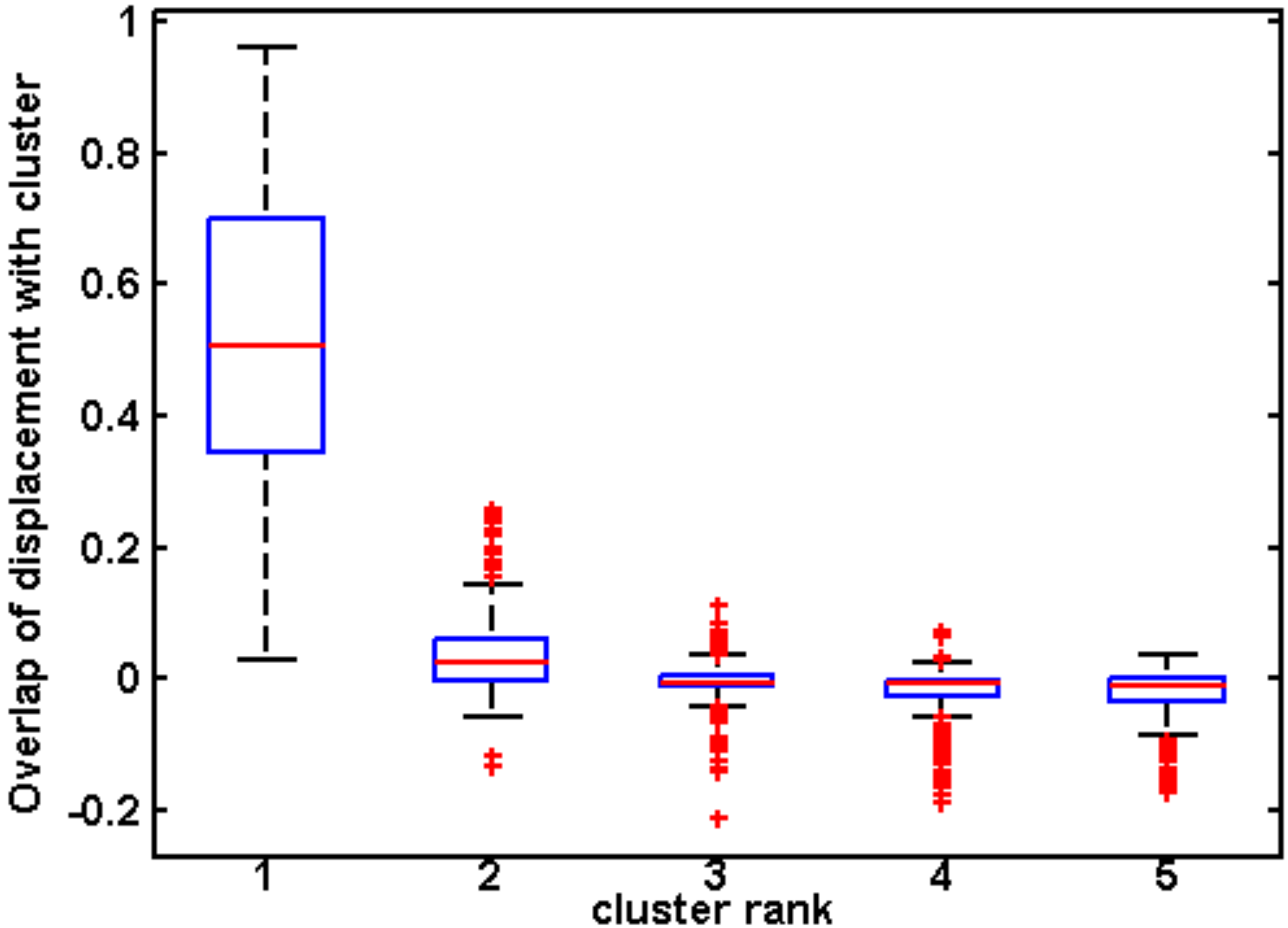
very sensitive metric (0.5 is a strong correlation!)

