Efficient determination of soft spots in amorphous solids *only* using local structural information

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Introduction

- Soft spots are structurally different.
- These differences could not be used to identify soft spots*.

*L. Manning & A. Liu, PRL **107**, 108301 (2011)

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- We propose a method that can efficiently predict regions vulnerable to rearrangement purely from local geometric quantities.
- We look at where rearrangements occur, and ask what was structurally different before the rearrangement.

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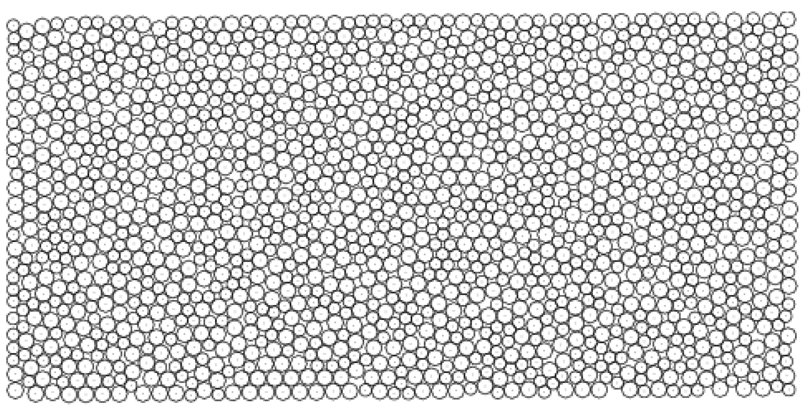

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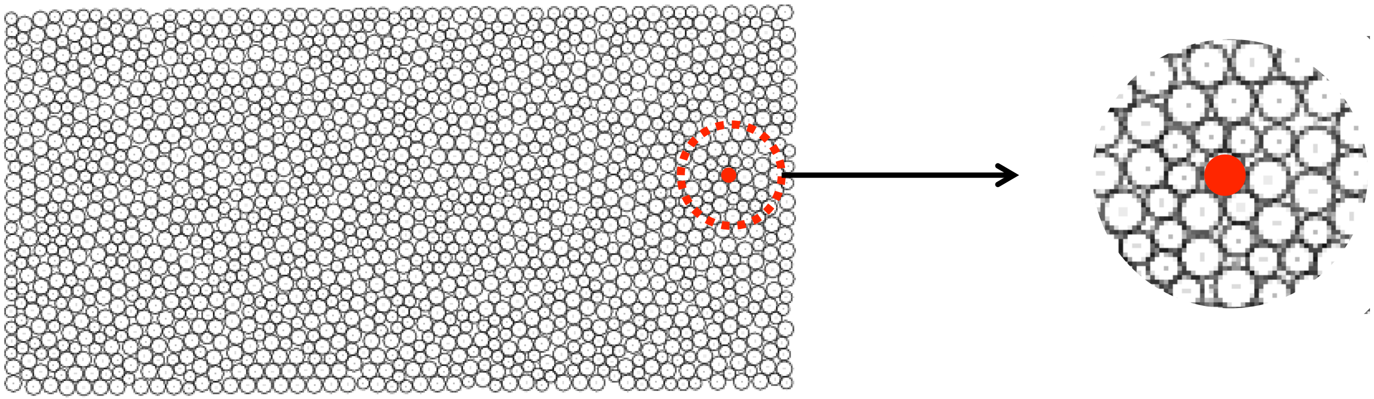

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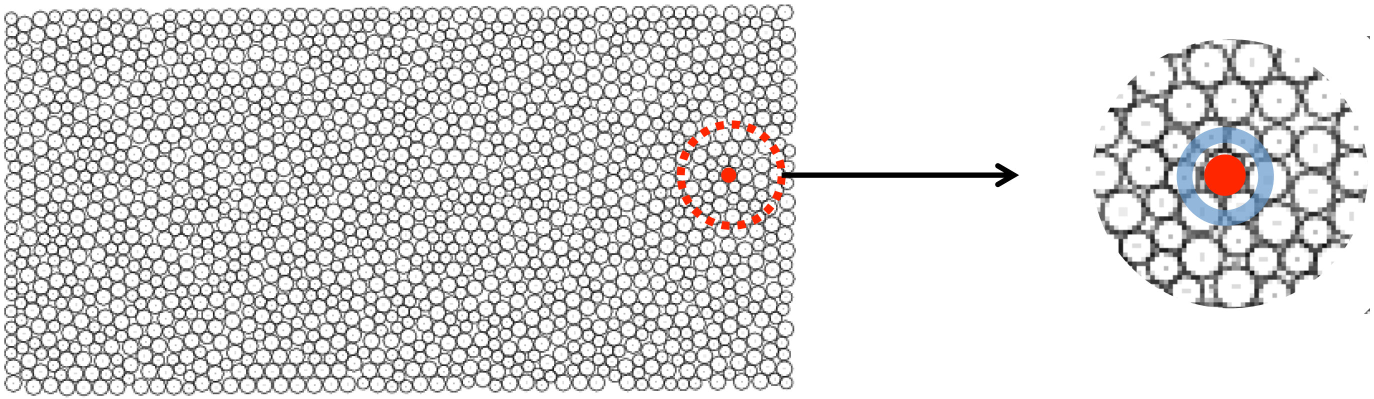

