2254-18

Workshop on Sphere Packing and Amorphous Materials

25 - 29 July 2011

Soft Modes in Hard Sphere Glasses

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Soft Modes in
Hard Sphere Glasses

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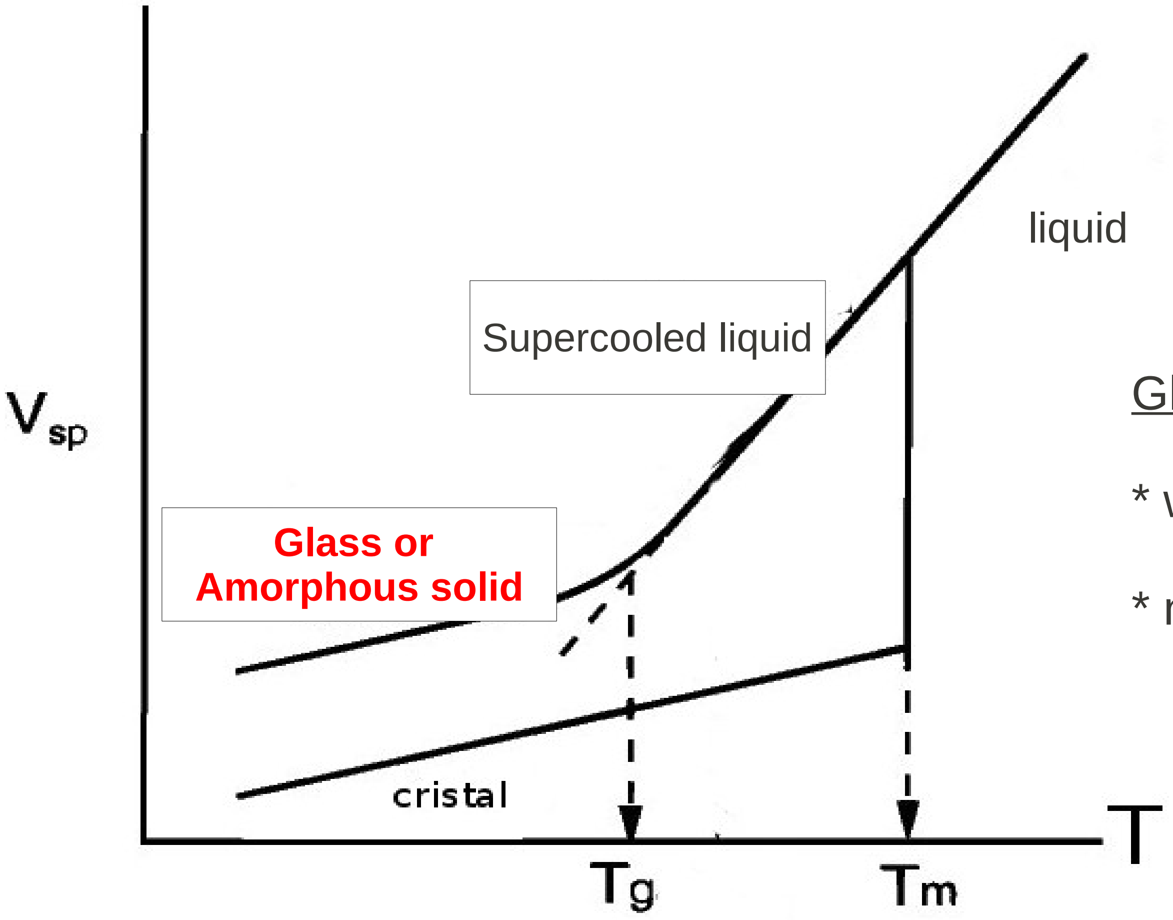
CAPES

Amorphous Solids

(structural glasses, granular material, colloids, dense emulsions)

How to obtain ?



Glass transition:

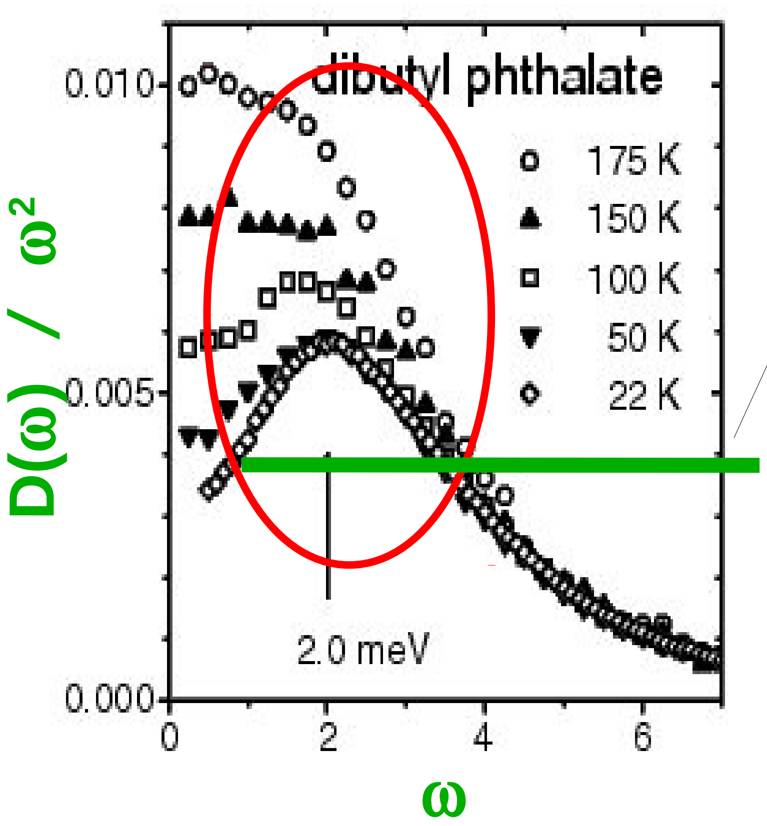
* without break of symetry between phases
(picture of a glass= picture of a liquid)
* no divergent static lengh scale

Amorphous solids have different behaviors compared to crystals

- properties of transport, force propagation
- Vibrational density of states $D(\omega) \equiv N(\omega) / V \omega$

``**Boson Peak**"

excess of modes of low frequency



In continuous solids :

$D(\omega) \sim \omega^2$ *Debye*

phonons are plane-waves

$\Rightarrow$ Nature of these modes in glasses ?

Outline of this presentation

- Vibrations in amorphous solids

- Vibrations in hard sphere glasses

    - How to compute the vibrational modes

    - What can we learn from them

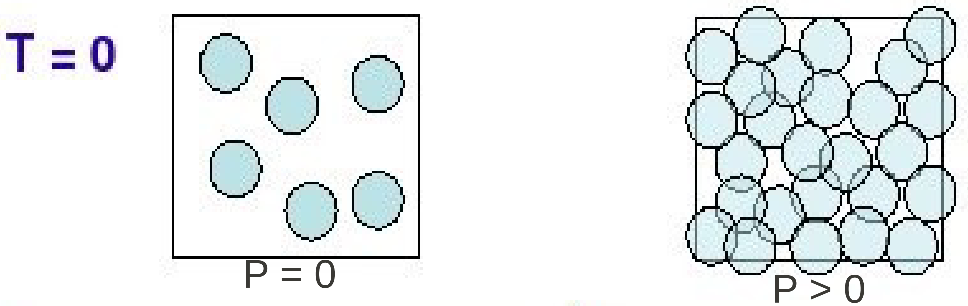
- Generalized isostaticity and avalanches

Model of amorphous solid

(O’hern, Silbert, Liu, Nagel, 2003)

soft spheres

- repulsive interaction,
- short range



$\phi = \phi_J$

(p→0)

jamming transition

$z = z_c$; $z_c = 2d$

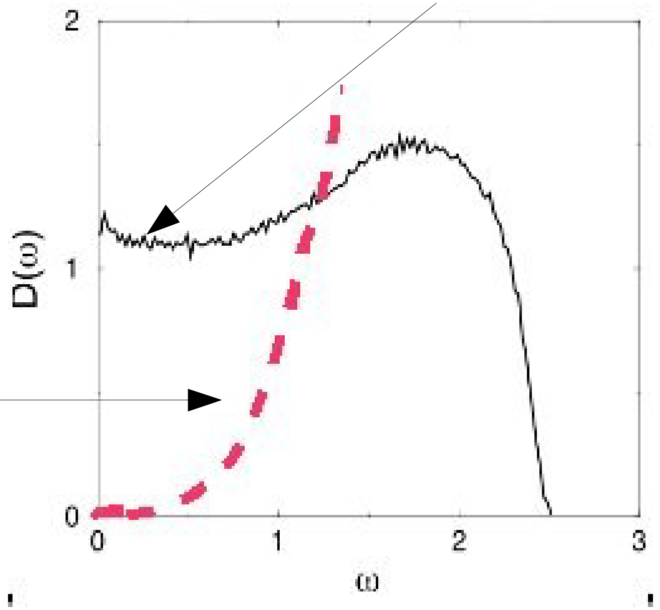
isostatic limit

in crystal: z=6(2d) ; =12(3d)

inherent difference between amorphous and crystals

excess of modes

Debye

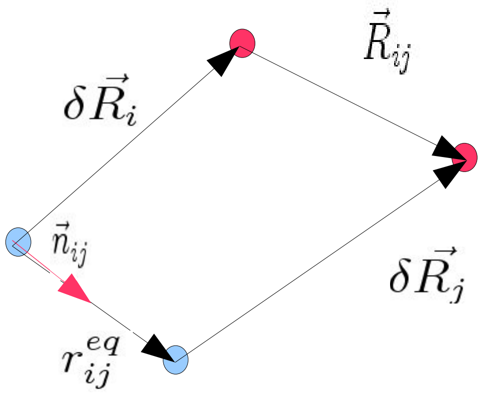


z : microscopic key parameter to describe vibrational properties in amorphous

Vibrations in amorphous solids

- **A** mechanical stability of a solid can be studied through its vibrational modes
- **B** rigidity & soft modes
- **C** Effect of the pre-stress term

mechanical stability of a solid can be studied through its vibrational modes



$$\delta E = \sum_{ij} V'(r^{eq}_{ij})\delta r_{ij} + \frac{1}{2}\sum_{ij} V''(r^{eq}_{ij})\delta r^2_{ij} + \mathcal{O}(dr^3_{ij})$$

$$\delta r_{ij} = ||\vec{R}_{ij}|| - ||\vec{r}^{eq}_{ij}|| = (\delta\vec{R}_j - \delta\vec{R}_i).\vec{n}_{ij} + \frac{[(\delta\vec{R}_j - \delta\vec{R}_i)^{\perp}]^2}{2r^{eq}_{ij}} + O(\delta\vec{R}^3)$$

(Alexander, RMP, 1999)

$$\boxed{\delta E = [\sum_{ij} V'(r^{eq}_{ij})\frac{[(\delta\vec{R}_j - \delta\vec{R}_i)^{\perp}]^2}{2r^{eq}_{ij}}] + \frac{1}{2}V''(r^{eq}_{ij})[(\delta\vec{R}_j - \delta\vec{R}_i).\vec{n}_{ij}]^2 + O(\vec{R}^3)}$$

$$\Downarrow$$

$$\boxed{\delta E = \langle \delta\mathbf{R}|\mathcal{M}|\delta\mathbf{R}\rangle}$$

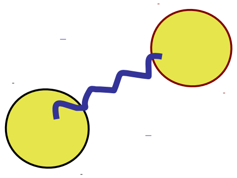
dynamic matrix

dN eigenvectors: **vibracional modes**

eigenvalues λ: **frequencies ω^2**

$e^{i\omega t} \Rightarrow$
ω real ⇒ *stable* mode ⇒ **$\omega > 0$**
ω imag ⇒ *unstable* mode ⇒ **$\omega < 0$**

rigidity & soft modes -- Maxwell



What garantees the rigidity of a system ?

$$\delta E = \frac{\kappa}{2}\sum_{\langle ij\rangle}[(\delta\vec{R}_j - \delta\vec{R}_i).\vec{n}_{ij}]^2 \longrightarrow$$

if $\delta E = 0$, system is NOT rigid
(Soft Mode)