Result: we CAN identify STZs



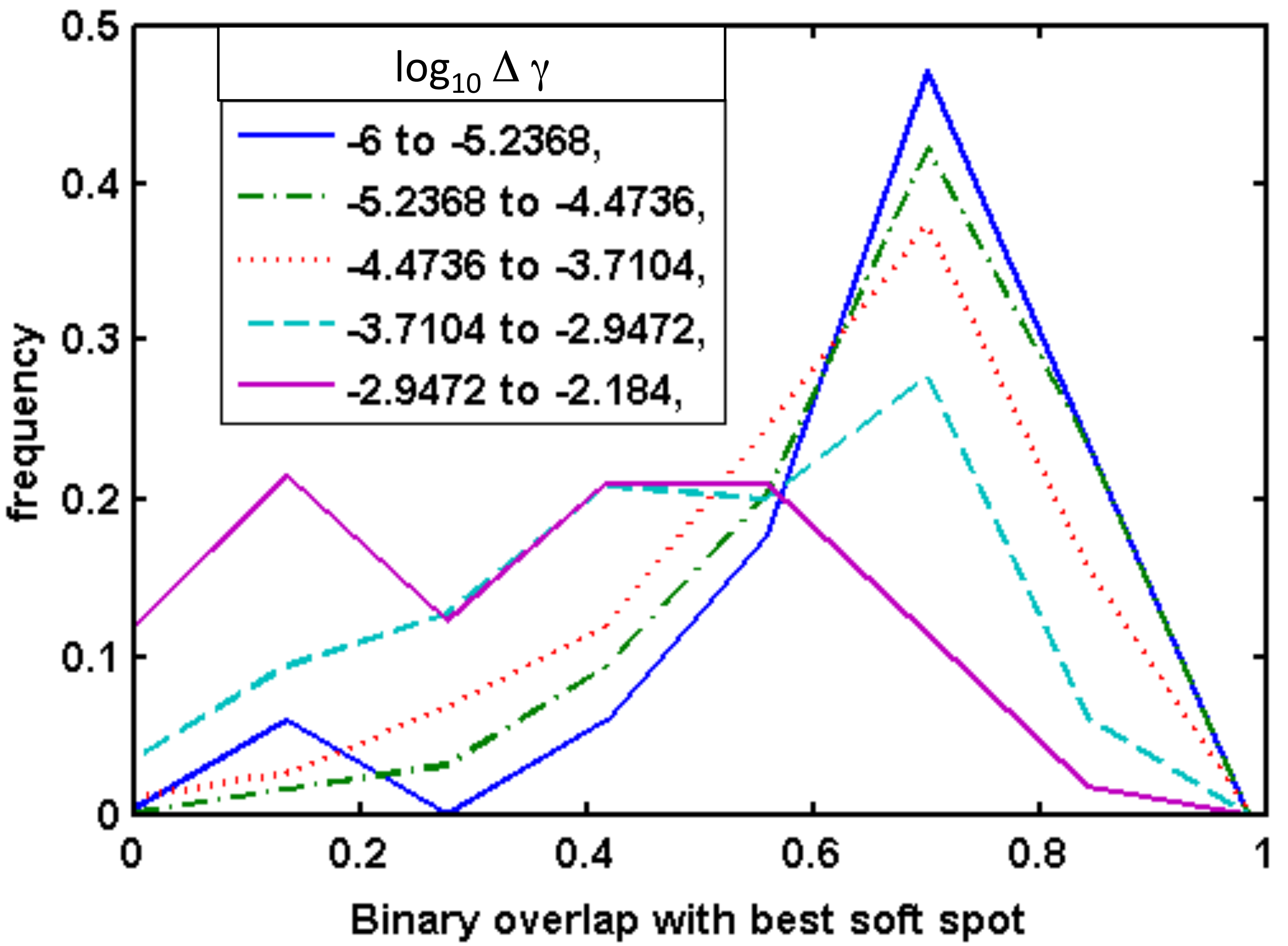
Plastic rearrangement strongly overlaps best soft spot for most events: total number of events is 1333