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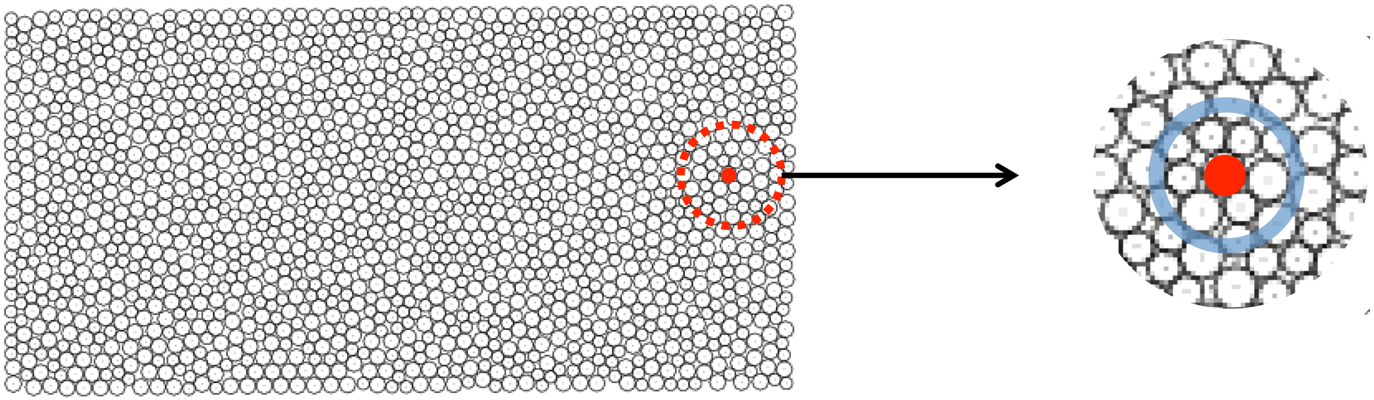

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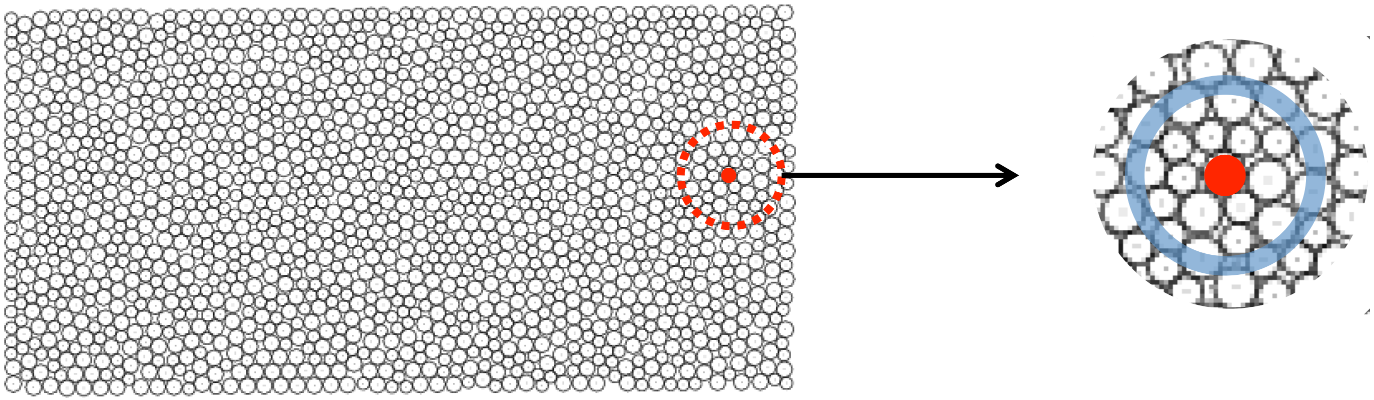

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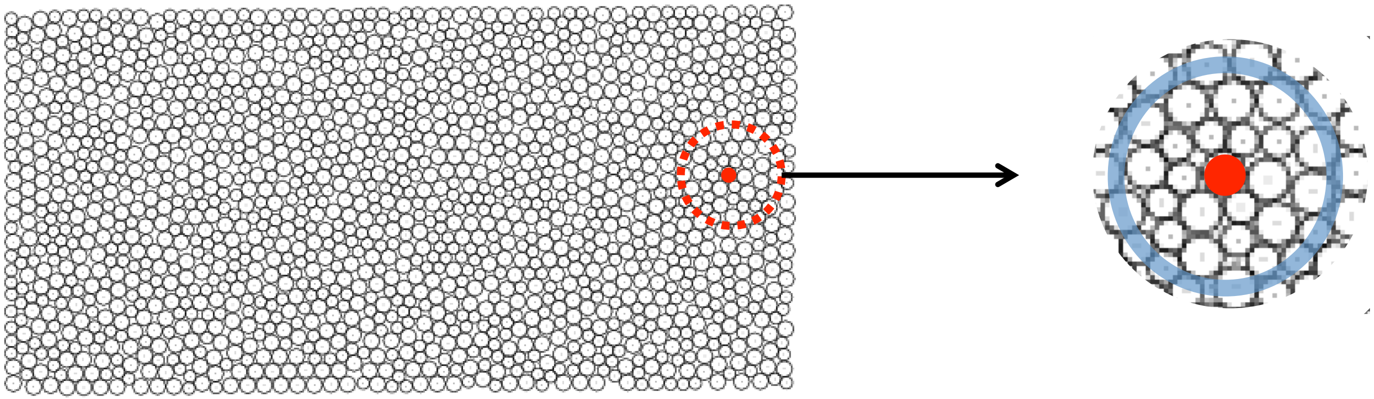

