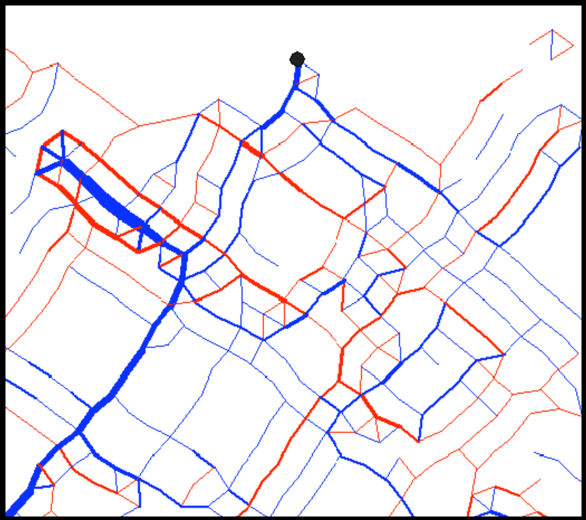
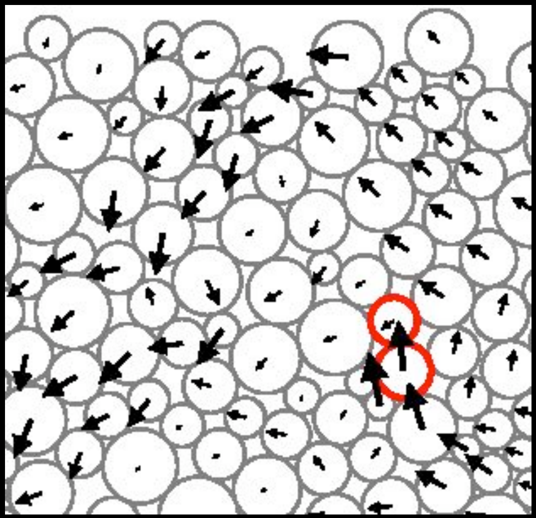
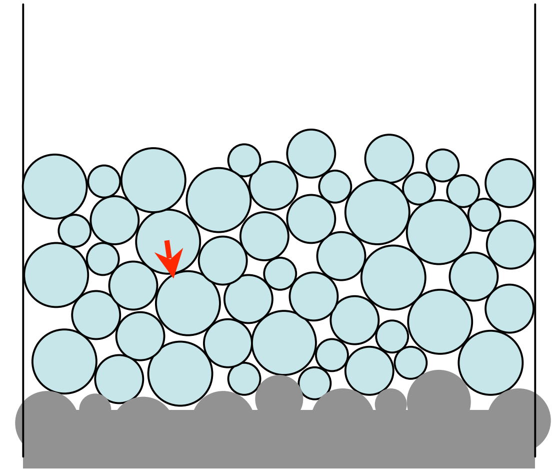
Indiana University, January 2007





T. Witten, University of Chicago

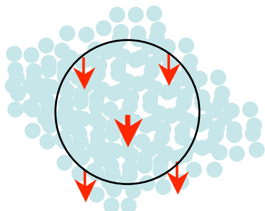
Force propagation in a simple solid: two pictures



Add circular beads to a container one by one

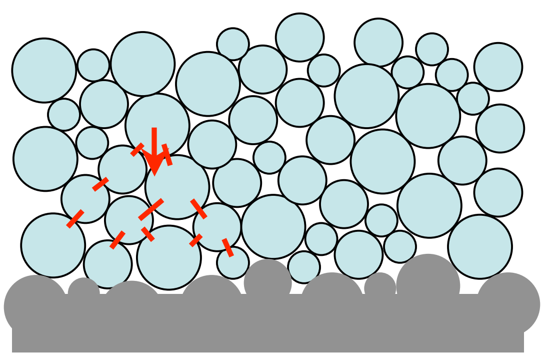
How does an added force reach the ground?

A: conventional solid: elasticity



Stresses above and below are *symmetric*

A: "bead-by-bead"



Stress go *asymmetrically* from source to boundary

Which picture is right?

Why study solids like this?

… kinetically *jammed:* each bead stays at the first place where it is stable

—unlike an equilibrium crystal

Important materials are kinetically jammed

Granular materials

Glasses: molecules get trapped in their positions as the liquid cools

Jammed vs equilibrium behavior is conceptually important

Forces in a jammed solid: solidity without elasticity

Alexei Tkachenko, David Head, Nagel group, Matthieu Wyart, T. Witten
University of Chicago

Anomalous force propagation

Minimal connectivity ⇒ *isostatic network*

⇒ Delicate stress balance is needed

⇒ Forces propagate along rays, not uniformly

Wild response to local perturbations ***free modes***

Anomalous vibration

Glasses have great excess of slow vibrational modes

Nagel-Liu jammed sphere pack has analogous slow modes

Wyart: why minimal connectivity entails anomalous slow modes

Implications

http://jfi.uchicago.edu/~tten/Glasperlenspiel/

Bead-by-bead packing makes minimal connectivity

Each bead was placed at a stable point. (no friction)
Adding one bead adds 2 contacts

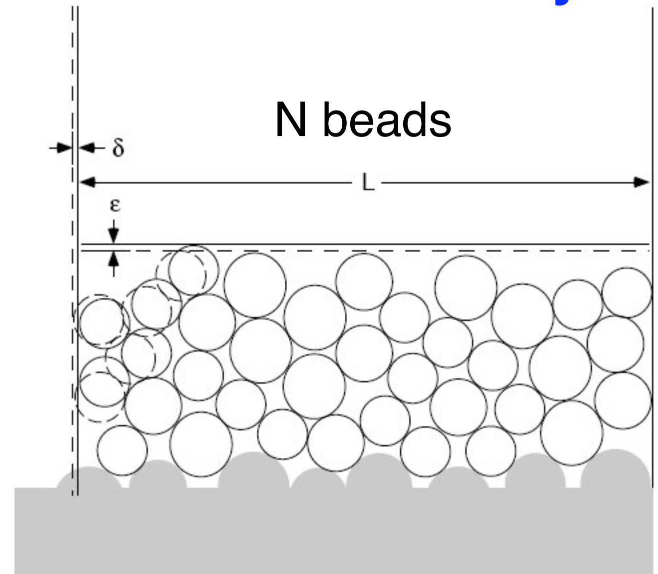
Number of contacts = 2N

Number of bead position variables (x, y) = 2N

Isostatic network:

contact constraints are just sufficient to determine bead positions.

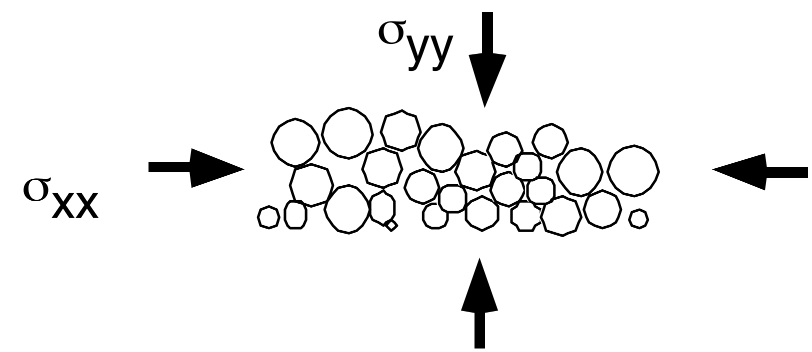
2N contact forces are just sufficient to balance forces on particles



Isostatic networks are *floppy*: if we rebuild the pile with walls shifted by δ,we create a deformation that costs no energy: a “free mode” where top shifts by ε

Internal stresses σ_{xx} σ_{yy}

must balance to avoid motion of free mode

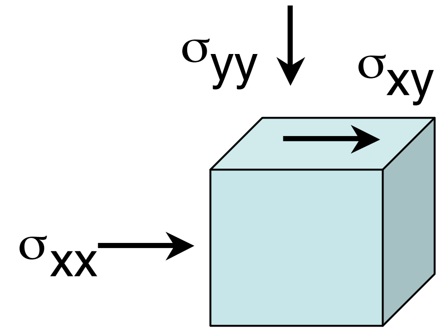


$$\delta\ \sigma_{xx} + \varepsilon\, \sigma_{yy} = 0$$

The medium must obey this *stress balance* condition.