“Best” soft spot really is the best



“Binary overlap” is a really strict metric; anything above ~0.2 is significant

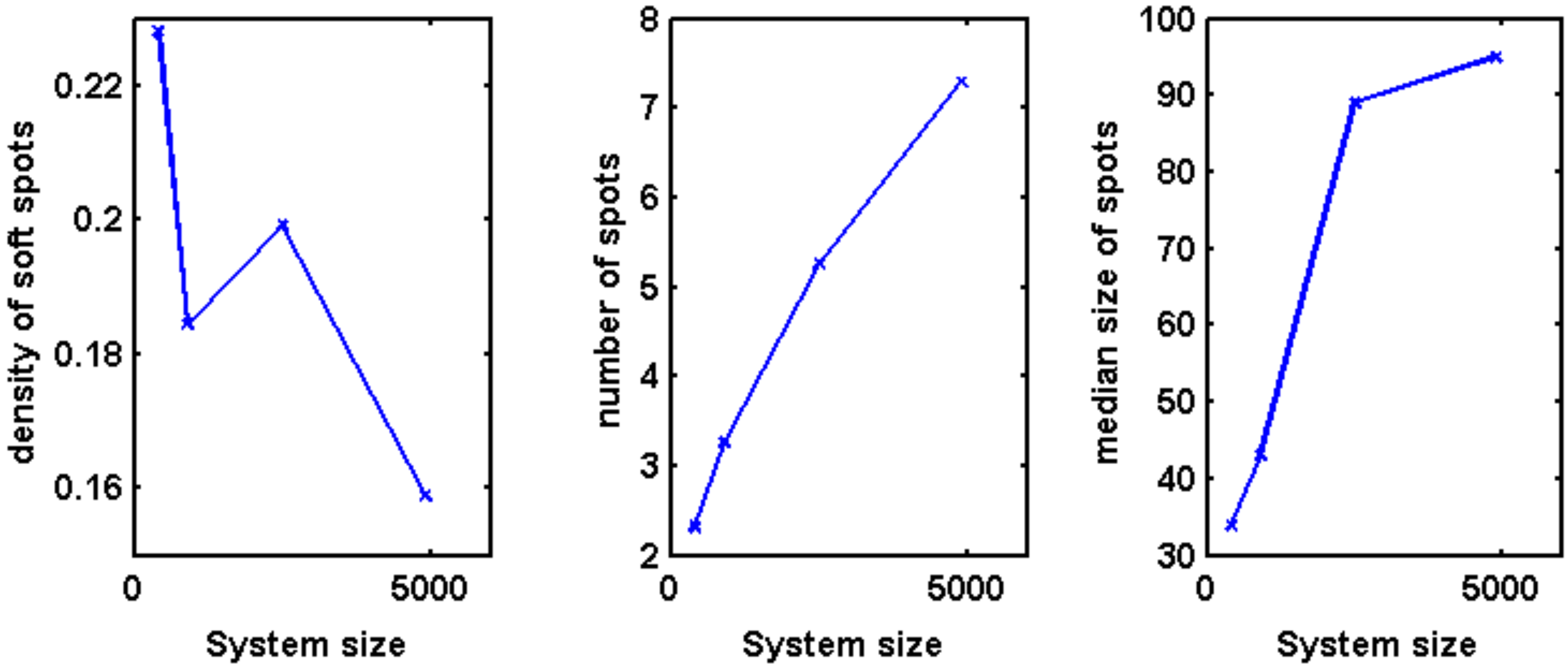
How does overlap change with distance to the plastic event?



average strain between rearrangements $\log_{10}\langle\Delta\gamma\rangle \approx -2.7$

The closer to the instability, the greater the overlap of the rearrangement with mode with best soft spot

Preliminary results: system size dependence



Conclusions

- The vibrational spectrum of amorphous solids includes "quasi-localized" modes which will eventually accommodate plastic rearrangements
- These modes mix together and mix with plane waves, but there are common "soft spots"
- We have developed algorithms and tools that allow us to identify soft regions or "STZs" that take up roughly 1/5th of the area in 2D binary mixtures
- It appears that these regions are clustered into spots with an average size

Thanks for your attention!