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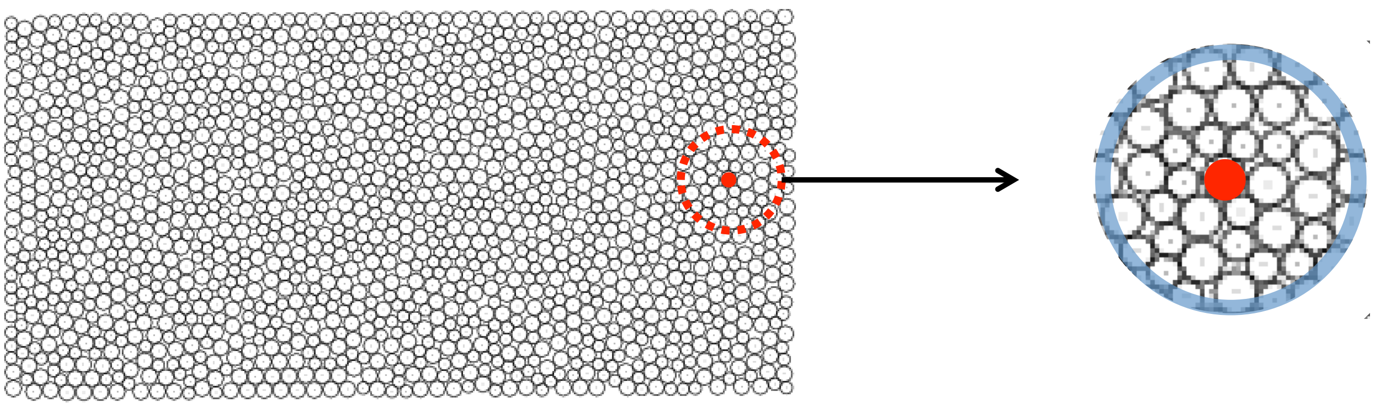

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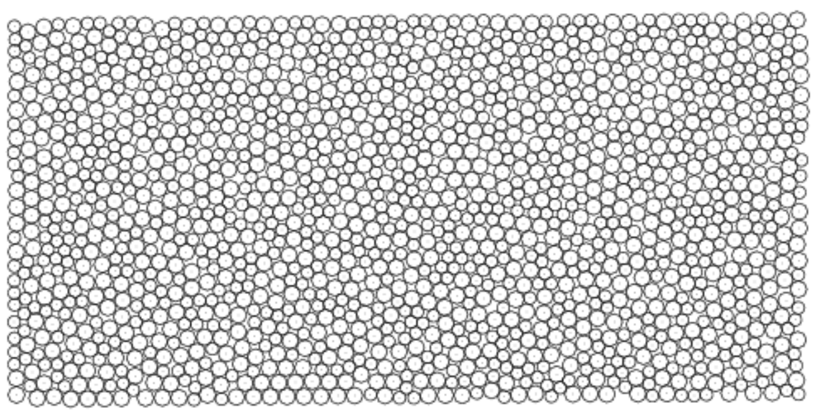
- calculate <u>many</u> descriptors for every particle's local environment
- observe the system and record plastic behavior



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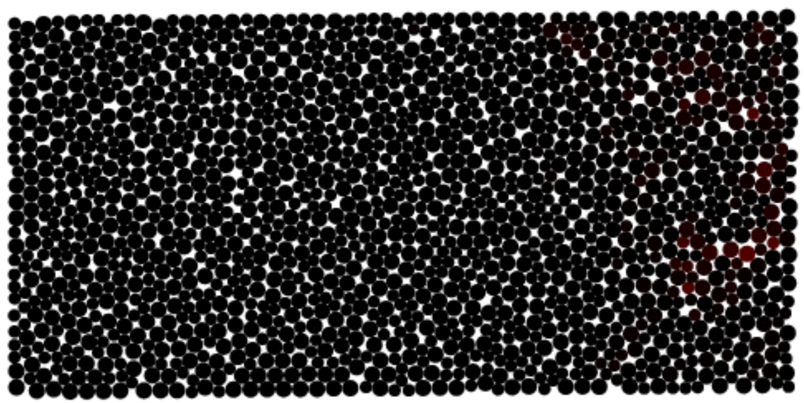

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- learn (from examples) the structural quantities that make up a soft spot

	Descriptors (t_0)	D^2_{Min} (t_0,ΔT)	Rearranged?
Particle 1	3.2,4.5,1.5	1.8	Yes
Particle 2	1.3,5.6,7.2	0.6	No
Particle 3	1.2,4.2,1.4	0.2	No
⋮	⋮	⋮	⋮

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Potential advantages of this method:

- Extremely fast, O(N) scaling
- Does not need vibrational modes
- The system does not need to be quenched
- Does not require the Hamiltonian

The local descriptors

- Calculate descriptors for each particle i
- They are sums over neighbors j and k of i
- Constants μ, λ, ζ and ξ are varied

$$G^1(i;\mu) = \frac{1}{\sqrt{2\pi\sigma^2}} \sum_j e^{-(R_{ij}-\mu)^2/2\sigma^2}$$

$$G^2(i;\xi,\lambda,\zeta) = \sum_{j,k} e^{-\xi(R_{ij}^2+R_{ik}^2+R_{jk}^2)}(1+\lambda\cos\theta_{ijk})^\zeta$$