\# constraints: N_c

\# degrees of fredom: Nd

$\longrightarrow$

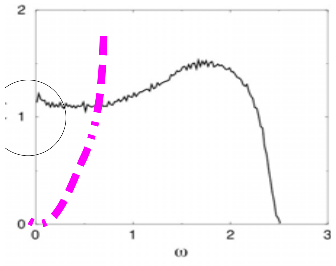
In order to *not* exist a solution:

$$\mathbf{N_c > Nd}$$

$$\boxed{z = 2\,N_c\,/\,N \;\geq 2d}$$

z_c=2d ***isostatic***

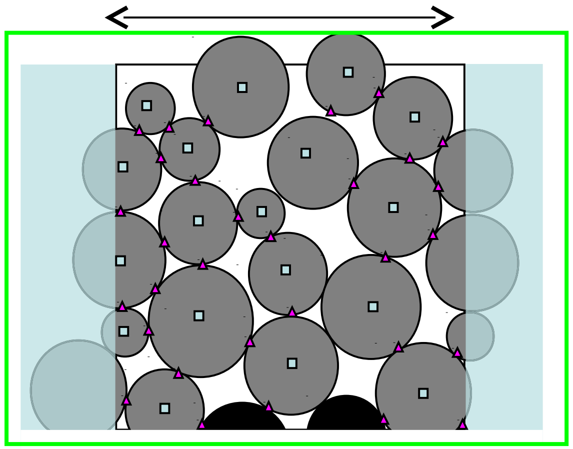
marginal rigidity

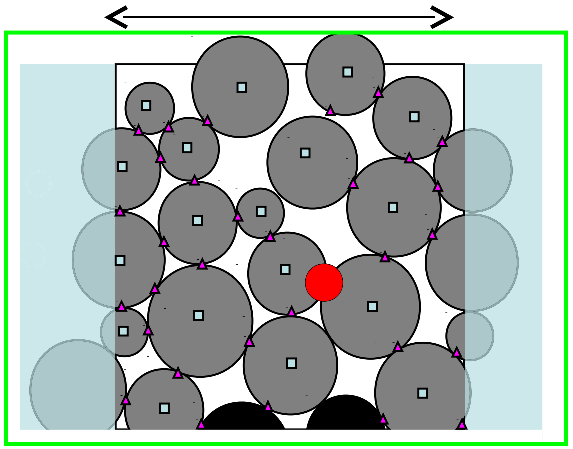


Excess of modes and marginal stability

- *“just” rigid:* ***remove 1*** *contacts …generates* ***1*** *soft mode*

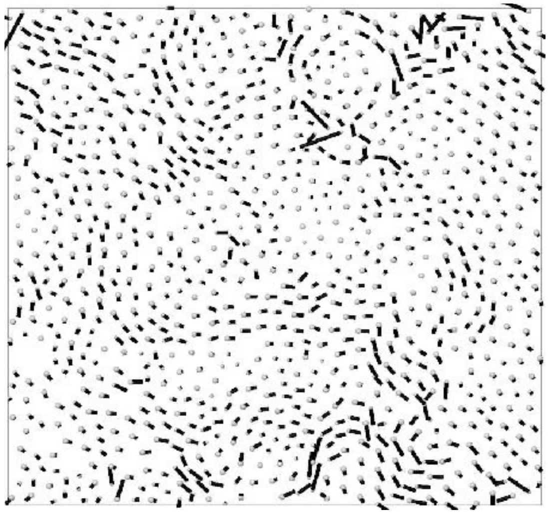
Original system





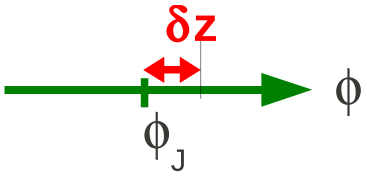
soft mode:
extended,
heterogeneous

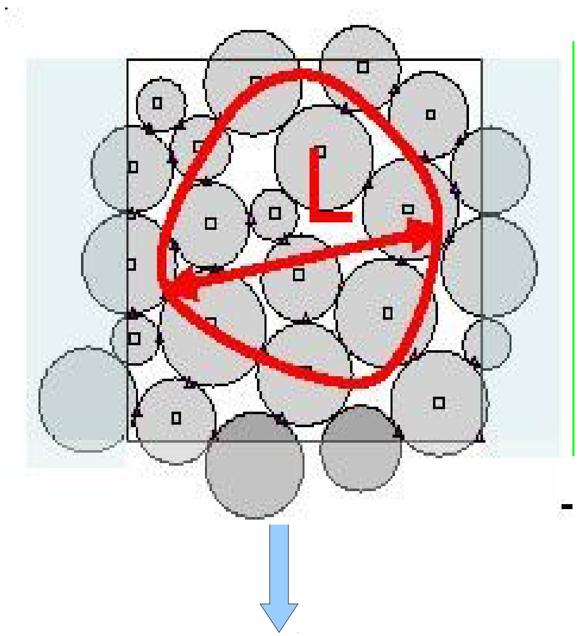
$z=z_c$ ⇒ marginally rigid



(Wyart, Nagel, Witten, 2005)

Modes of the original system



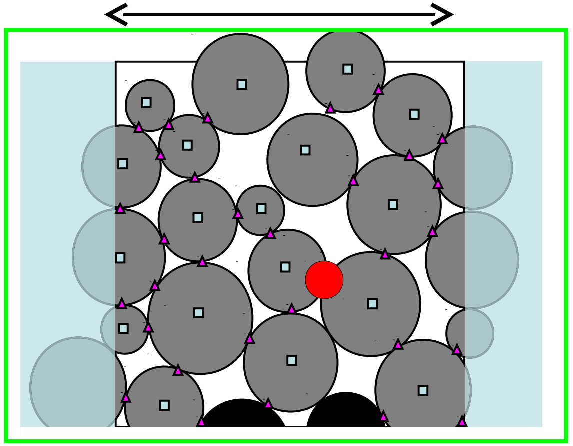


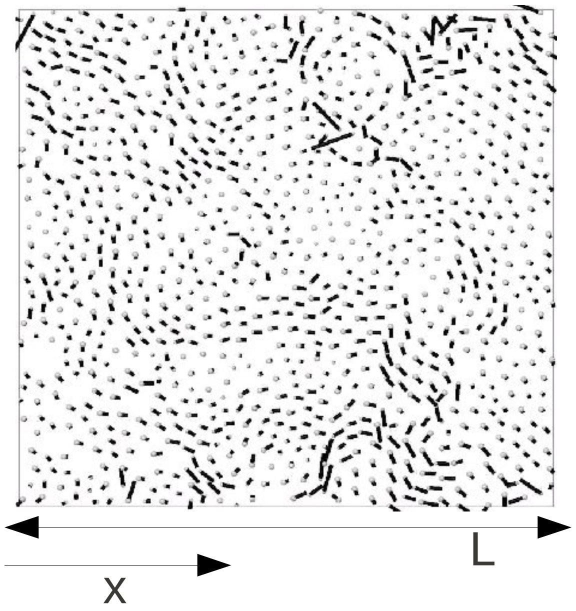
anomalous modes:

soft modes modulated by sin(x/L)

- ✔ $\omega^* \sim B^{1/2}\,\delta z$
- ✔ extension $L^* \sim \delta z^{-1}$

$\delta z = z - z_c$





Effect of the pre-stress term: extended Maxwell criterion

$$\boxed{\delta E = [\sum_{ij} \underbrace{V'(r_{ij}^{eq}) \frac{[(\delta\vec{R}_j - \delta\vec{R}_i)^{\perp}]^2}{2r_{ij}^{eq}}}_{\text{pre-stress}}] + \frac{1}{2}V''\underbrace{(r_{ij}^{eq})[(\delta\vec{R}_j - \delta\vec{R}_i)\,.\vec{n}_{ij}]^2}_{\text{harmonic}} + O(\vec{R}^3)}$$

$V' \sim - f_{ij}$

$\Rightarrow$ repulsive system: $f_{ij}>0$

decreases the energy of the system:

$\Delta E \sim V' \sim -f$

It decreases the frequency of the modes:

$$\boxed{\omega_a{}^2 = (\omega*)^2 - A_1 f = A_0 B\, \delta z^2 - A_1 f}$$

Effect of the pre-stress term: extended Maxwell criterion

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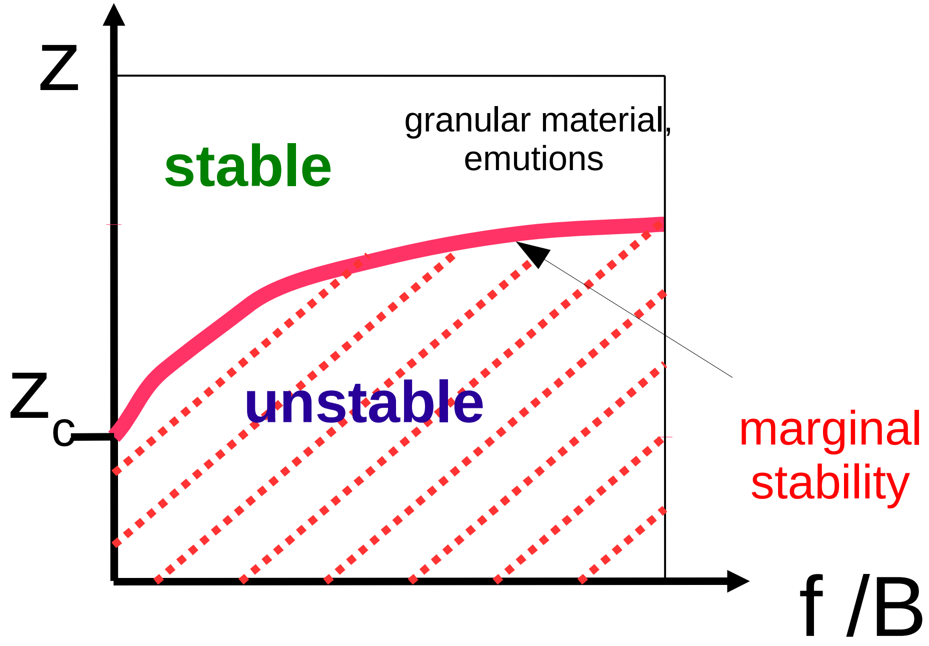


- stability ⇒ $\omega_a > 0$ ⇒

$$\boxed{\delta z^2 \geq f/B}$$

∀ subsystem with L>L*

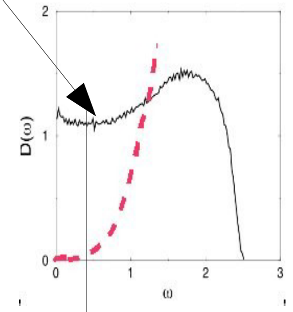
Summary so far:

- rigid material ⇔ all vibrational modes are stable

- rigidez *vs* z: Maxwell: necessary condition to be rigid?

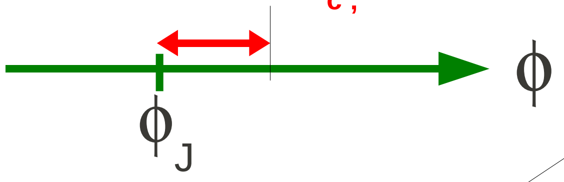
$$\boxed{z \geq z_c = 2d}$$

⇨ at the jamming transition: the solid is *marginally* rigid
boson peak: = excess of modes on the *verge* of instability



- And when $\phi > \phi_c$?