M. L. Manning, A. J. Liu (manuscript in preparation, 2010)

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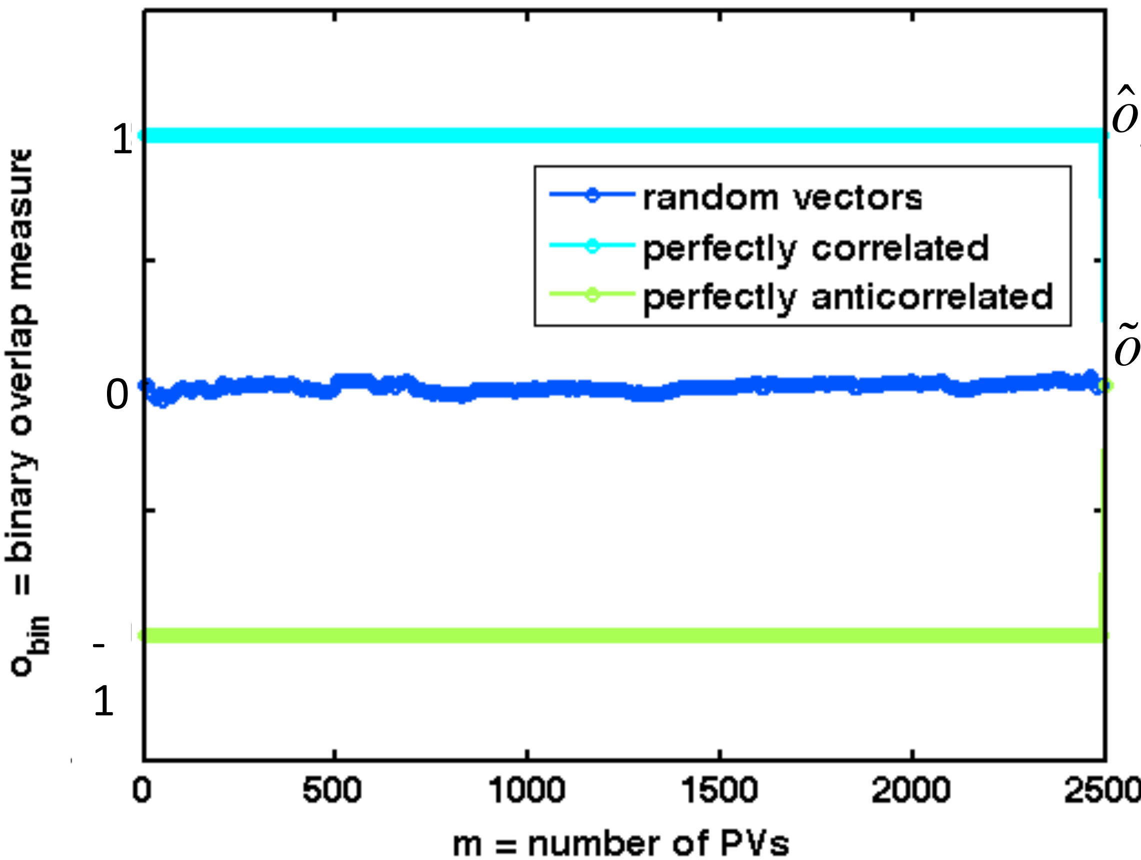
Funding: Princeton Center for Theoretical Science,