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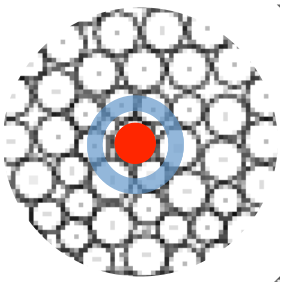

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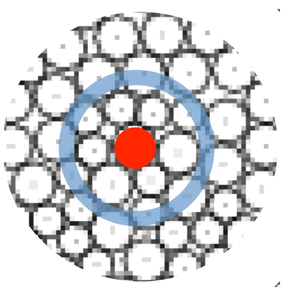

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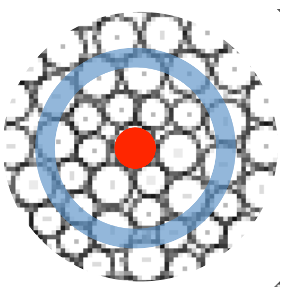

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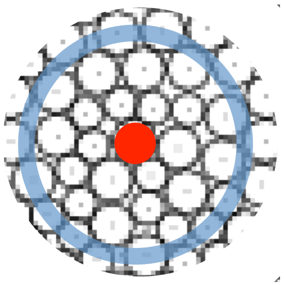

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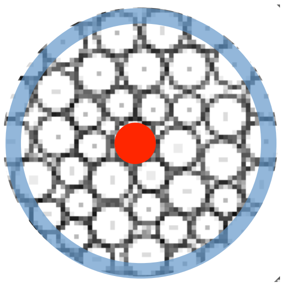

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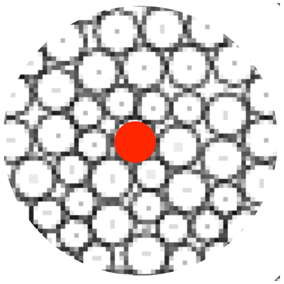

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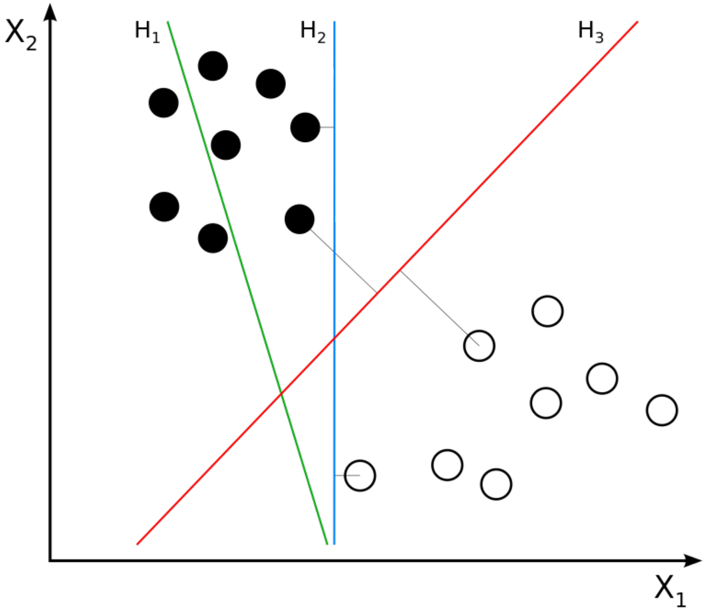
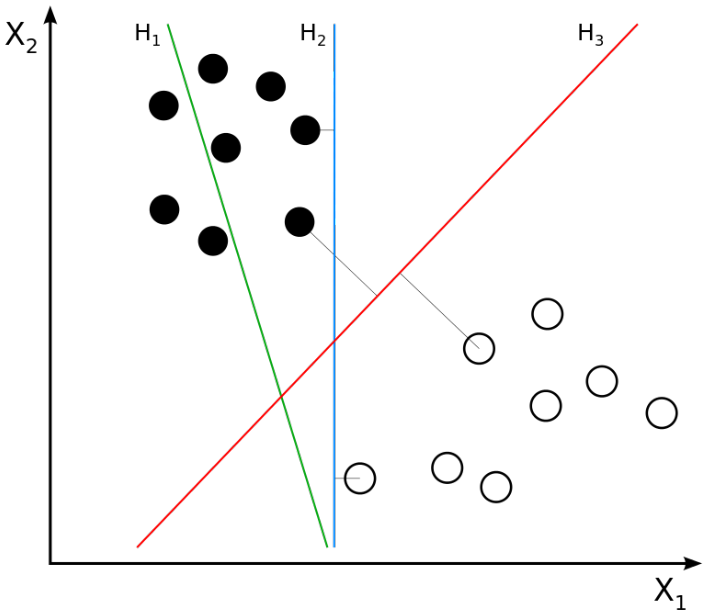
Support Vector Machines

- A simple supervised learning model.