$\delta z = z - z_c$; $p \sim V' > 0$

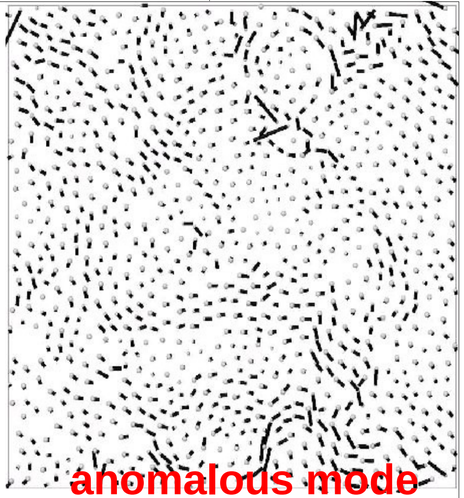


$$\boxed{\delta z \geq (p / B)^{1/2}}$$

Maxwell extented criterion

Solids at the limiar of stability
(marginal solids)
excess of low frequency modes:

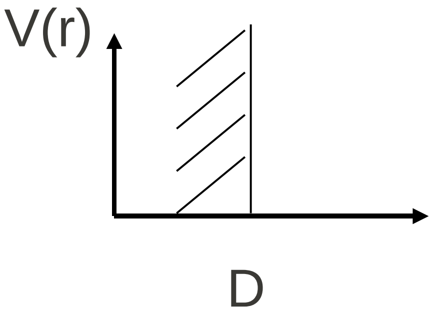
- extended $L^* \sim (\delta z)^{-1}$
- heterogeneous
- $\omega^* \sim B^{1/2}/L\hat{}^* \sim B^{1/2}\ \delta z$



anomalous mode

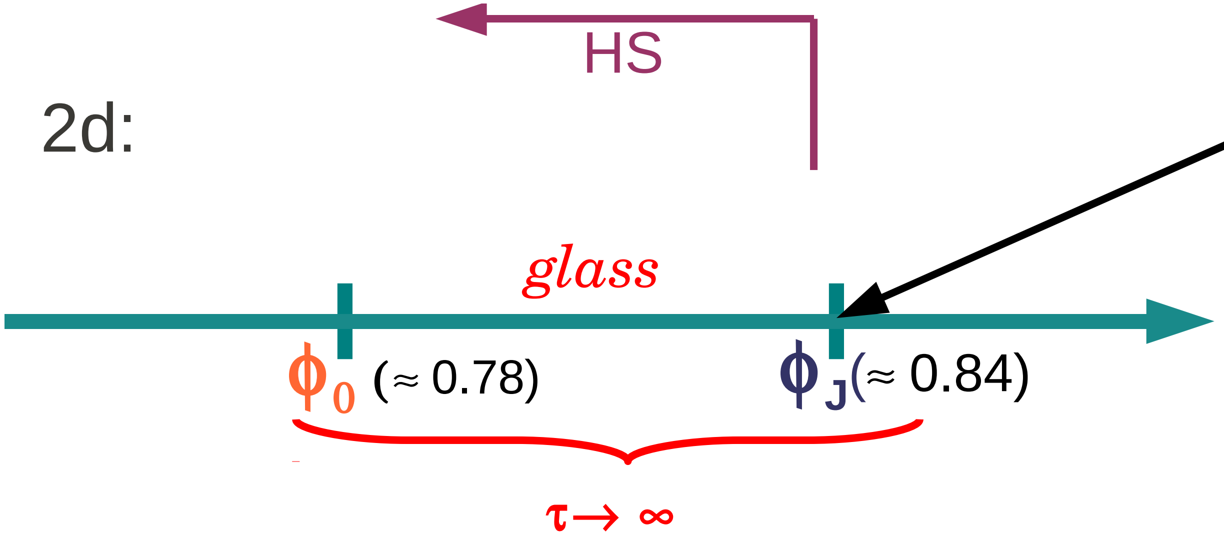
Vibrations in hard sphere glasses

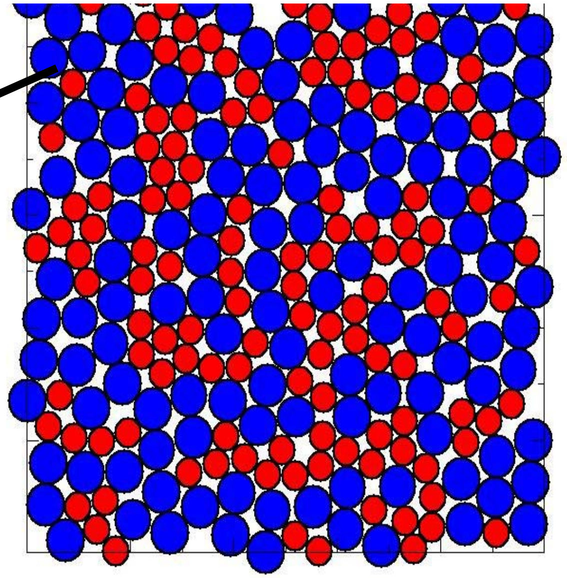
- How to compute modes in HS systems



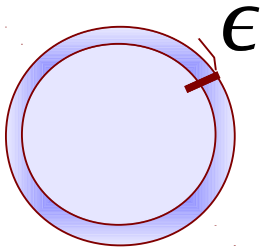
- What can we learn from / with them?

2d:





(ϕ_J)



- ✓ *Event-driven simulation*
- ✓ $< v^2 > =$ const
- ✓ Periodic boundary conditions

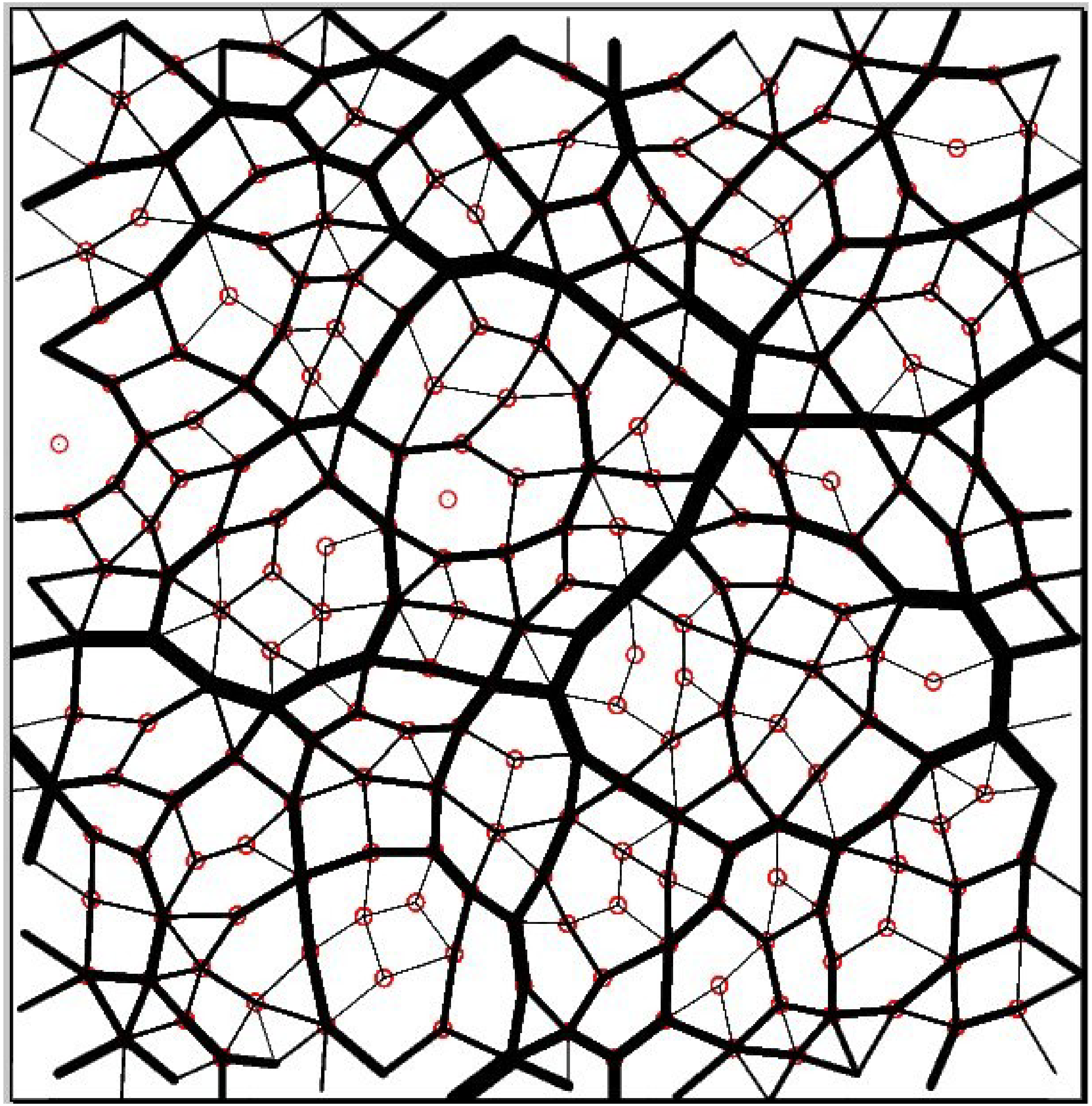
⇒ during $t_c \ll t_1 \ll \tau$, one defines:

contact, contact forces $\mathbf{f}_{ij}$

Z: if i,j touch each other, they are in contact

$$\vec{f}_{ij} = \frac{1}{t_1} \sum_{n=1}^{n=n_{col}} \Delta \vec{P}_n$$

(A. Donev et al, JCP (2005) , A. Ferguson et al, PRE (2006).)

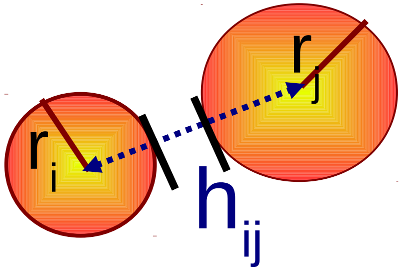


$\epsilon = 10^{-4}$

N = 256

$t_1 \approx 100N$

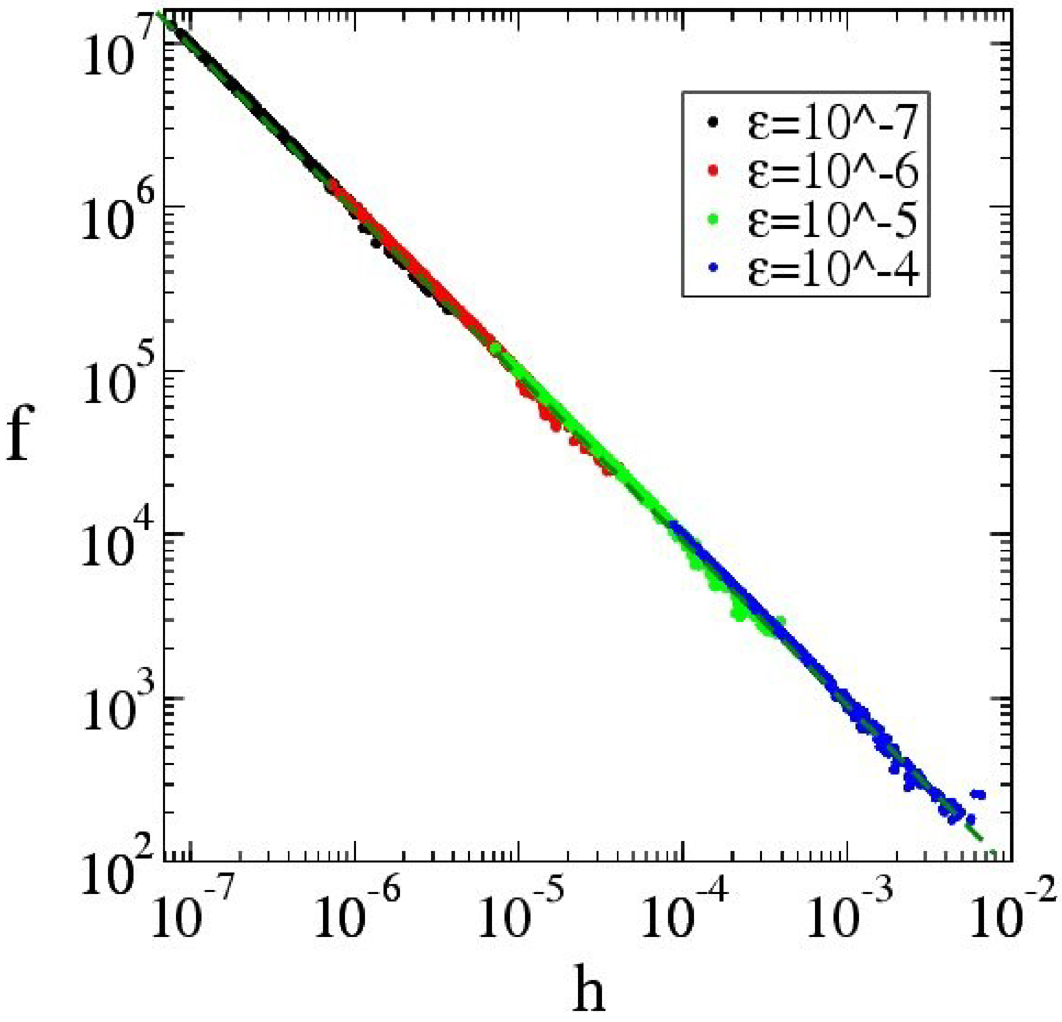
Effective potential – scale argument



$$\boxed{f_{ij} = \nu \, t_1 \, \frac{||\Delta P||}{t_1}}$$

$$\nu \sim \frac{v}{\langle h_{ij} \rangle}$$

$$||\Delta P|| \sim mv$$



$$\boxed{f_{ij} \sim \frac{\langle v^2 \rangle}{\langle h_{ij} \rangle} \sim \frac{1}{\beta \langle h_{ij} \rangle}}$$