DOE DE-FG02-03ER46087

Binary overlap

- Need two terms to handle correlated AND anti-correlated



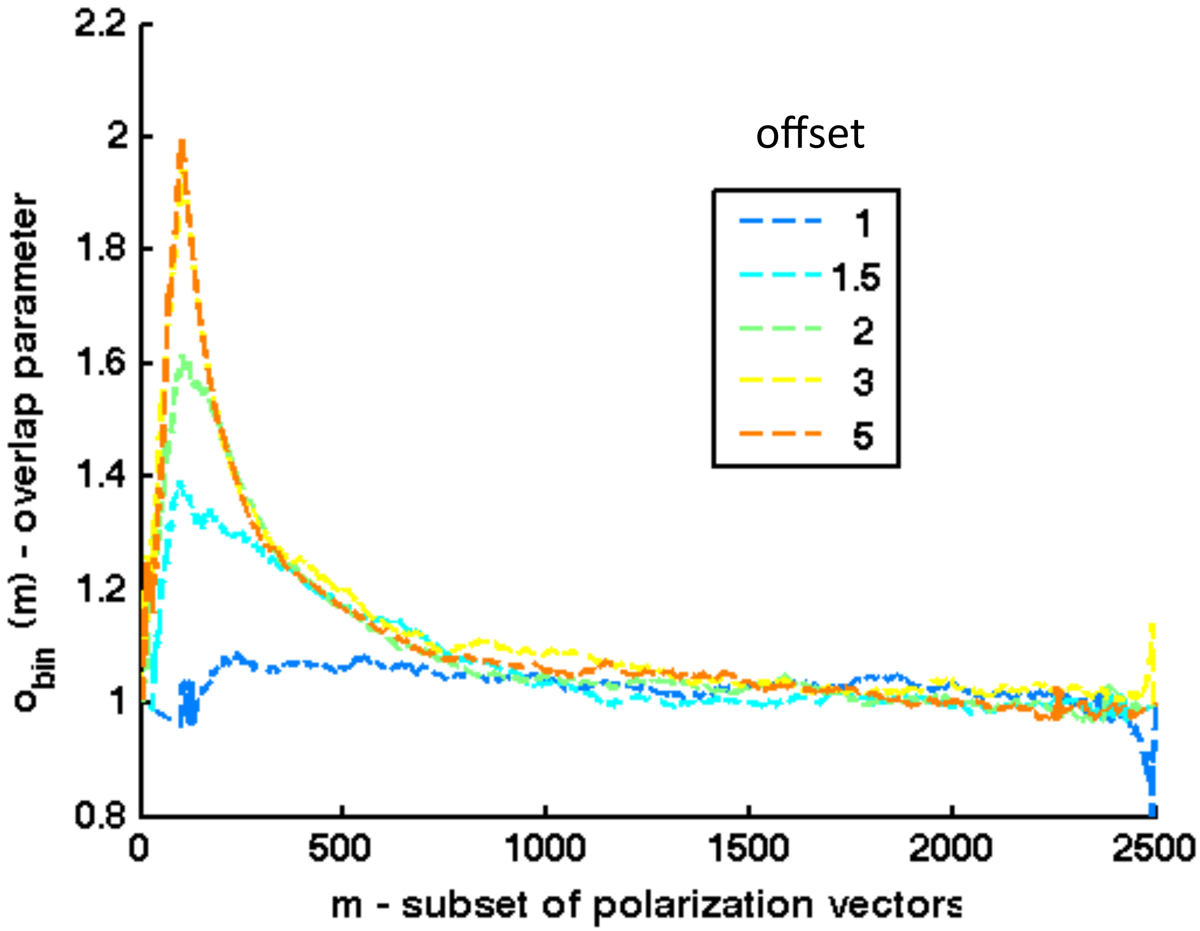
$$\hat{o}_{bin} = \frac{1}{2}\left(\frac{b_1 \bullet b_2}{m} + \frac{(1-b_1)\bullet(1-b_2)}{N-m}\right)$$

$$\tilde{o}_{bin} = \frac{1}{2}\left(\frac{b_1 \bullet \tilde{b}_2}{m} + \frac{(1-b_1)\bullet(1-\tilde{b}_2)}{N-m}\right)$$

$$o_{bin} = \begin{matrix} \hat{o}_{bin}, & \hat{o}_{bin} > \tilde{o}_{bin} \\ -\tilde{o}_{bin}, & \tilde{o}_{bin} > \hat{o}_{bin} \end{matrix}$$