Support Vector Machines

- A simple supervised learning model.
- Find the hyper-plane that separates the two different classes for future predictions



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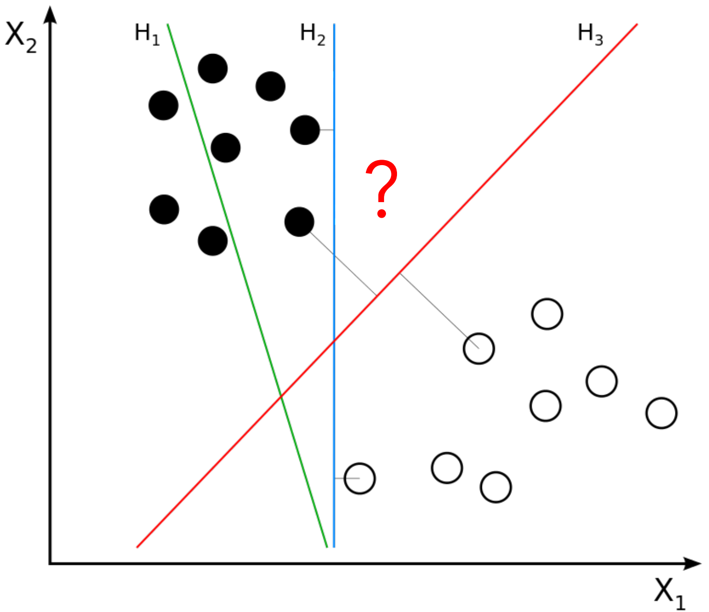

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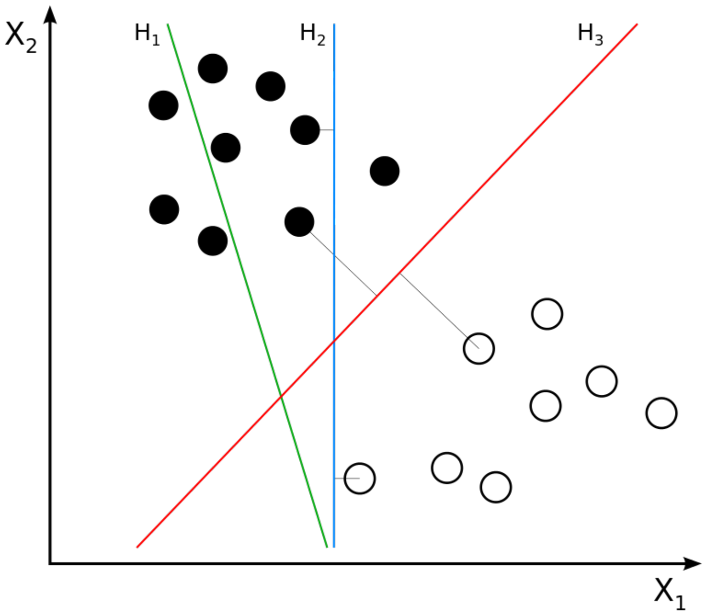

Sheared glass

Simulation of a 2D glass being sheared (LJ temperatures 0.1 to 0.4).

MD simulations done by Joerg Rottler.

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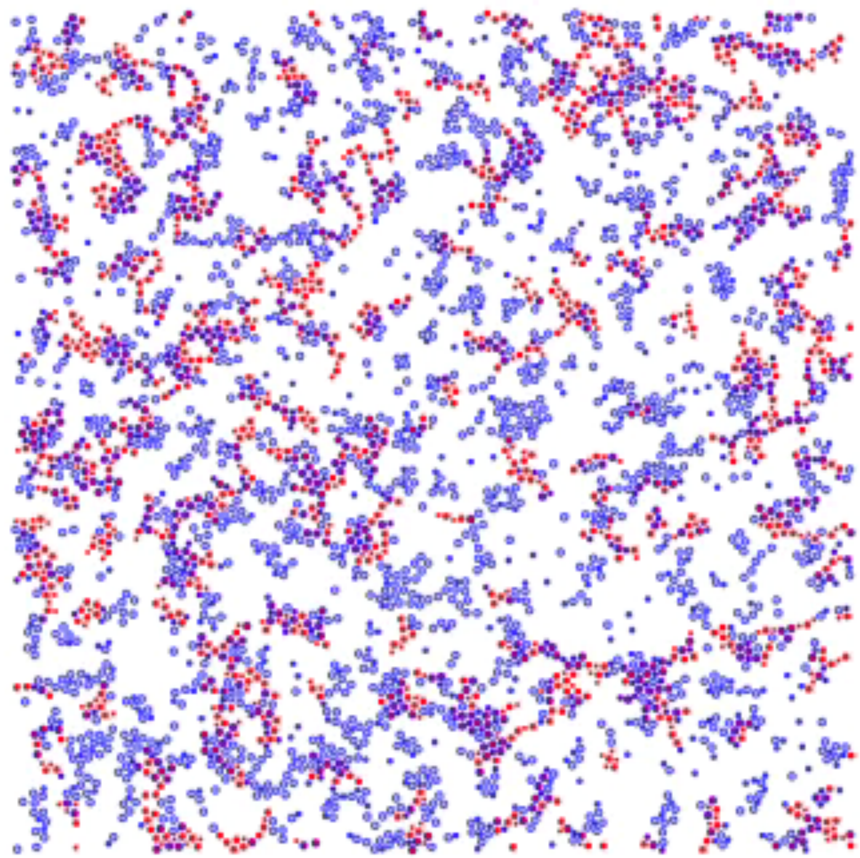
Blue →machine learning soft spots
Red → phonon method soft spots

Our soft spots are very robust until rearrangement.