(CB and M. Wyart, EPL 2006)

Effective potential

Tonks, PR (1936)

1d, p=*cte*

$$\mathcal{Z} \sim \prod_i \int_0^\infty dh_i e^{-\beta p h_i} \longrightarrow p = k_b T / \langle h \rangle$$

d>1, in the isostatic limit:

$$\mathcal{Z} = \prod_{\langle ij \rangle} \int_{h_{ij} \geq 0} dh_{ij} e^{-f_{ij} h_{ij} / k_b T} . \longrightarrow f_{ij} = \frac{k_b T}{\langle h_{ij} \rangle}$$

d ≥ 3, numerically: P. Charbonneau et al, arXiv:1107.4666

Effective potential

- In the isostatic limit:

$$\begin{cases} V_{ij}(r) = \infty & \text{If } \langle h_{ij} \rangle < 0 \\ V_{ij}(r) = -\frac{1}{\beta}\ln(\langle h_{ij} \rangle) & \text{If } i \text{ and } j \text{ are in contact} \\ V_{ij}(r) = 0 & \text{If } i \text{ and } j \text{ are } \textit{not} \text{ in contact} \end{cases}$$

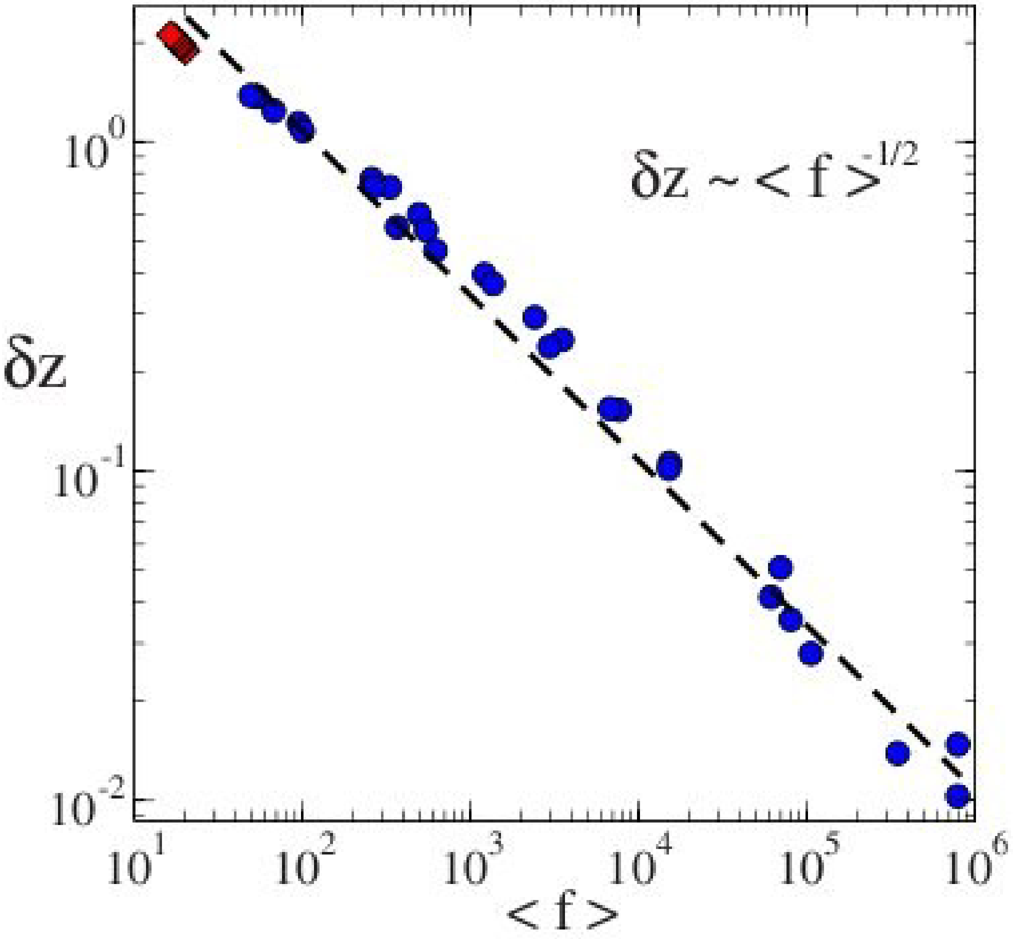
- when $\delta z = z - z_c > 0$, correction to the force

$$f_{ij} = \frac{k_b T}{\langle h_{ij} \rangle}(1 - c\,\delta z)$$

Mechanical stability

Rigidity criterion $\Rightarrow$ **$\delta z^2 \geq f/B$** $\Rightarrow$ $(B \sim V'' \sim f^2)$ $\Rightarrow$ **$\delta z \geq f^{-1/2}$**

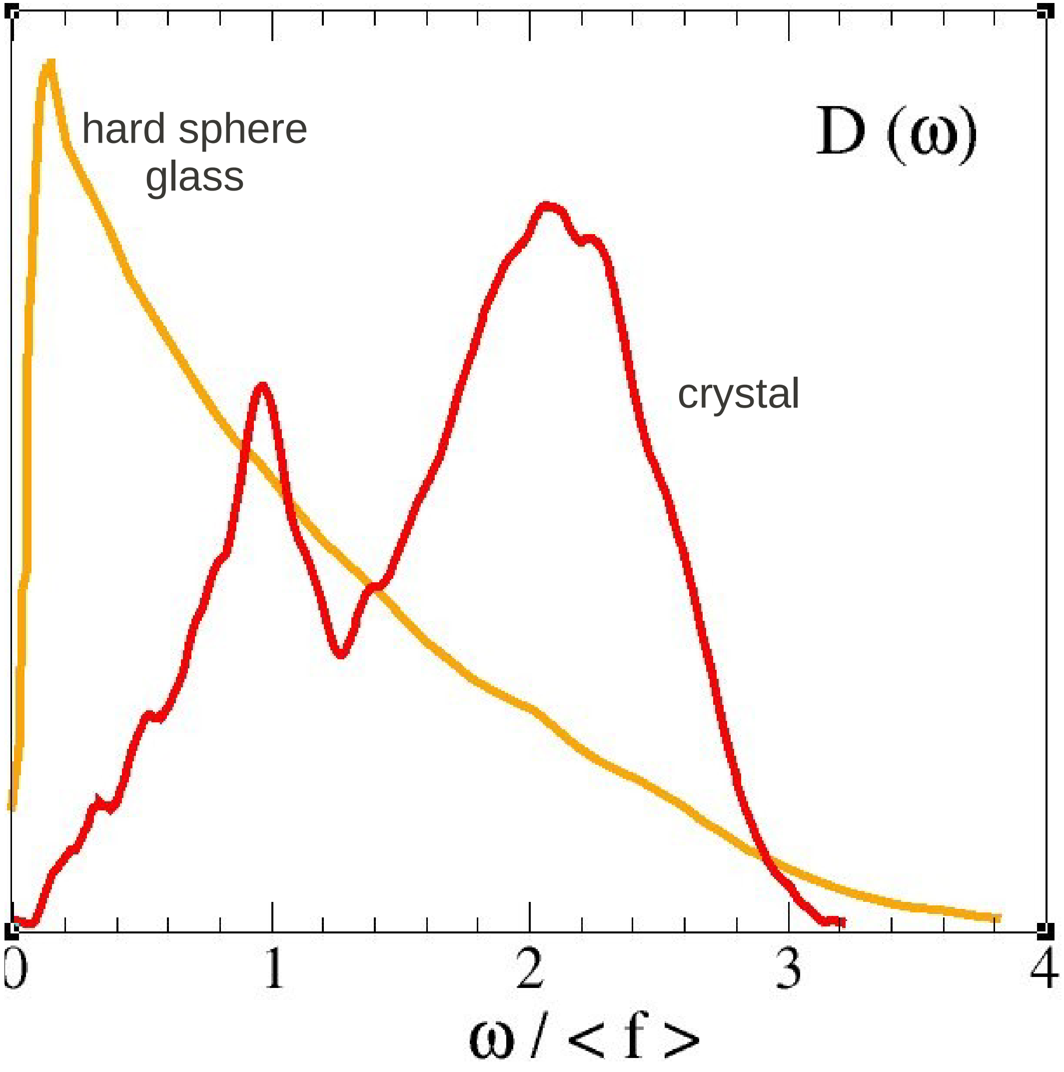
HS glass is *marginally* rigid !



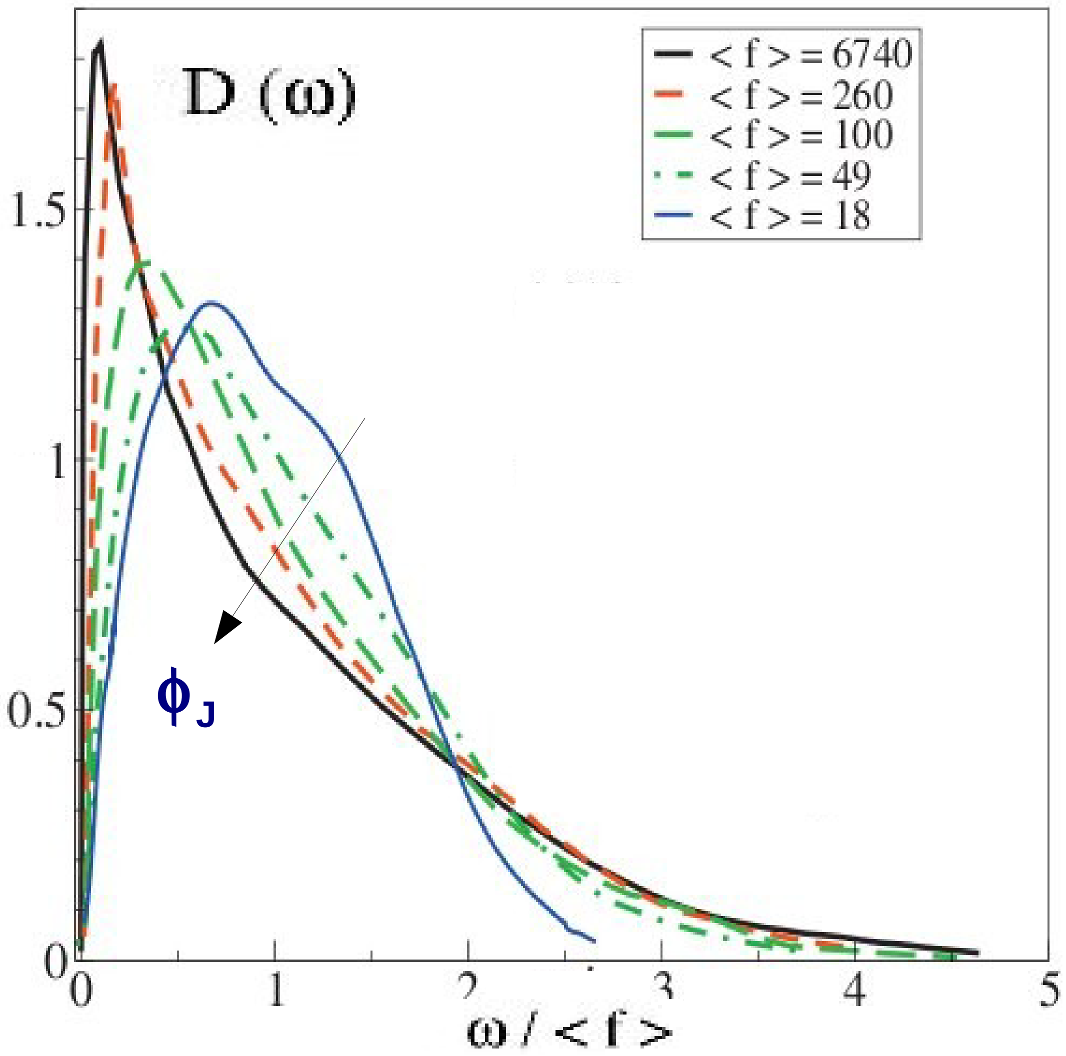
number of contacts is *exact* to keep rigidity