Cf. Cates Bouchaud, Claudel, Wittmer, 1990’s

Stress-balanced medium has ray-like force propagation



Equilibrium: net force on box must vanish

Eg. If σ_{xx} changes with x, the other σ 's must change to compensate

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} = 0$$

and likewise

$$\frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{xy}}{\partial x} = 0$$

Stress balance condition allows use to find stress: $\delta\ \sigma_{xx} + \varepsilon\, \sigma_{yy} = 0$

Combining these three equations to eliminate all but σ_{xx},

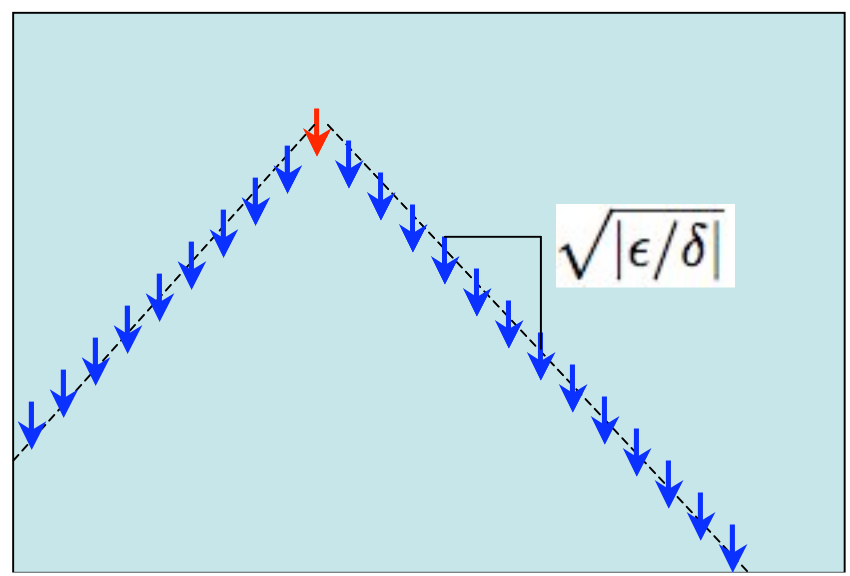
$$\frac{\partial^2 \sigma_{xx}}{\partial x^2} - \left|\frac{\delta}{\epsilon}\right| \frac{\partial^2 \sigma_{xx}}{\partial y^2} = 0$$

…*wave equation! So…*

Stress propagates from a point (x, y) like a pulse of *light at (x, t)*

Force is concentrated along oblique *rays*

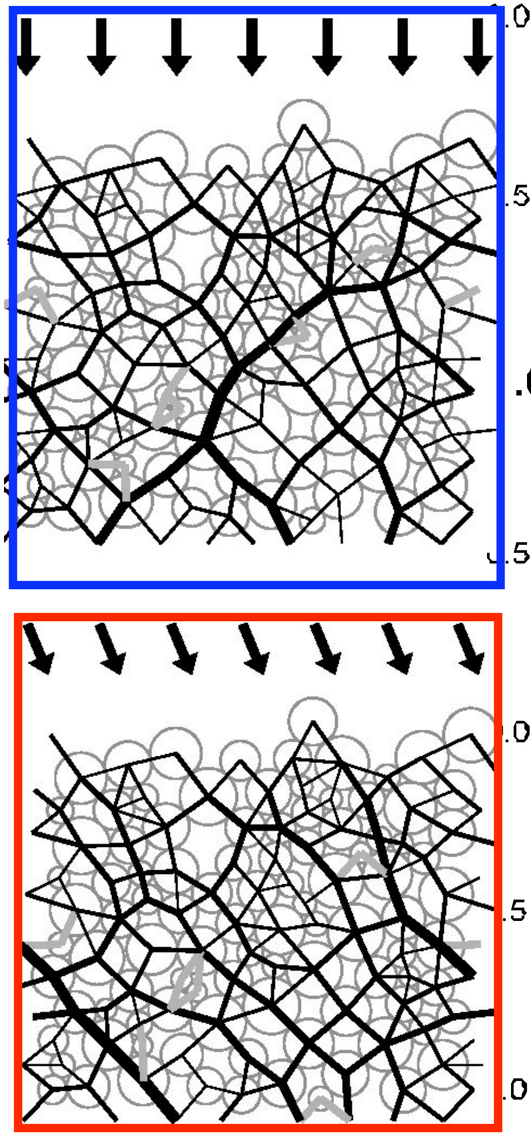
This oblique propagation is observed in sand piles

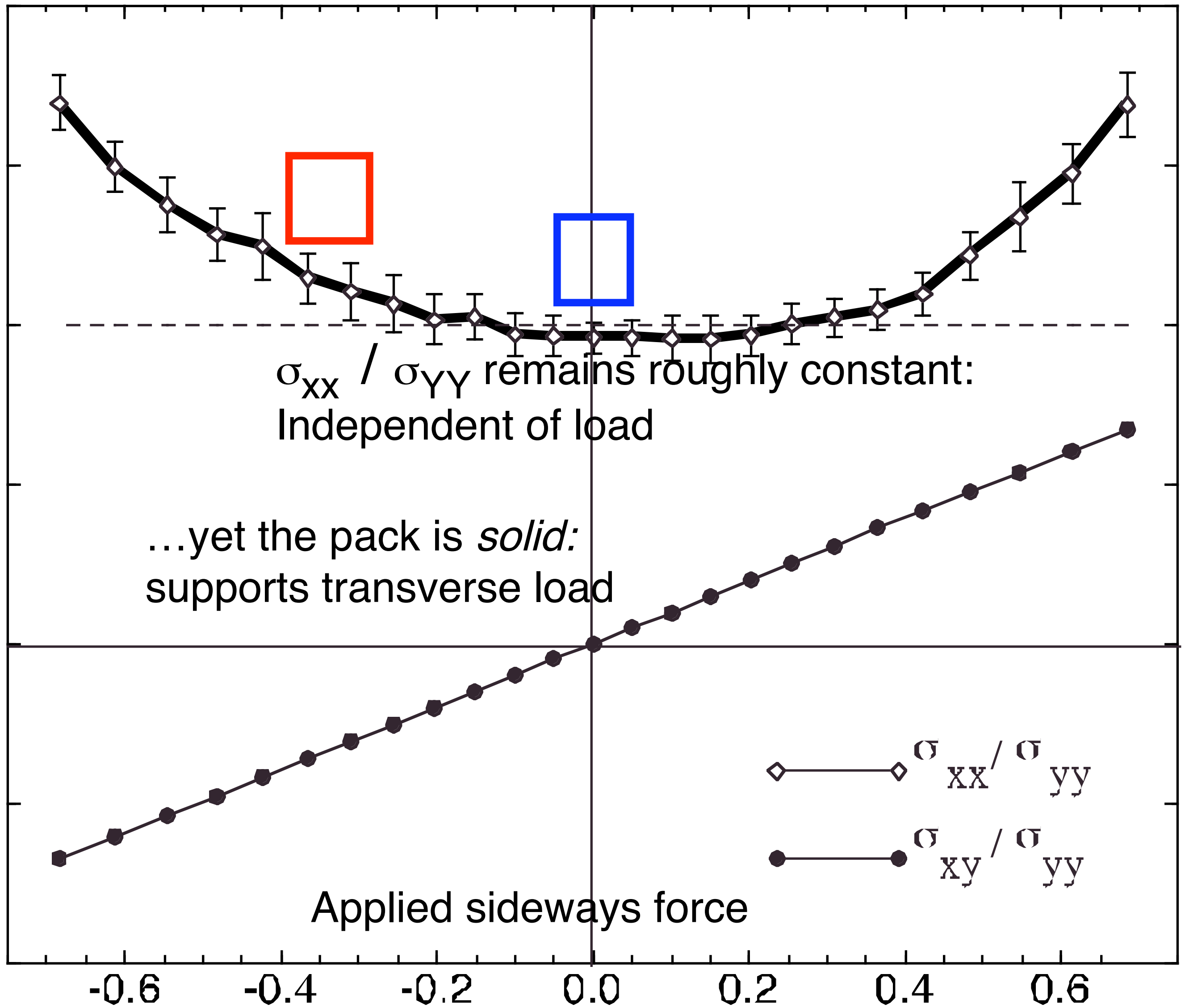


Simulation verifies stress balance condition

D. Head, A. Tkachenko, T. Witten

400 frictionless beads packed sequentially in 2-dimensional container
Beads are shifted slightly to make contact forces compressive