Results (sheared system)

- For the simulation of a sheared glass, (for T = 0.1, 0.2, 0.3 and 0.4) we correctly predict
    - 78% of the rearrangements
    - with a 24% soft spot coverage

20K training samples
20M test samples
Tg = 0.33

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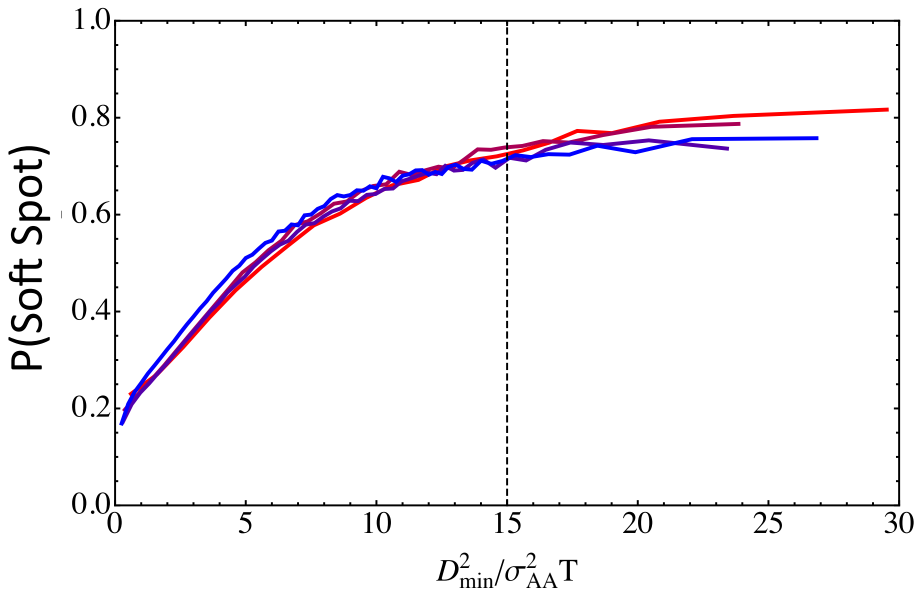

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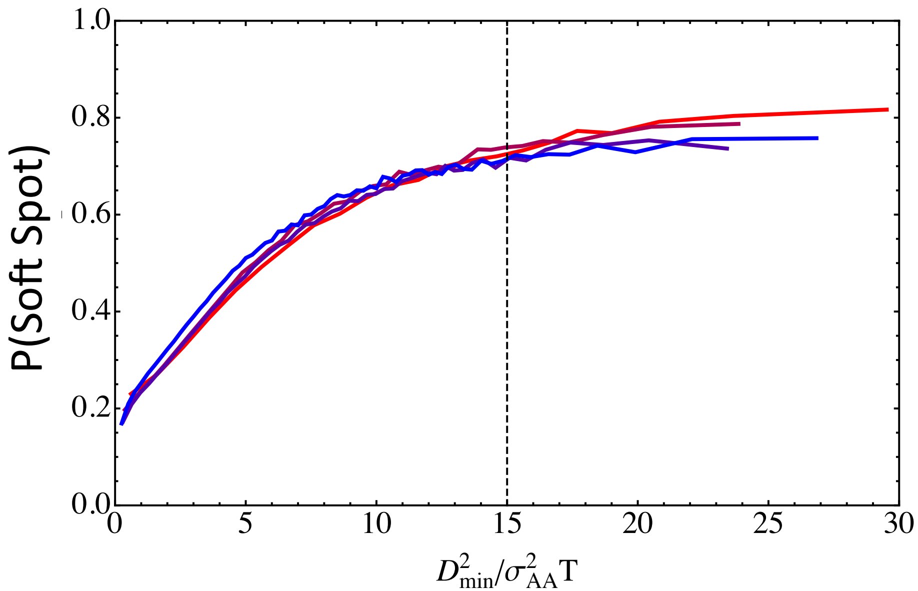