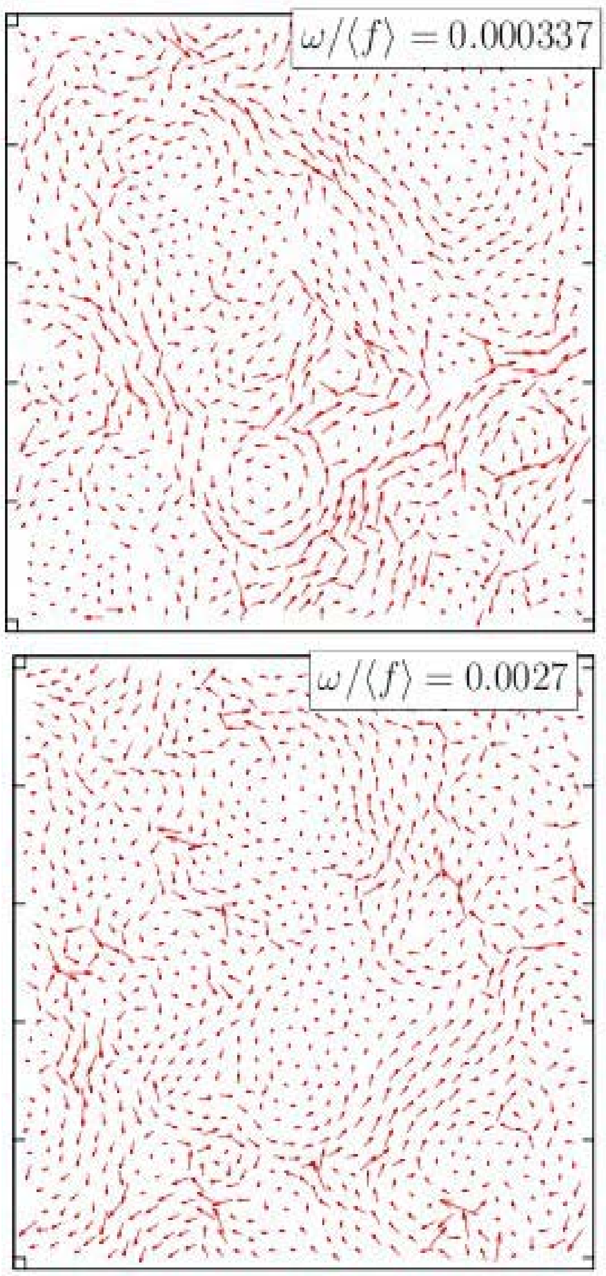
excess of low frequency modes:
on the verge of becoming soft...

Microscopic dynamics: the vibrational density of states

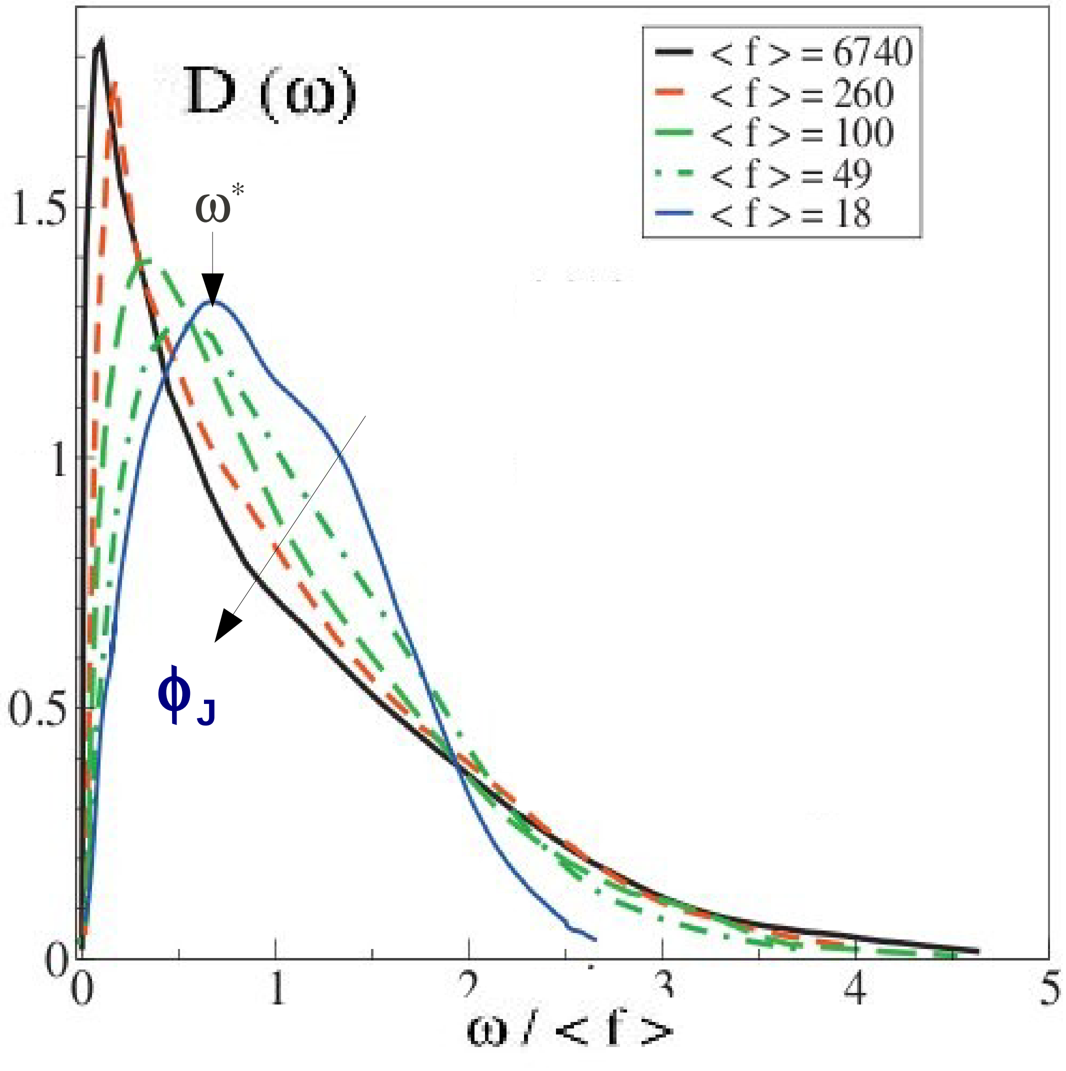


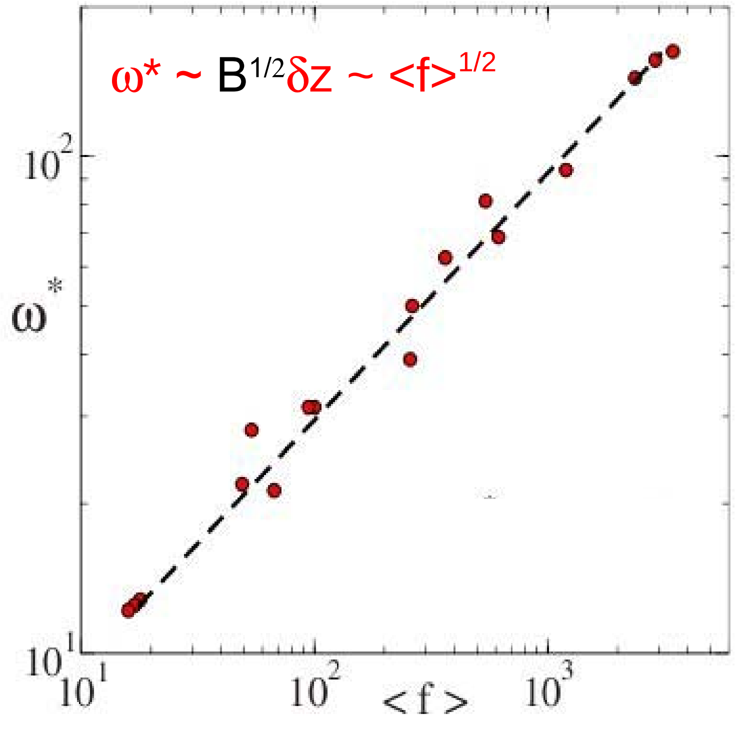
Microscopic dynamics: the vibrational density of states





Microscopic dynamics: characteristic frequency





$\omega^* \sim B^{1/2}\delta z \sim \langle f \rangle^{1/2}$

Microscopic dynamics: mean square displacement

$$\langle \delta\vec{R}^2\rangle \sim \int_0 \frac{D(\omega)}{\omega^2} d\omega \geq \int_{\omega^*} \frac{D(\omega)}{\omega^2} d\omega$$

- Amorphous:

$$D(\omega) \sim \frac{1}{B^{1/2}} \qquad \omega > \omega^*$$

$$\boxed{\langle \delta\vec{R}^2\rangle \geq \frac{D(\omega^*)}{\omega^*} \sim \langle f\rangle^{-3/2} \sim h^{3/2}}$$

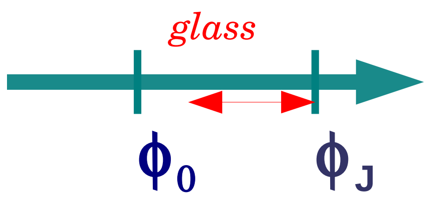
- Crystal :