Simulation confirms ray-like propagation

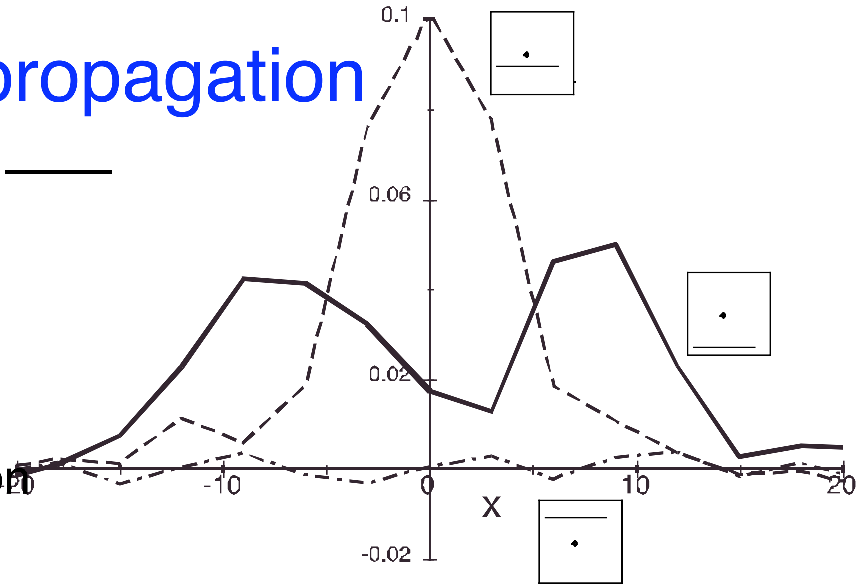
Extra force is applied at • and measured at ——

No force above •, as predicted

Unlike elastic material

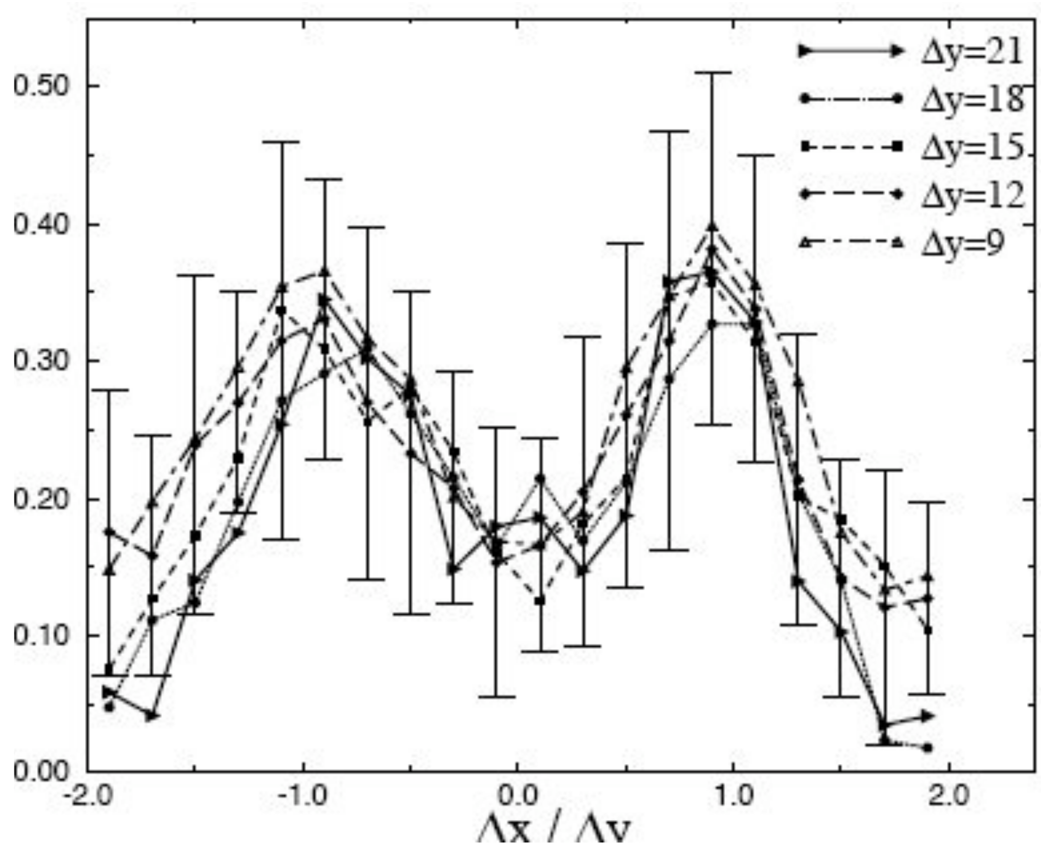
Force beneath is maximal in oblique direction

Not directly below •



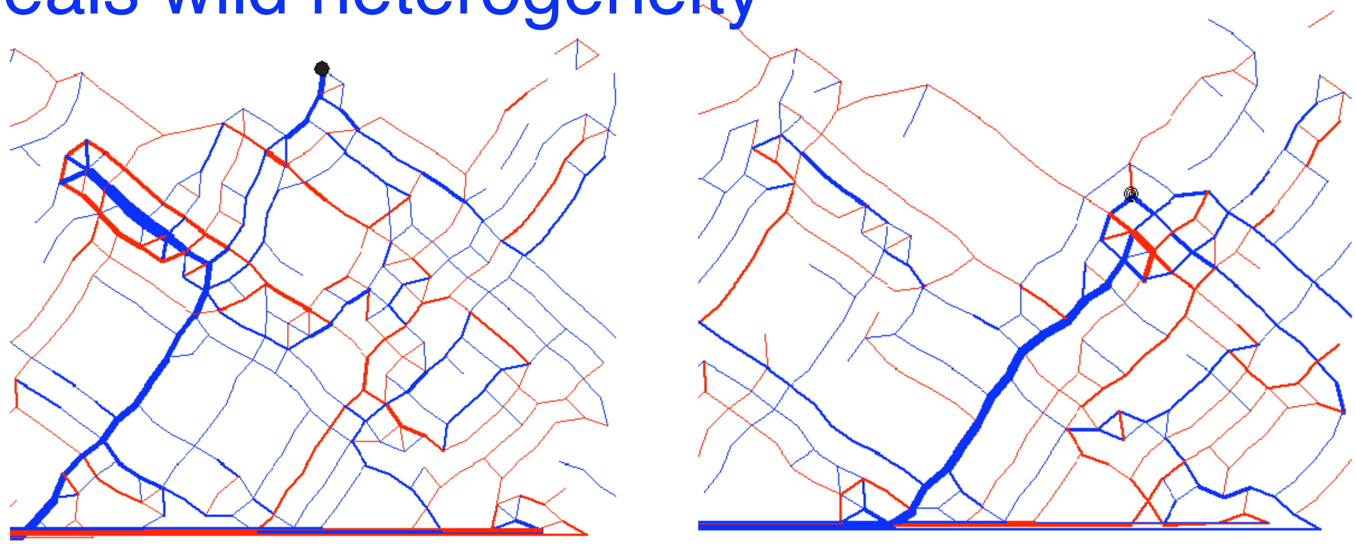
Locus of max force is along *oblique rays*

