

Hidden static length-scales of super-cooled liquids

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How to unveil “hidden order”?

The story of glassy systems
(super-cooled liquids)

Glassy systems are everywhere!

Condensed and soft-matter systems,...., computer science (optimization problems), economics (agent based models)...



glasses,



plastic bottles,



granular materials,

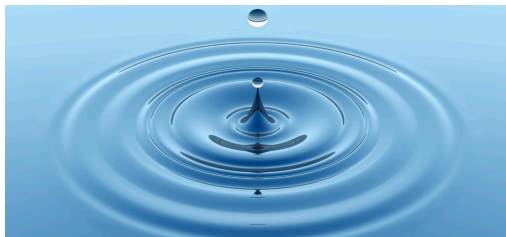
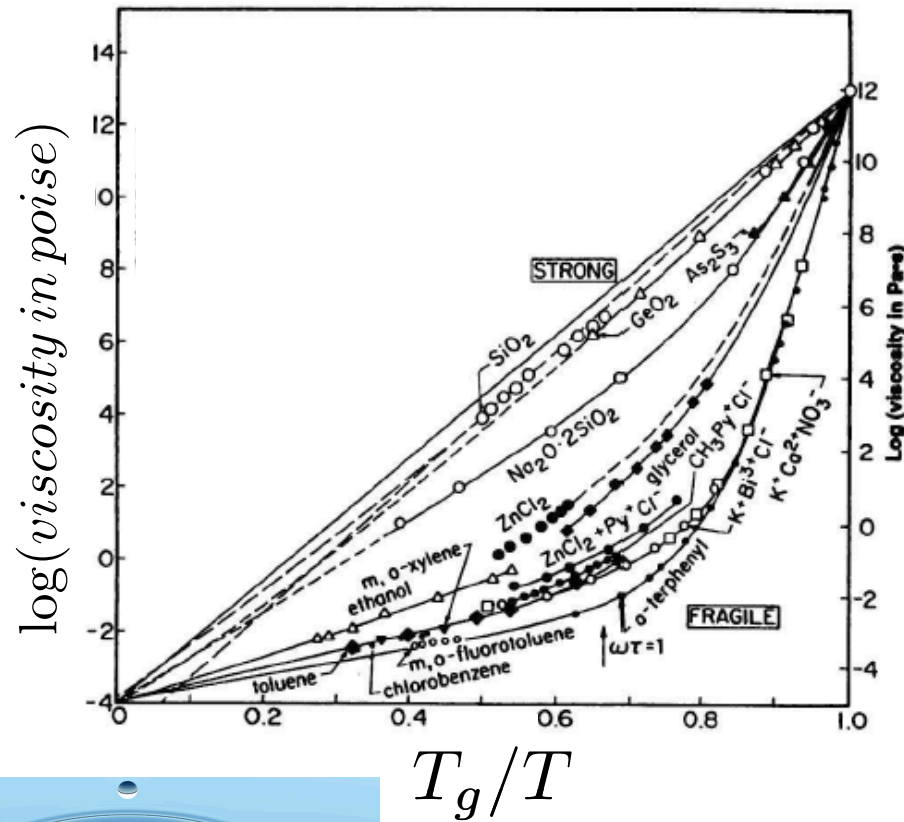
$(x_1 = 1 \text{ OR } x_2 = 0 \text{ OR } x_4 = 1)$
AND $(x_1 = 0 \text{ OR } x_3 = 1 \text{ OR } x_4 = 0)$
AND $(x_2 = 1 \text{ OR } x_3 = 1 \text{ OR } x_4 = 1)$
AND $(x_1 = 0 \text{ OR } x_3 = 0 \text{ OR } x_4 = 1),$

random K-satisfiability

....bosons and fermions with quenched disorder, ...

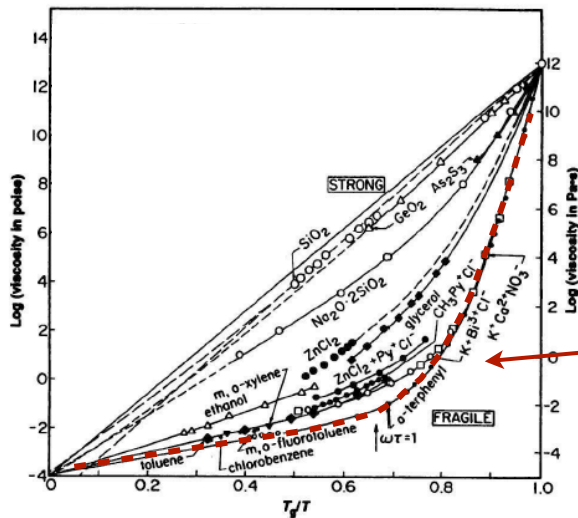
Hallmarks: ultra-slow dynamics and disordered structure

Slow Dynamics and the Glass Transition



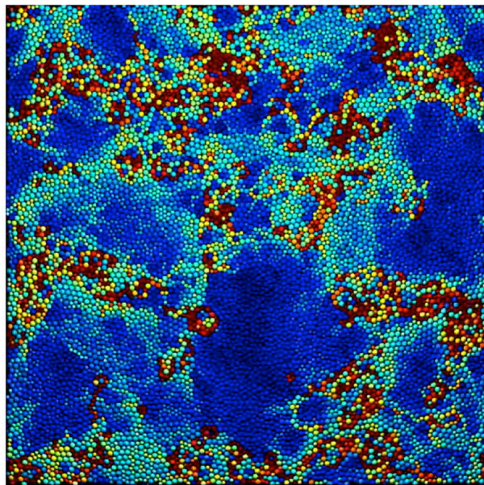
- Relaxation time: picoseconds \rightarrow days
- It takes one second to a molecule to move of one Angstrom!