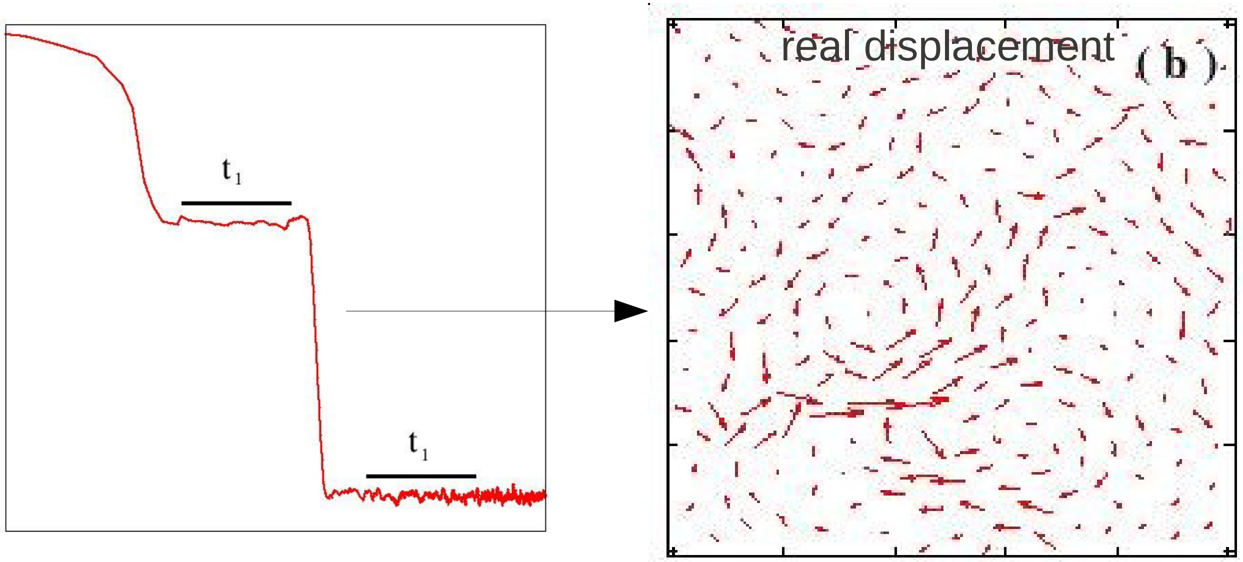
$$D(\omega) \sim \omega \qquad \text{(2d)}$$

$$\boxed{\langle \delta\vec{R}_i^2\rangle \sim \langle f\rangle^{-2} \sim h^2}$$

The existence of anomalous modes implies much higher fluctuations around a meta-stable state

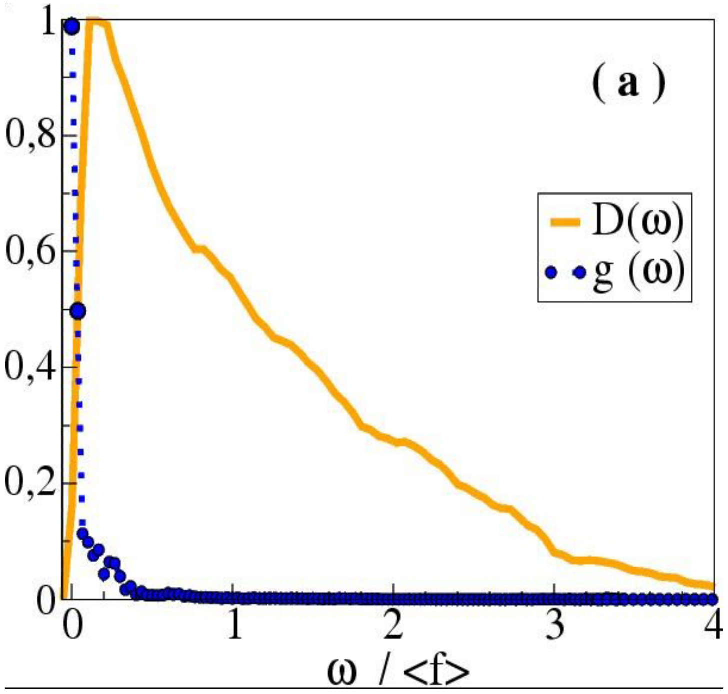
Structural relaxation and the anomalous modes

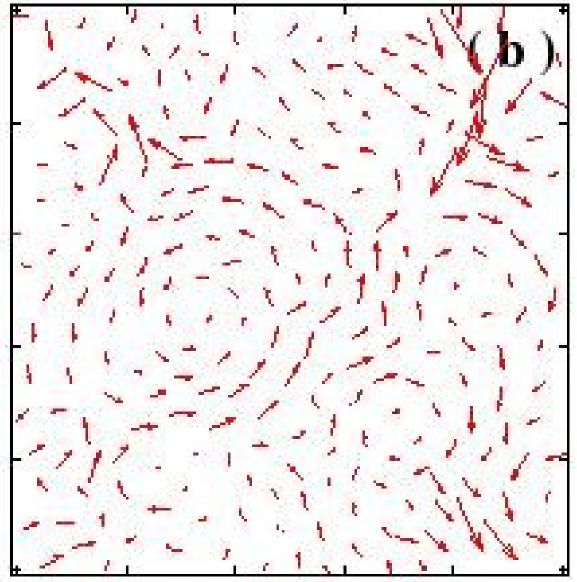




$g(\omega) = \langle c^2(\omega) \rangle$

$c(\omega)$ =projection on the mode w

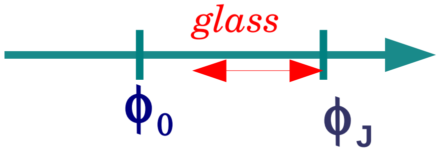




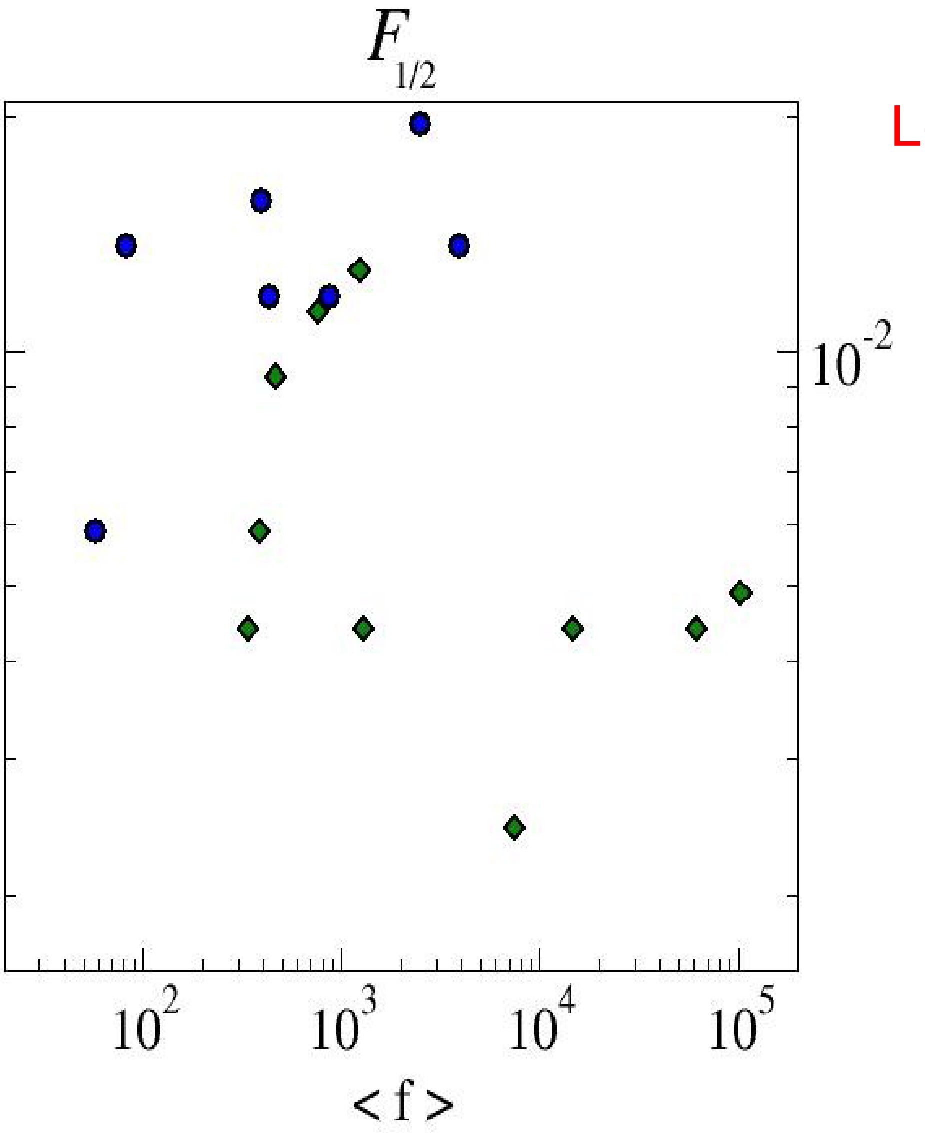
softest mode

⇒ structural relaxation happens alond the softest modes in the glass phase

sistematically …

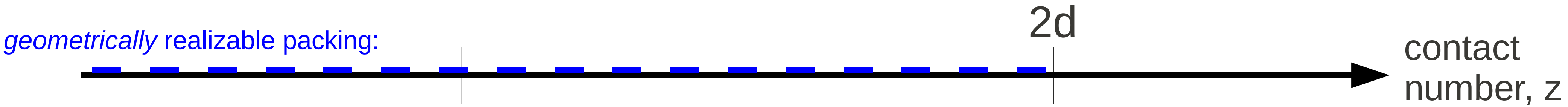


$F_{1/2}$:= fraction of the most important modes that contribute to 50% of the relaxation events

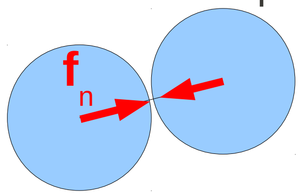


Less than **2%** of the modes contribute to the relaxation events

Avalanche in a granular packing & Generalized isostaticity



frictionless packings:



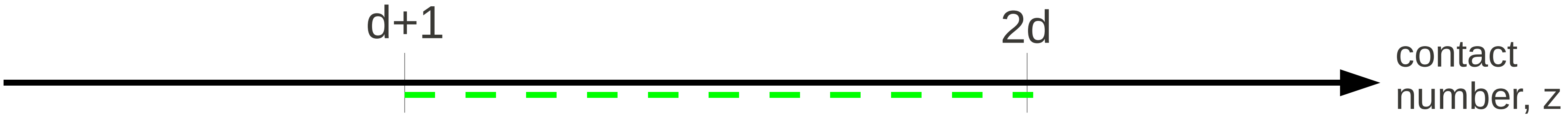
constraints
(from the mechanical stability of the pile)

$$Nd$$

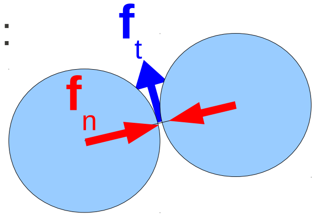
dof of force
(linear system of eqs of total force)

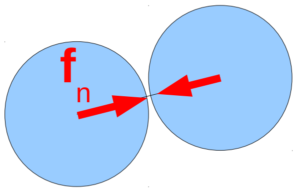
$$\underbrace{N_c}_{z \geq 2d \equiv z^0_{iso}}$$

Avalanche in a granular packing & Generalized isostaticity



frictional
packings:





constraints
(from the mechanical
stability of the pile)