Averaged over 100 cases

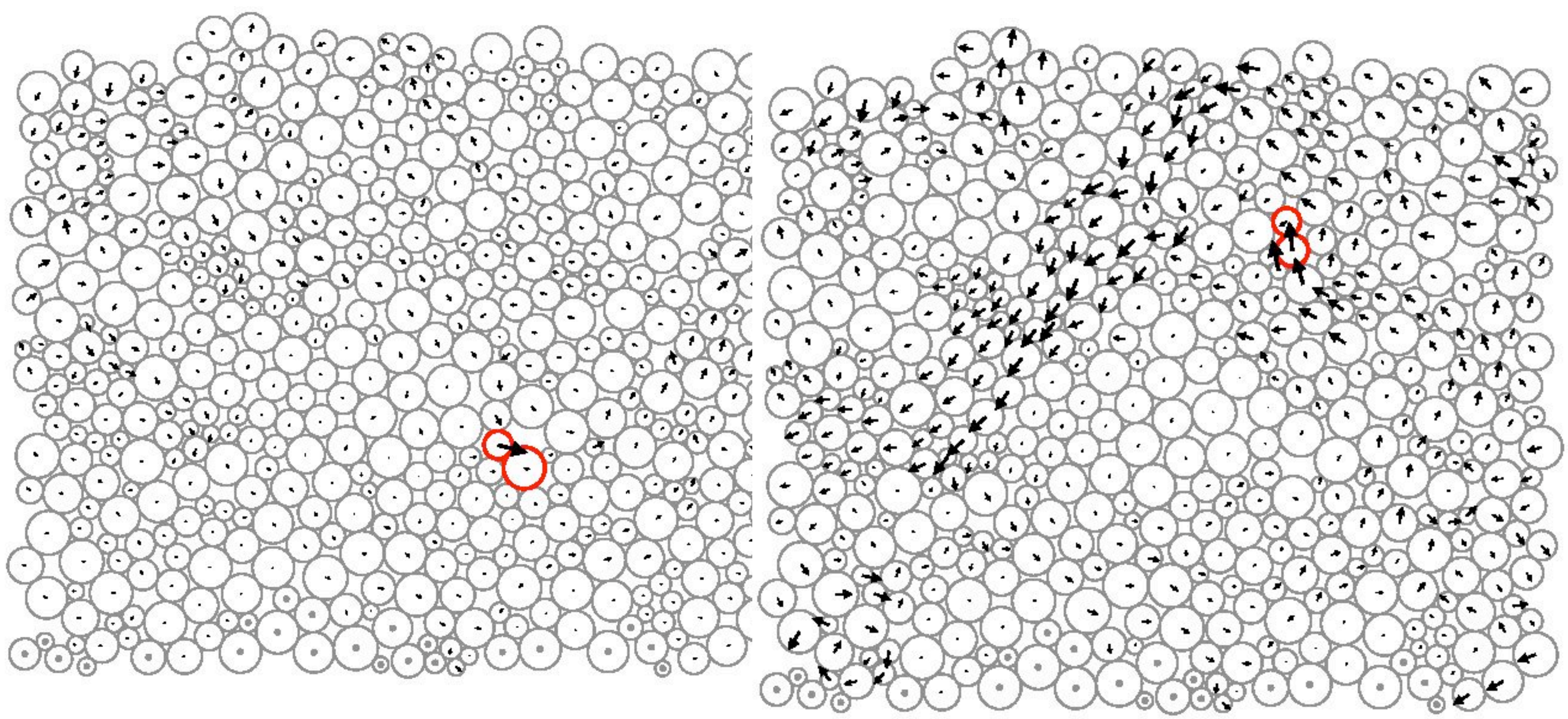


Simulation reveals wild heterogeneity

Lines show extra compressive/ tensile contact forces from extra bead force at •



Free modes resulting from removal of one contact

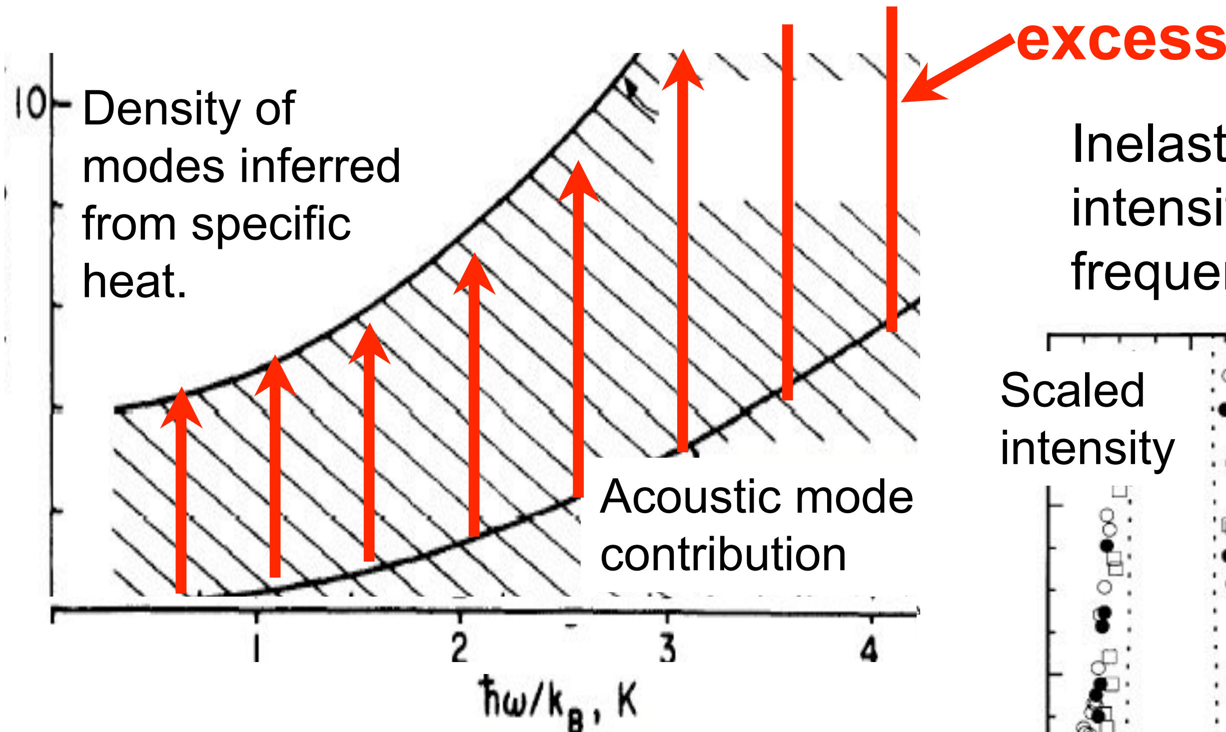


Summary: forces in jammed solids

- Solid is uniform, but forces are heterogeneous
- They propagate asymmetrically, unlike an elastic solid
- These properties arise from their minimal connectivity, which requires a delicate balance of stresses.

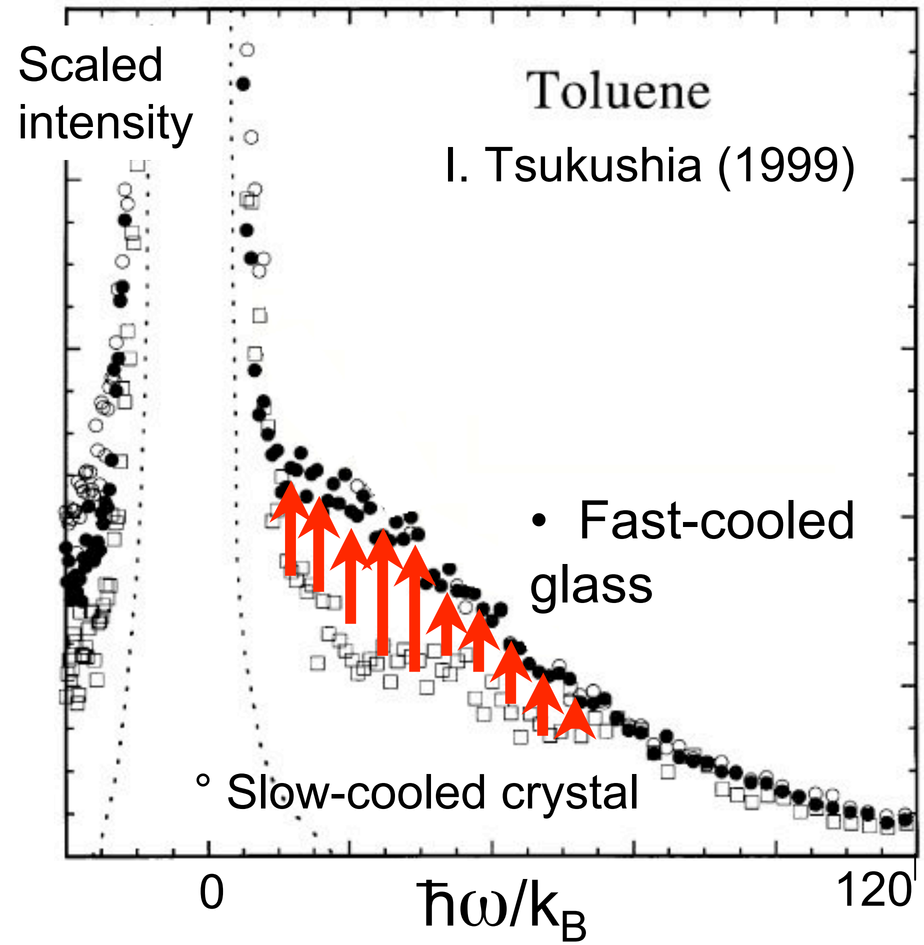
Vibrations: another anomalous feature of jammed materials

Fast-frozen liquids have excess slow vibrations



SiO_2, R. B. Stephens (1973)

Inelastic neutron scattering intensity measures vibrational frequency spectrum.