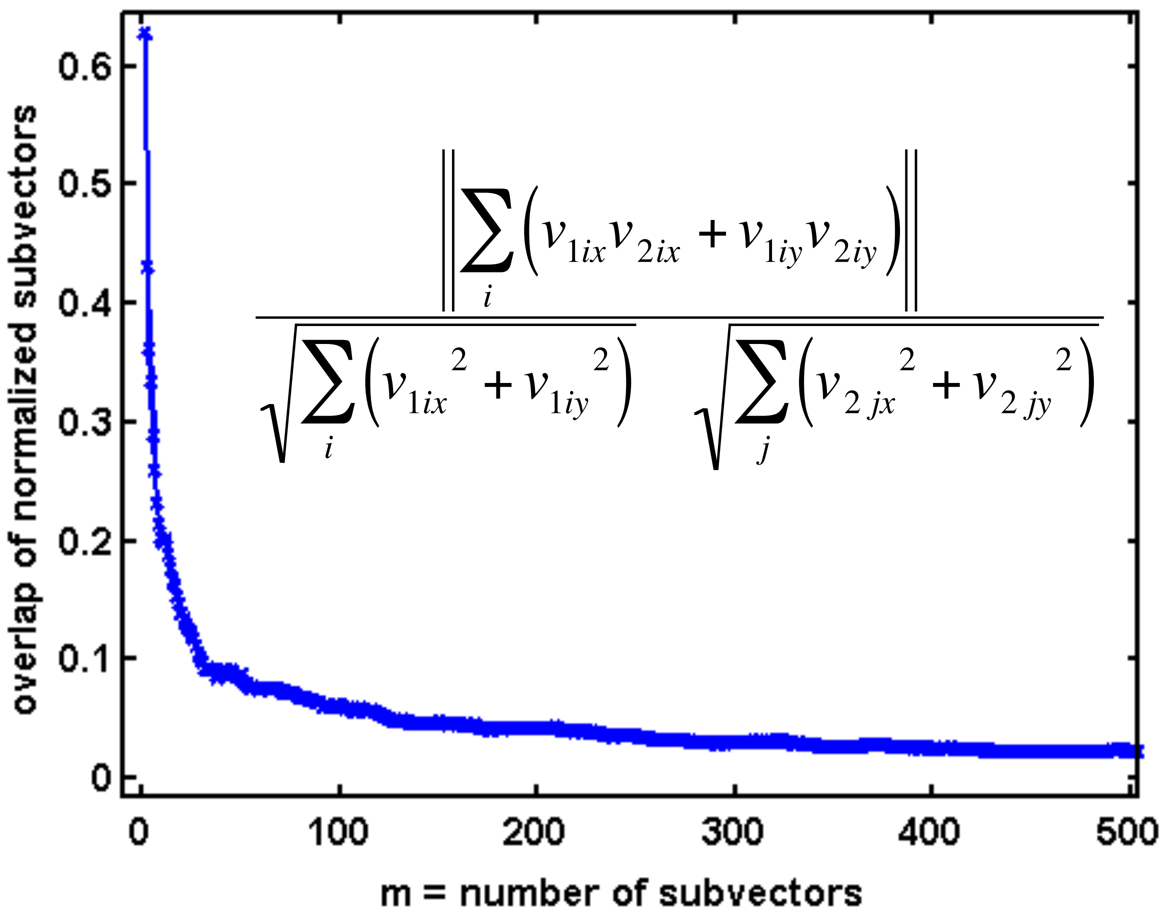
Binary overlap

- Synthetic tests on features of size = 50 particles
- sum fixed vector from U[0,1] with random vector on U[0, offset]