$Nd + Nd(d-1)/2$

Nd

dof of force
(linear system of eqs
of total force)

$$\underbrace{N_c + N_c(d-1)}_{z \;\geq\; d+1 \,\equiv\, z^{\mu}_{iso}}$$

$$\underbrace{N_c}_{z \geq 2d \,\equiv\, z^{0}_{iso}}$$

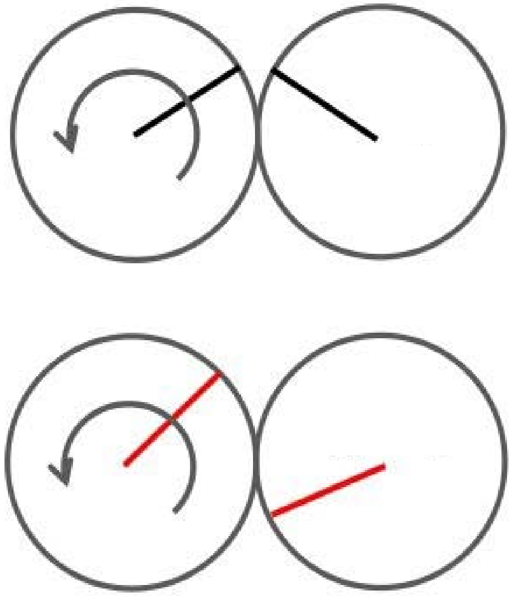
Critical (or fully mobilized) contacts

Coulomb's law
for friction:

$$|f_t| \leq \mu f_n$$

If $|f_t| < \mu f_n$: no slip motion

If $|f_t| = \mu f_n$: contacts slip



Fully mobilized

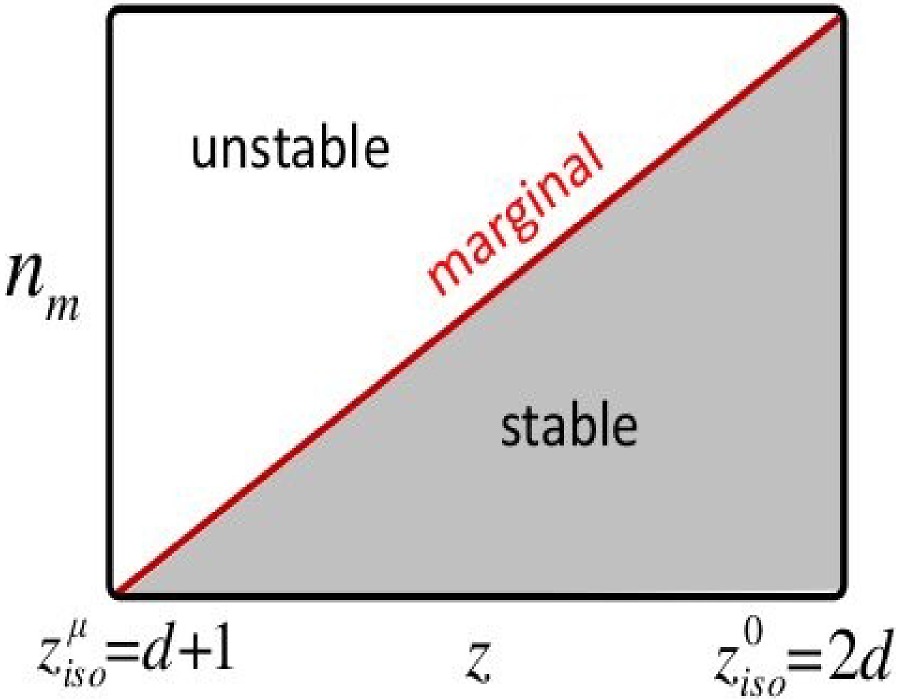
Generalized isostaticity

K. Shundyak et al., PRE (2007)
L. Silbert et al., PRE (2002)
J.-P. Bouchaud, Les Houches (2002)

If $F_t = \mu f_{n\ t}$ the number of *dof* of forces is smaller!

$$\left.\begin{array}{ll}\textbf{constraints} & Nd(d+1)/2 \\ \textbf{dof of force} & N_c d - N\boxed{n_m}\end{array}\right\} \quad z \geq \underbrace{(d+1)}_{z^{\mu}_{iso}} + 2n_m/d \equiv z^{m}_{iso}$$

mean number of critical
contacts per particle



Generalized isostaticity

K. Shundyak et al., PRE (2007)
L. Silbert et al., PRE (2002)
J.-P. Bouchaud, Les Houches (2002)

If $F_t = \mu f_{n\ t}$ the number of *dof* of forces is smaller!

constraints $Nd(d+1)/2$

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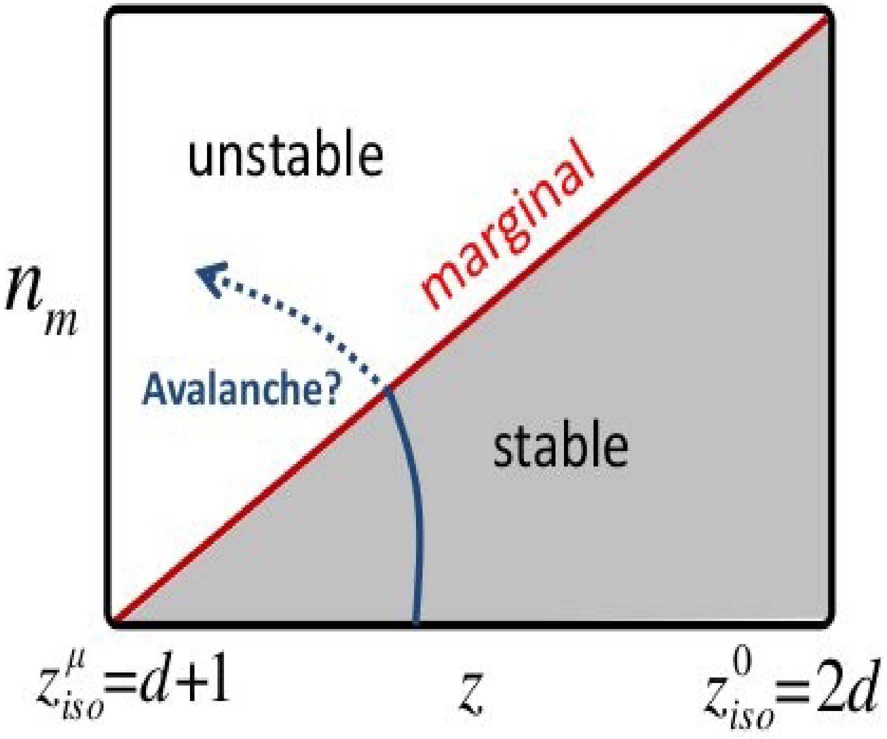
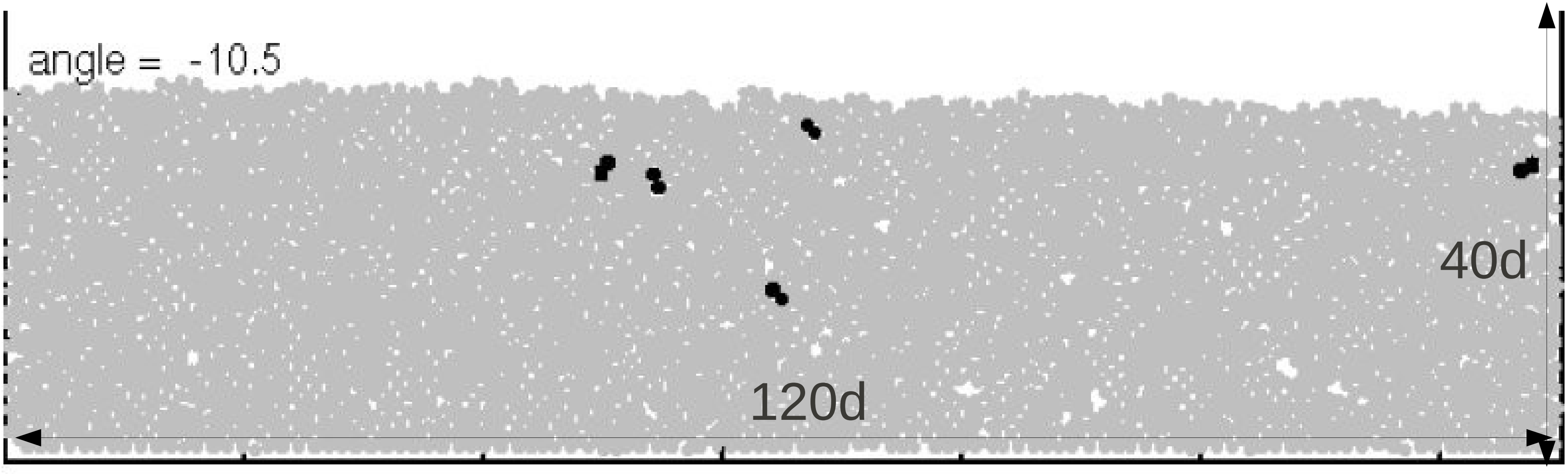


System: simulation of frictional grains

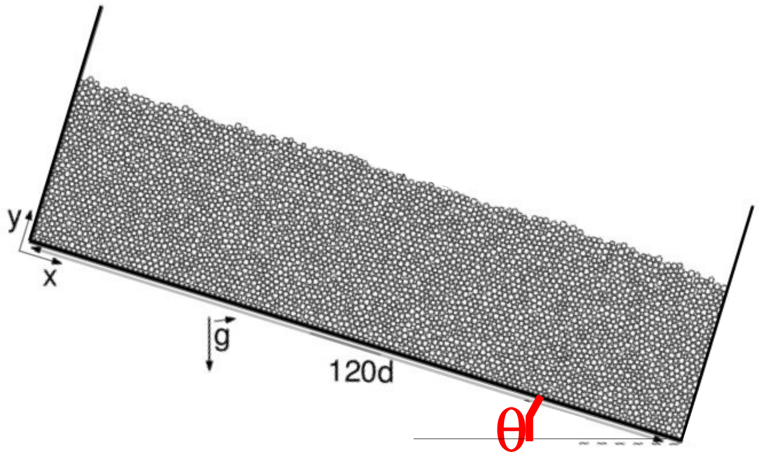


- Simulation method: contact dynamics
- Bed is slowly tilted (0.001 degree/frame)
- From -11 degree to +30 degree
- Average over 50 different initial condition
- 4000 particles, polydisperse

● Particle with critical contact

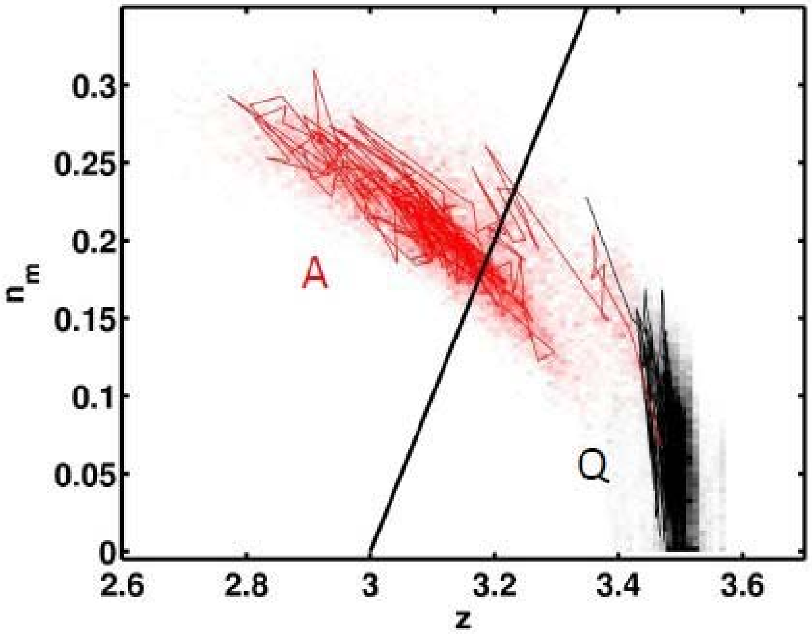
Simulation:
L. Staron and
S. Leboeuf (O. Dauchot)

(CB, S. Henkes, O Dauchot and W van Saarloos)



- criterion to identify the **quiet period** and the **avalanches**
- we define θ_m as the start of the avalanche
- 50 different Initial condition: $\theta_m \in (17°, 21°)$
- all ensemble averages are performed as a function of $\theta - \theta_m$