Fast-cooling makes extra low-frequency modes

Two potential reasons for excess low-frequency modes

DISORDER

Rapid freezing traps atoms in random positions

makes localized modes (doesn’t explain excess modes)

makes quantum tunneling modes (two-level systems)

MARGINAL TRAPPING

Freezing: motion stops as soon as atoms are trapped.

Thus system is in a state adjacent to mobile state: *marginally trapped.*

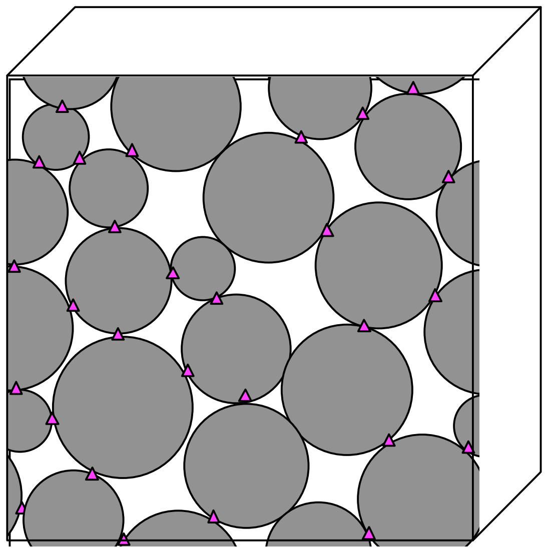
Marginally trapped states have just enough constraints to be trapped:
suggests *weak connectivity*

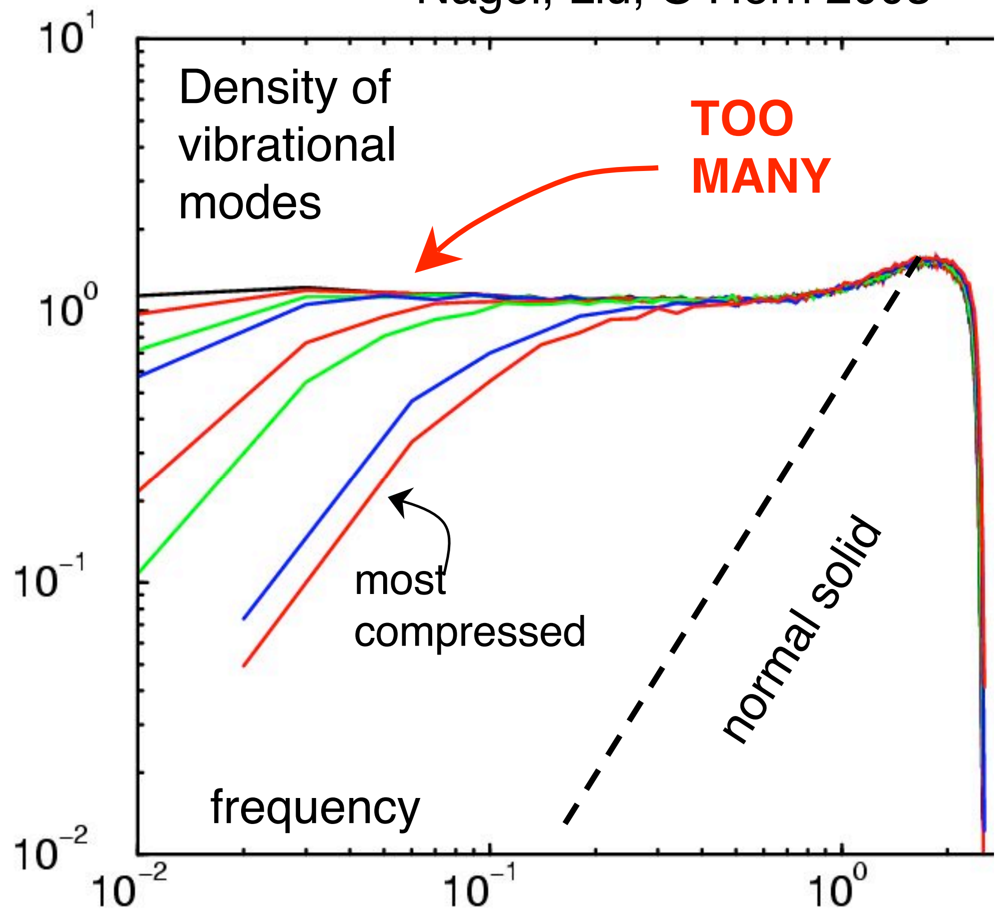
U of C: find an ideal case of marginal trapping:
adiabatically jammed spheres.

Squeeze-jammed grains ⇒excess slow vibrations

—Nagel, Liu, O'Hern 2003

simulated random packing





Why *constant* density of modes?

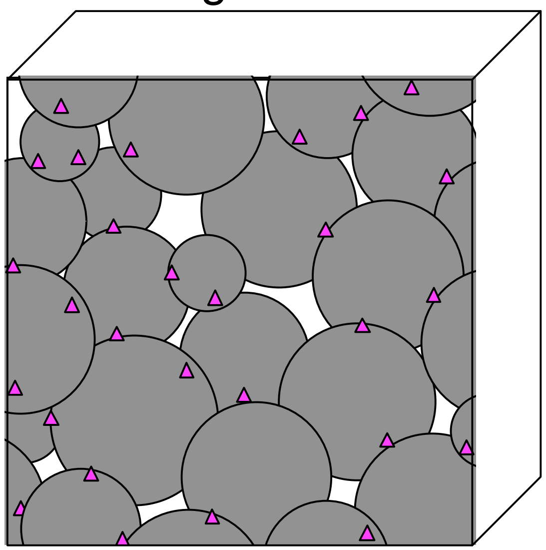
NORMAL SOLID : **acoustic modes** :: JAMMED SOLID : ?

O’Hern simulation: simple path to marginal jamming

Place soft frictionless spheres in a box at random at high density

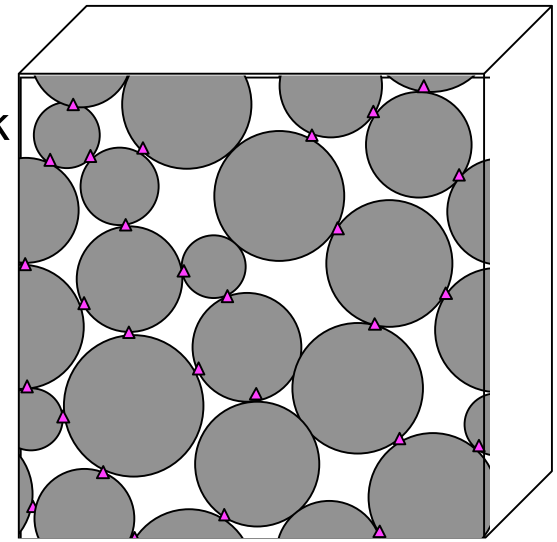
Find closest configuration of minimum energy