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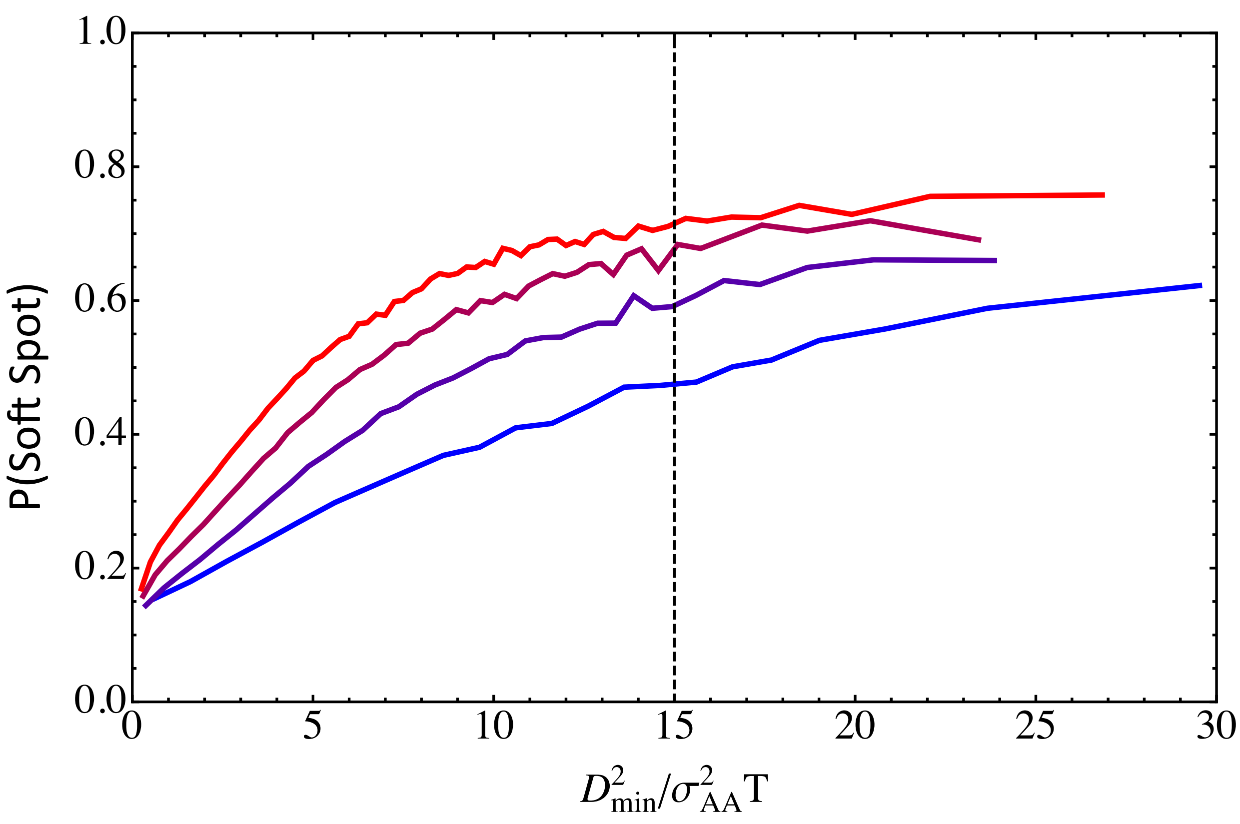
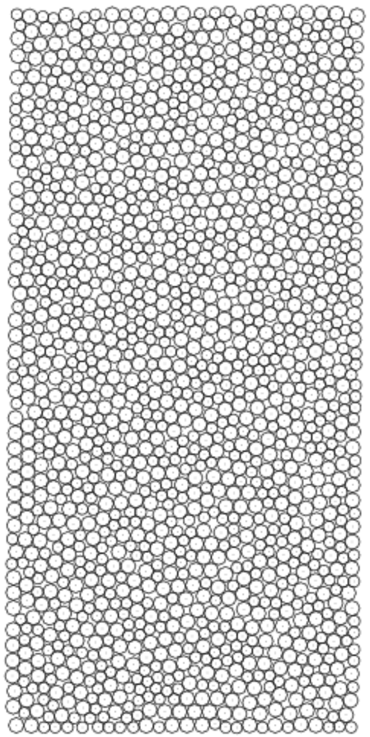
Soft spots predict rearrangements just as well for T>Tg as for T<Tg !!!!

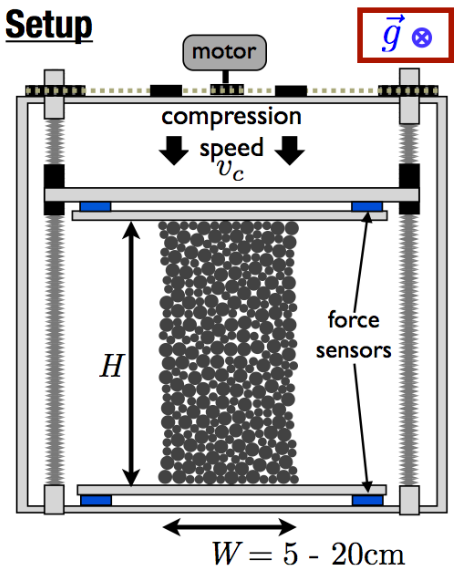
Results (sheared system)

- Results are transferable:
  train on T = 0.4, test on T = 0.1, 0.2, 0.3 and 0.4



Results (granular pillar)



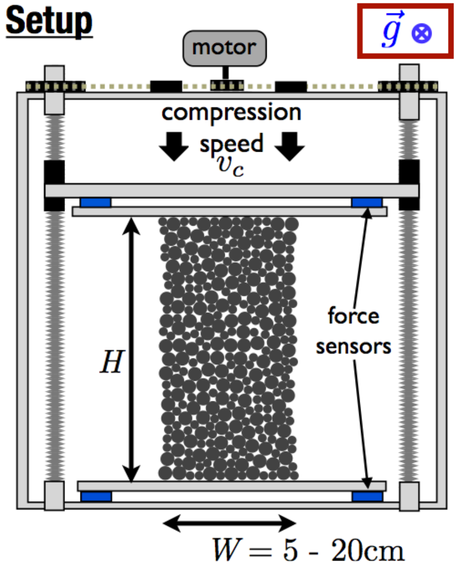


Cannot be analyzed with the phonon method!