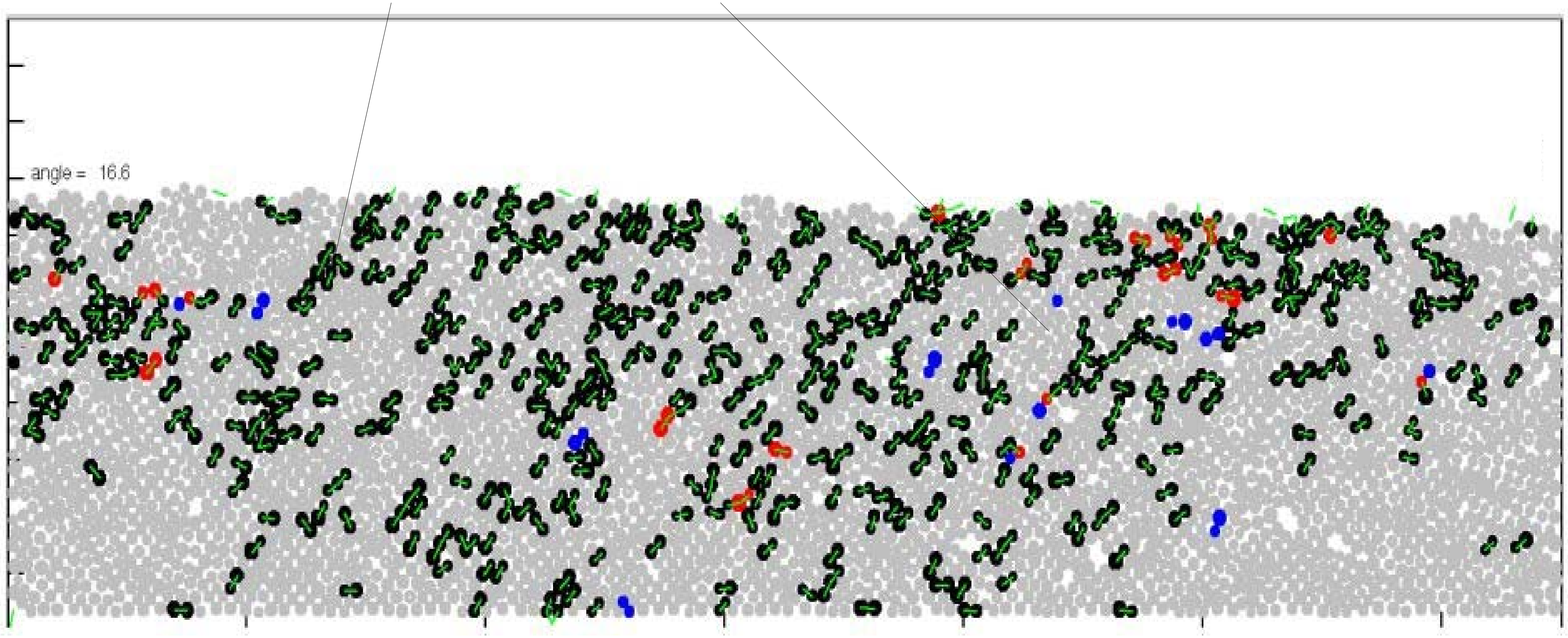
System becomes unstable before crossing isostaticity line!



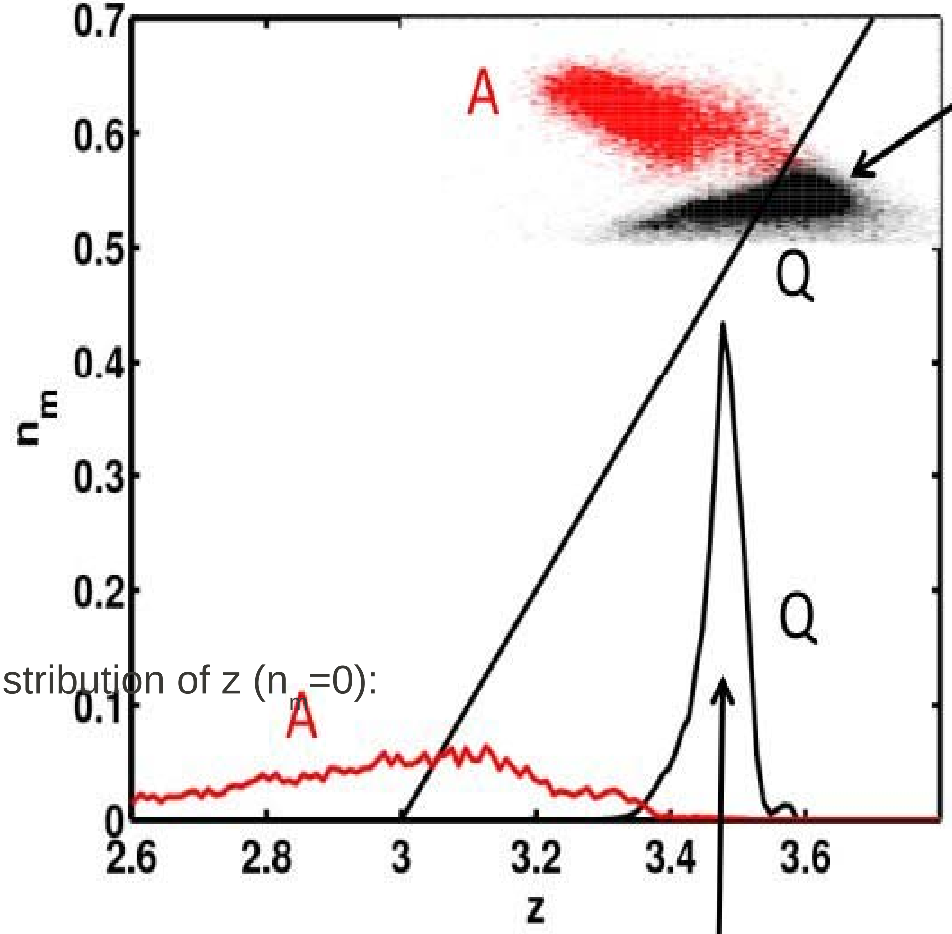
This picture supposes that the distribution of critical contacts is homogeneous, but ...

Separation into two populations:

with and **without** critical contacts



Generalized isostaticity for both subpopulation



Distribution of z (n_r=0):

Clusters:

Around stability line during quiet period

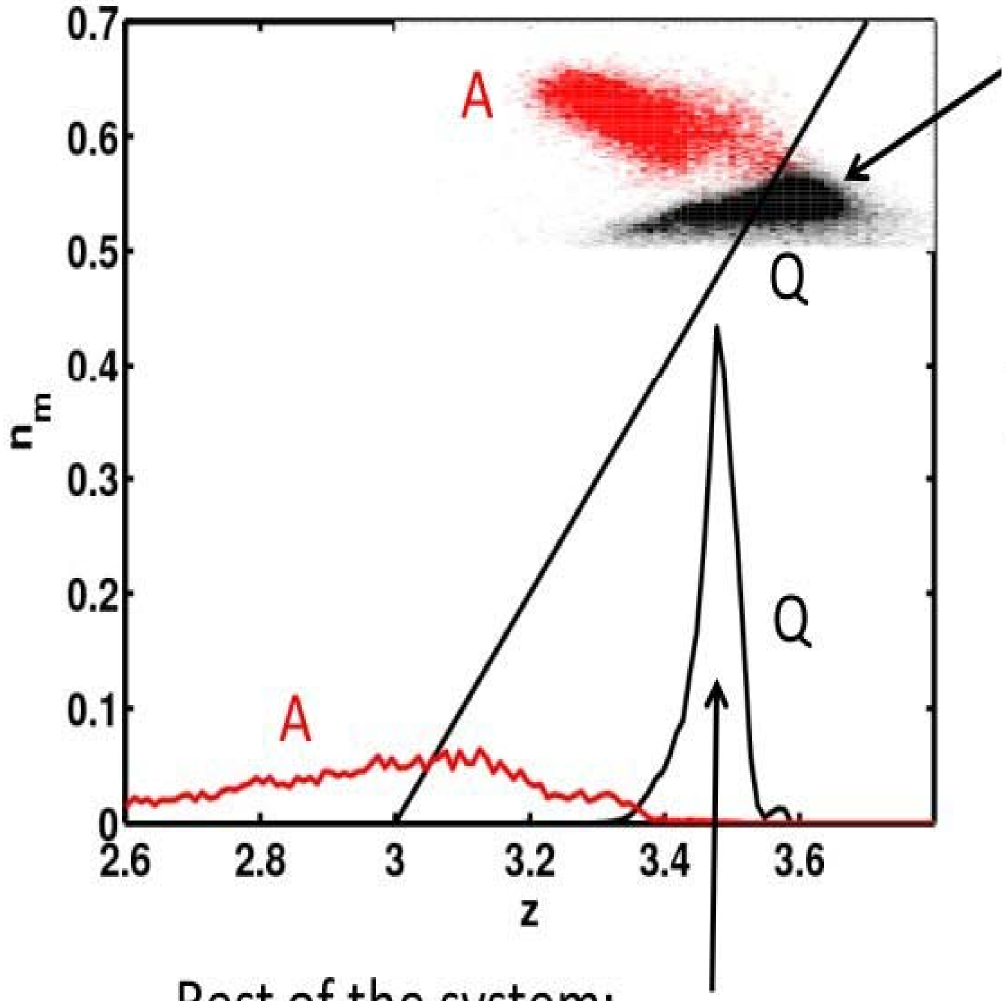
In unstable region during avalanche

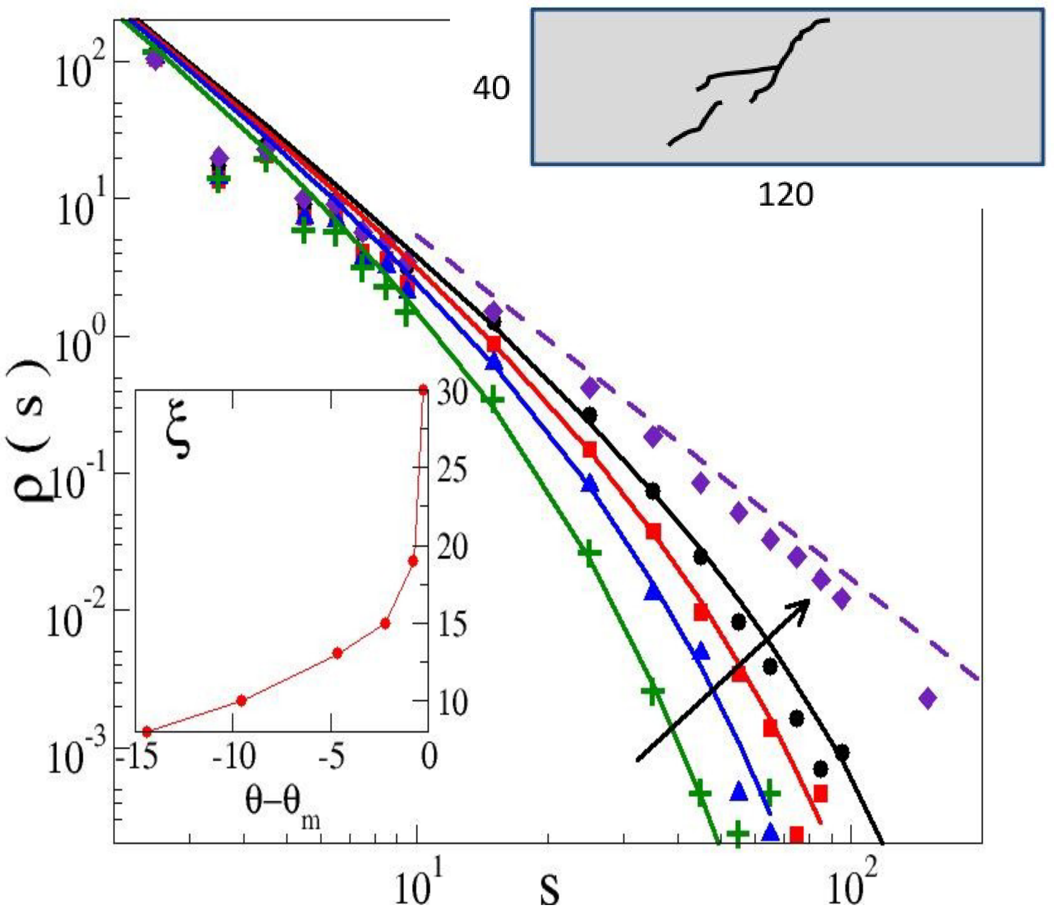
The dynamics is dominated by clusters appearing, failing, and reappearing.

Rest of the system:

Stability determined by z only

Generalized isostaticity for both subpopulation





Rest of the system:

Stability determined by z only

Summary and Conclusions

Description of the amorphous solids:
properties emerge from fact that the system is about to loose its mechanical stability

➔ Study of the HS system

- Computation of an effective potential
- HS glass is marginally rigid
  - excess of vibrational modes
  - amplitude of the fluctuations around a meta-stable state is anomalously big
  - structural relaxation happens along the softest modes

➔ Application of the diagram of rididity to understand more complex situations

➔ Statistical properties of these modes are needed!

Obrigada !

Porto Alegre