compressed



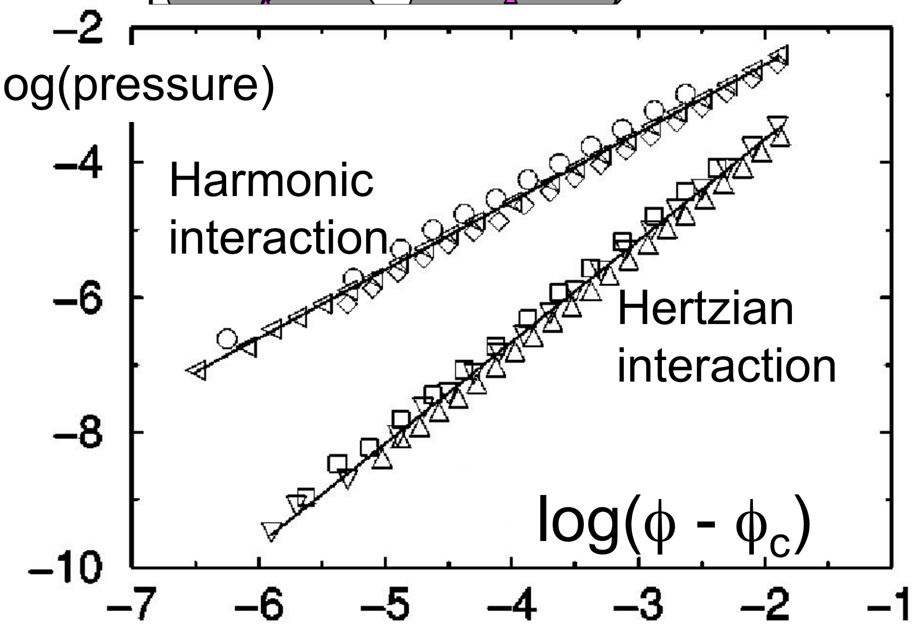
Slowly shrink spheres until pressure→0

Maintain equilibrium



marginally jammed

volume fraction $\phi \equiv \phi_c$



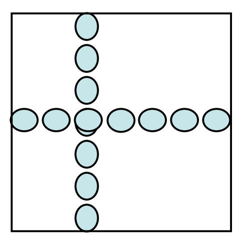
Scaling properties near jamming threshold ⇒ well characterized.

Marginally jammed particles are *isostatic*

- Threshold: some particles feel forces
- All N forced* particles must have *balanced* forces.
  - d N constraints on contact forces in d dimensions
  - Requires** *at least* d N contacts.
- Adiabatic jamming suggests *minimal* increase of contact number with compression
- … expect marginally jammed state to have just d N contacts: *isostatic*
  - *i.e. minimal number of contacts to fix particle positions.*
- *Observed in simulation*

* Unforced particles (floaters) appear to play a minor role

** Exceptional angles allow fewer contacts
not observed



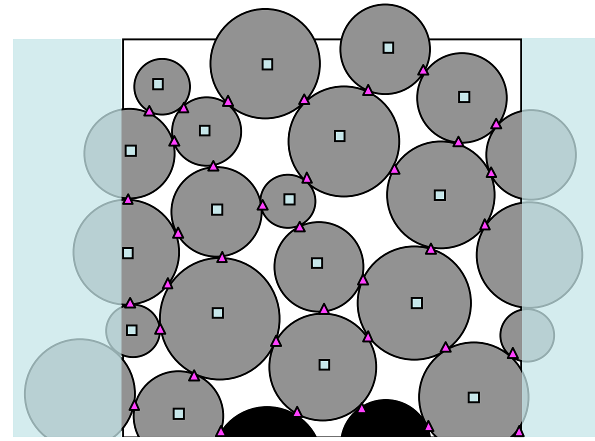
Nearly isostatic packings have *free modes*

ISOSTATIC …

just enough contacts N_c to fix all N particles

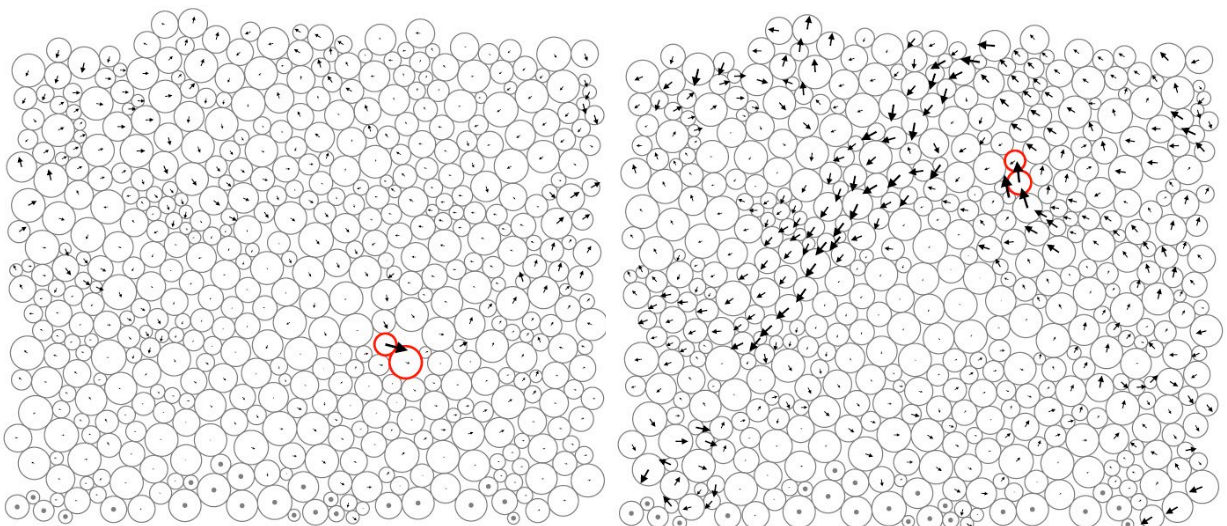
i.e. 2N contacts (in 2 dimensions)

N=18; N_c = 36

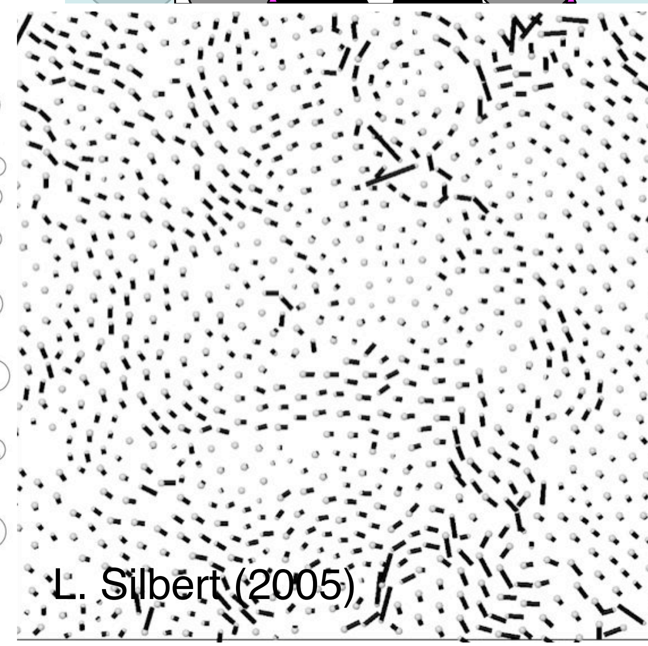


not quite jammed: ***remove*** **1** contact

…liberates **1** FREE MODE…e g



D. Head (2003)



L. Silbert (2005)

Free modes are … *extended* (like acoustic modes), *heterogeneous* (unlike acoustic).

Can 0-frequency **free** modes explain **low-frequency** modes of jammed system?