Jennifer Rieser
Doug Durian

Results (granular pillar)

- Train on 10 pillars.
- For 10 test pillars, we correctly predict
  - 80% of the rearrangements
  - with a 22% soft spot coverage



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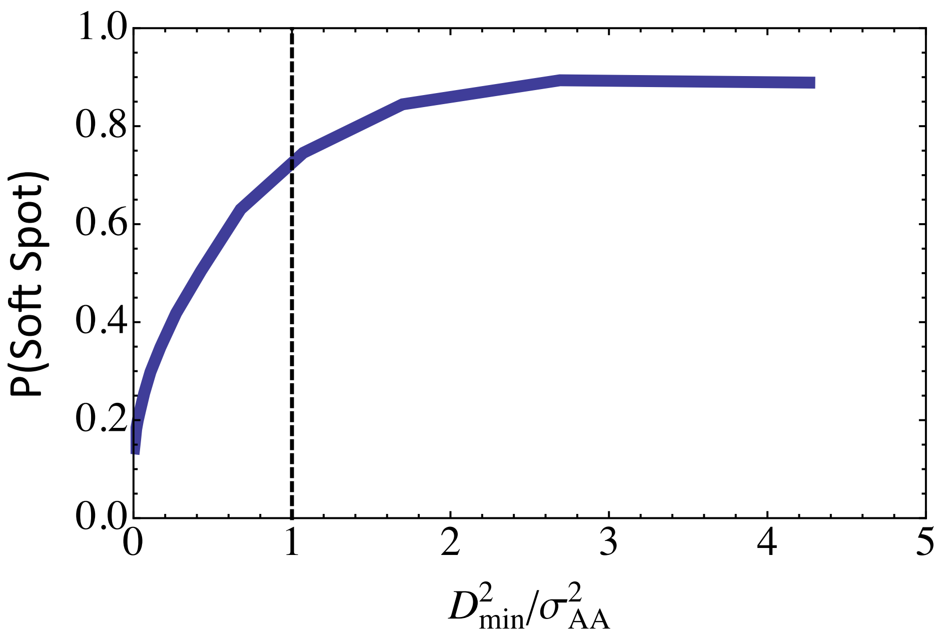

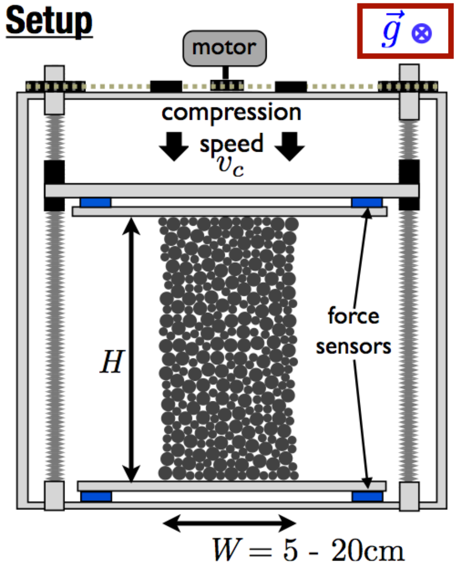

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- Can be applied to a large variety of systems (experimental/computational, quenched/thermal, 2D/3D).

Ongoing work

- What in the structure determines if a spot is soft?
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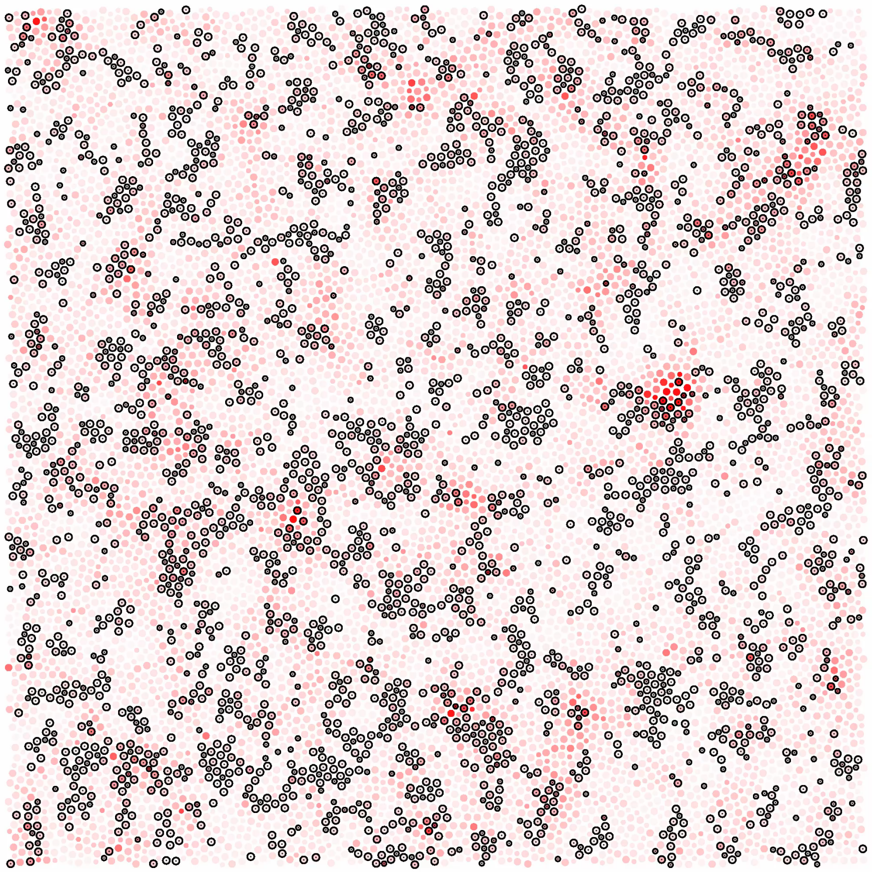

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