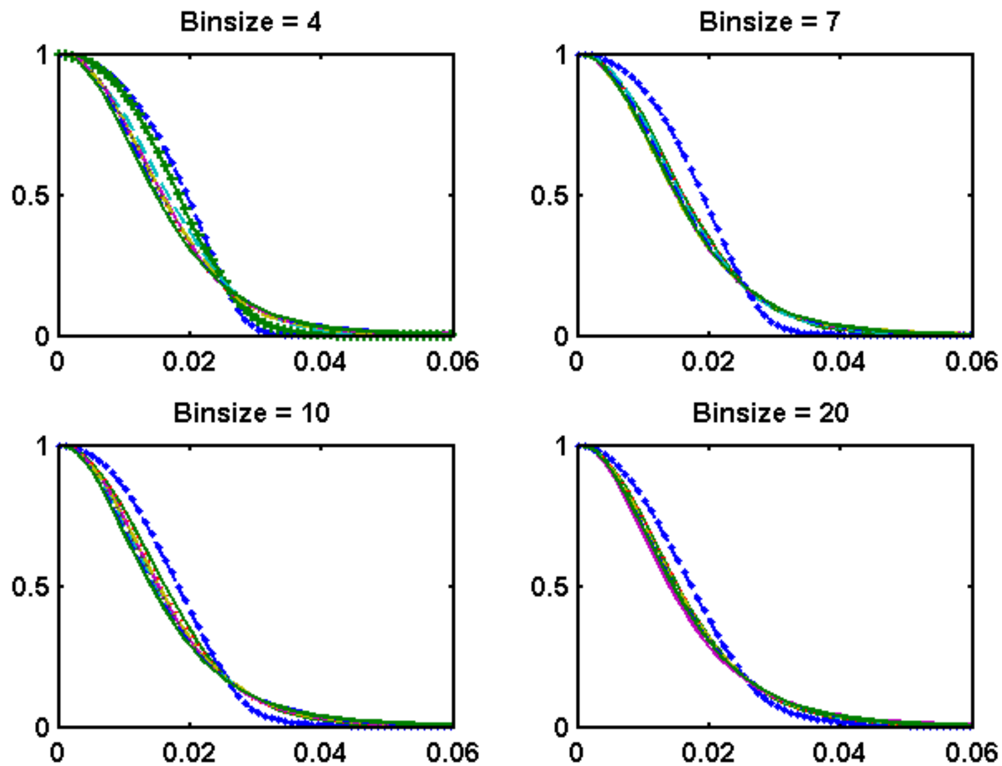
Binary overlap

- Why don’t you just take the dot product?
- x to –x, y to –y symmetry of dynamical matrix means there is an m-dependence



How many modes to analyze?

- Currently: Analyzing lowest 8 eigenvectors



- still an open question how this scales with system size

How many modes to analyze?

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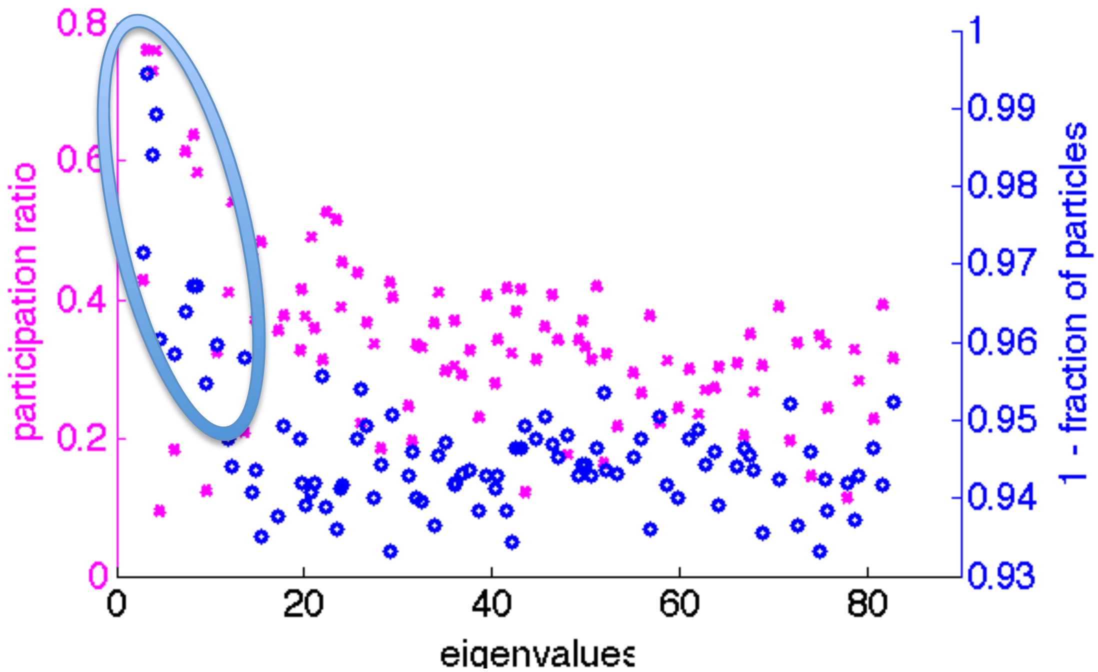

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