Energy → dynamical matrix → normal modes

Contact energy V for particles i and j: $V = 1/2\,(1 - r)^2$ $\quad r < 1$

particle diameters separation

…expressed in terms of displacement δR_i, δR_j, this gives energy

$$\delta E = \left\{ \frac{1}{4} \sum_{\langle ij \rangle} \left[({r_{ij}}^{eq} - 1)(\delta\vec{R}_j - \delta\vec{R}_i)^{\perp} \right]^2 \right\} + \frac{1}{2} \sum_{\langle ij \rangle} [(\delta\vec{R}_j - \delta\vec{R}_i) \cdot \vec{n}_{ij}]^2$$

…a quadratic form in the displacements:

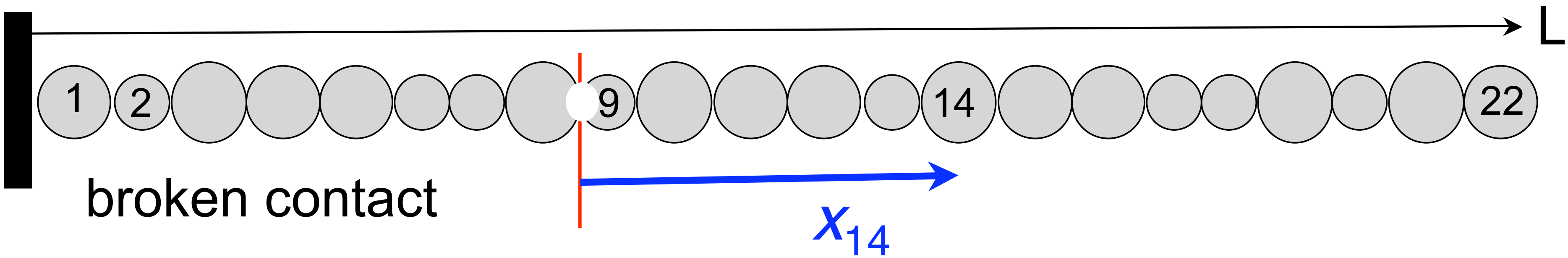
$\delta E = \langle \delta \mathbf{R} |\ M\ | \delta \mathbf{R} \rangle$ vector of all 3N displacements

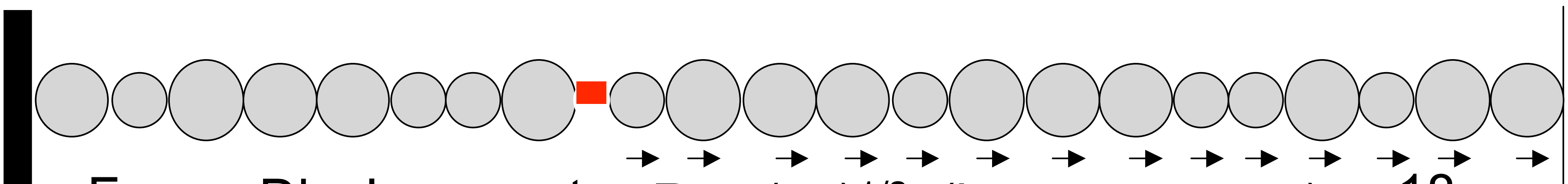
dynamical matrix

Eigenstates of *M* are the **normal modes;**
eigenvalues are **squared frequencies** ω^2 (for particles of mass 1)

Variational bound: for *any* displacement field $|\delta \mathbf{R}^*\rangle$ with $\langle \delta \mathbf{R}^* |\ 1\ | \delta \mathbf{R}^* \rangle = 1$
lowest eigenvalue $\omega_0^2 \leq \langle \delta \mathbf{R}^* |\ M\ | \delta \mathbf{R}^* \rangle$

Deforming a free mode can make a *slow* mode of low frequency



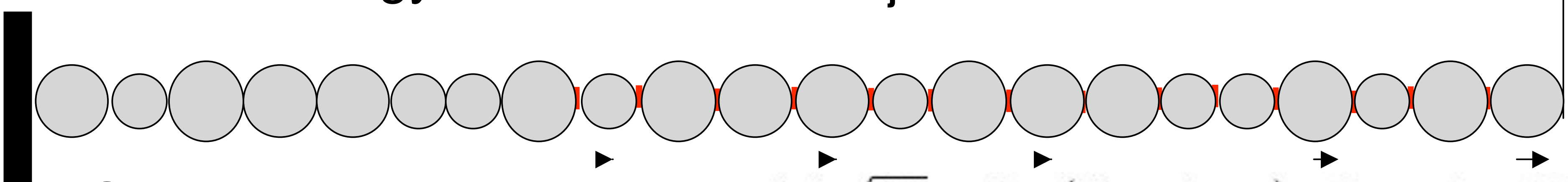


Free mode

Displacement: $\delta R_i = (18)^{1/2}$ $(i = 9, 10, \ldots 22)$

18 particles

Energy: $\delta E = \sum(\delta R_{j+1} - \delta R_i)^2 = 1/18$



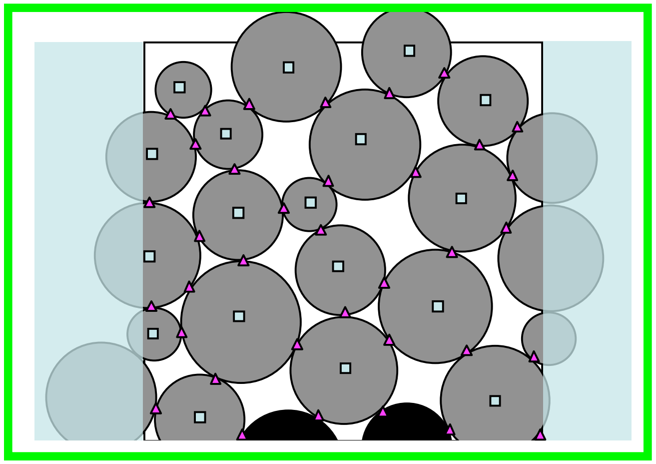
Slow mode

Displacement: $\delta R_i^* = 1/\sqrt{18}\ \ \sin\left(\frac{\pi}{2} x_i / x_{22}\right)\ \ (i = 9 \ldots 22)$

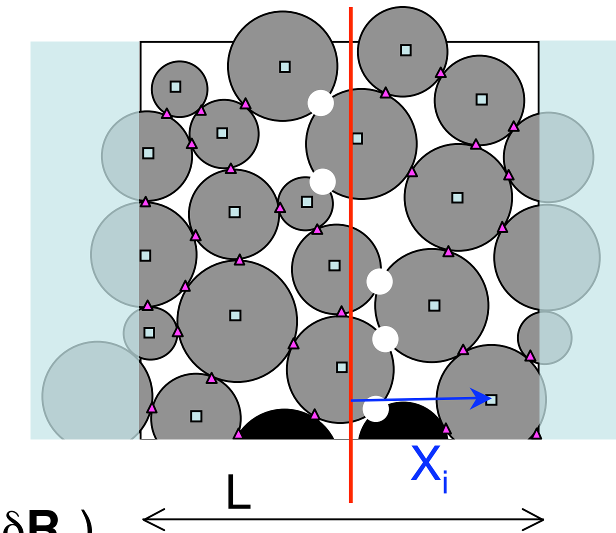
$$\delta E \simeq \sum_{j=9}^{22} \left(\frac{1}{\sqrt{18}} \times \frac{1}{18}\right)^2 = \frac{1}{18} \times 18 \times \left(\frac{1}{18}\right)^2$$

Energy ~ 1/L²; frequency ~ 1/L

Constructing slow modes of



from *free* modes of



1. Make an independent set of free modes ($\delta\mathbf{R}_1,\ldots\delta\mathbf{R}_5$).
   These create gaps (only) at the 5 contacts ○

2. Construct *trial modes* ($\delta\mathbf{R}^*_1,\ldots\delta\mathbf{R}^*_5$) from ($\delta\mathbf{R}_1,\ldots\delta\mathbf{R}_5$) to *close* these gaps

   E g, displacement of particle i for mode 1 $\quad \delta R^*_{1,i} = \delta R_{1,i}\ \sin(2\pi X_i/L)$

3. Select ($\delta\mathbf{R}_1,\ldots\delta\mathbf{R}_5$) so that ($\delta\mathbf{R}^*_1,\ldots\delta\mathbf{R}^*_5$) are *orthogonal.*

4. Trial modes have low energy, hence low average frequency $\omega(L)\sim 1/L$

   …about as low as lowest *acoustic* modes of these particles

Thus there are 5 **normal** modes with average frequency $< \omega(L)$

Trial modes account for excess slow modes

Lowest frequency modes:

For system size L (in 3D) there are $\mathcal{N}(L) \sim L^{2}$ trial modes

Their frequency $\omega_0(L) \sim 1/L$ as in a normal system.

The density of lowest modes $D_0(\omega) \sim \mathcal{N}/(\omega L^{3}) \sim L^{0}$ .... *as observed*

In d dimensions, there are $\mathcal{N}(L) \sim L^{d-1}$ trial modes; $D(\omega) \sim \mathcal{N}/(\omega L^{d}) \sim L^{0}$

Higher-frequency modes:

For subsystem of size L/2, this argument $\Rightarrow D(\omega) \approx D_0(\omega)$ up to $\omega(L/2) \approx 2\,\omega_0$

Extending to L $\approx$ few x particle size $\Rightarrow D(\omega) \approx D_0(\omega)$ for nonzero fraction of modes.

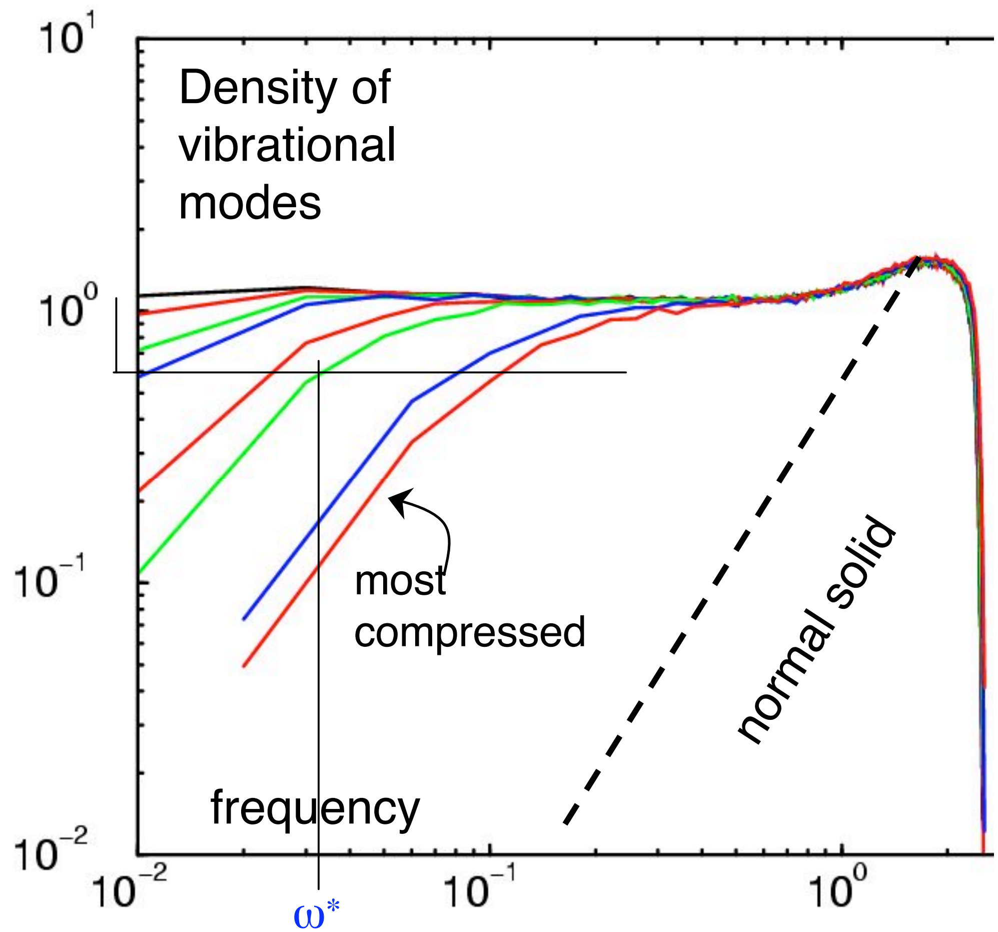
Deformed free mode picture agrees with marginally jammed simulation

- density of modes independent of frequency and system size for d=2, 3

- lowest normal modes are extended, heterogeneous …like free modes.

Can the deformed free modes explain the effects of *compression?*

i.e…how does crossover frequency ω^* Grow with compression?



How compression modifies the free modes

Compression adds contacts-per-particle **z** above the isostatic number **6** (in 3D)

Each new contact blocks one of the L^2 free modes

Number of added contacts ~ (z - 6) L^3

When (z - 6) L^3 > (constant) L^2, excess modes are removed

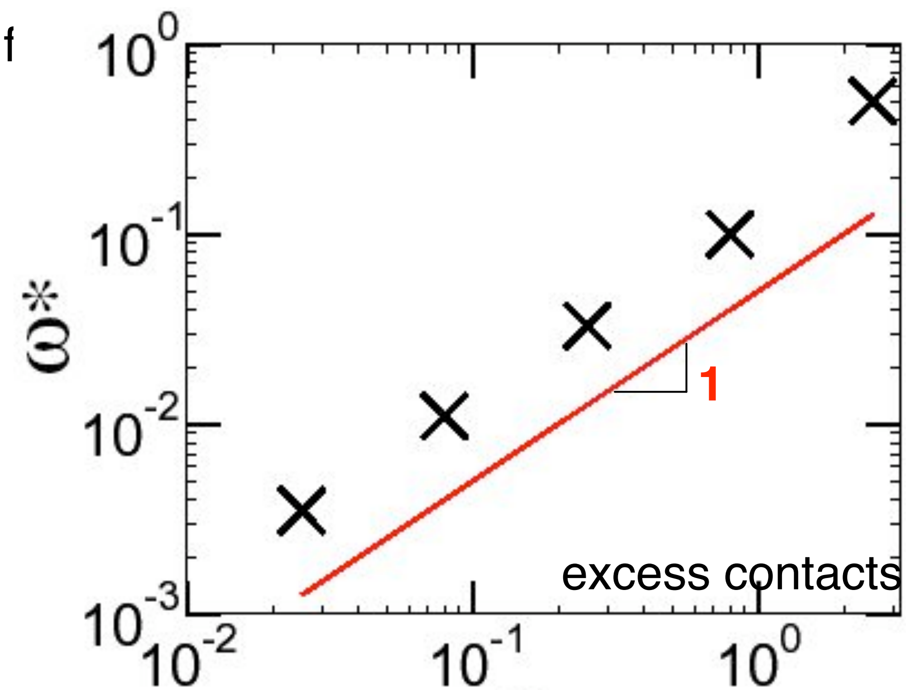
Still, small subregions of size L^* < (constant) /(z-6) are ~unperturbed

Thus the density $D(\omega)$ is ~ unperturbed f

$\omega > \omega^* \sim 1/L^* \sim (z\text{-}6)$

Simulation confirms prediction:

$\omega^* \propto$ excess contacts per particle



Further implications of deformed free modes

NORMAL SOLID	:	**acoustic modes**	::	JAMMED SOLID	:	deformed free modes

shown

How anomalous modes disappear under compression

Why shear modulus $\propto$ number of excess contacts

Why compression $(\phi - \phi_c) \propto$ (excess contacts)^2

hoped

Scaling of thermal conductivity, acoustic damping of jammed particles

How coupling of deformed free modes leads to *melting*.

Marginal jamming makes a new kind of solid

Internal forces

Supports transverse stress like a solid

Forces propagate differently from elastic solid

Dictated by required balance of internal stresses

Vibrational modes

Great excess of anomalous slow modes not possible in an elastic solid.

Relevance

Granular materials and glasses get trapped away from equilibrium state.

Marginal jamming is the extreme limit of maximal trapping.

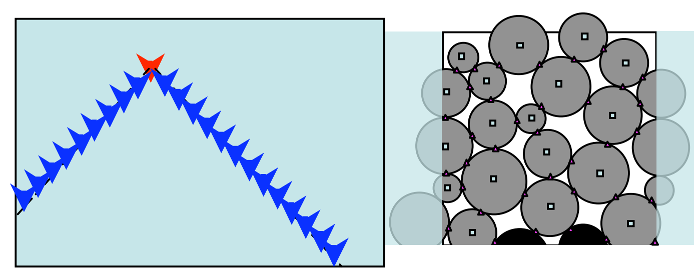
Questions

Does marginal jamming explain slow modes in real glasses?

Cf accepted picture: quantum mechanics

Do rays-like forces occur in isotropic jammed solids?

Can jamming ideas explain *melting?*



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