Growing time-scale and cooperativity



Super-Arrhenius behavior of the relaxation time

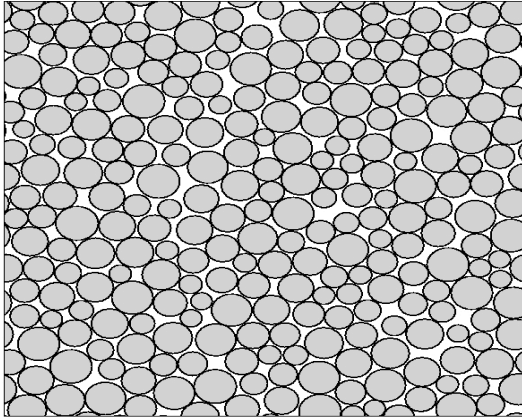
$$\eta \propto \tau \propto \exp\left(D \frac{T_0}{T - T_0}\right)$$



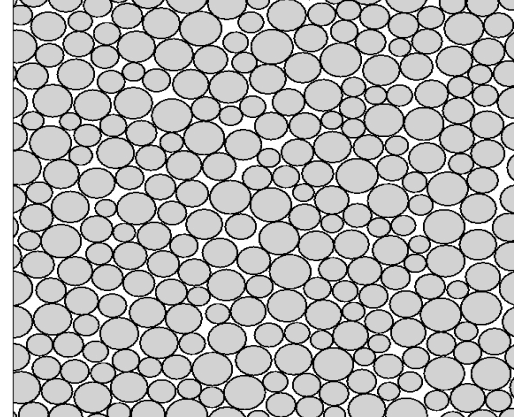
Dynamical heterogeneity grows approaching the glass transition

Hedges et al, 3D KA liquid

Are glasses statically ordered?

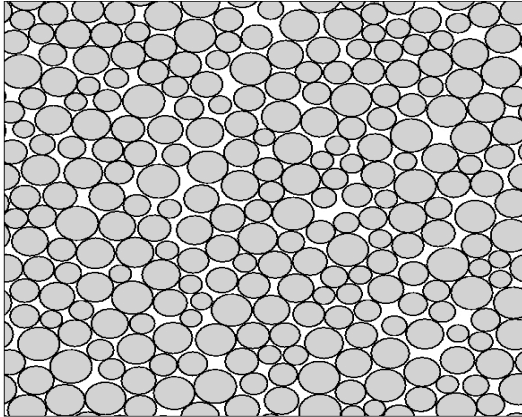


Liquid

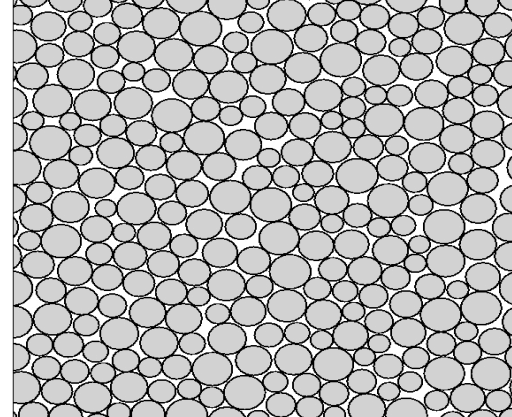


Glass

Are glasses statically ordered?



Liquid

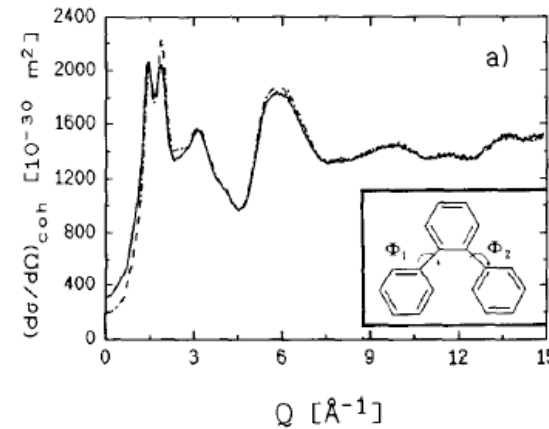


Glass

PW Anderson 1983: “Some--but not all--transitions to rigid, glasslike states, may entail a hidden, microscopic order parameter which is not a microscopic variable in any usual sense, and describes the rigidity of the system. This is the fundamental difficulty of the order-parameter concept: at no point can one be totally certain that one can really exclude a priori the appearance of some new hidden order.”

No evidence from usual probes

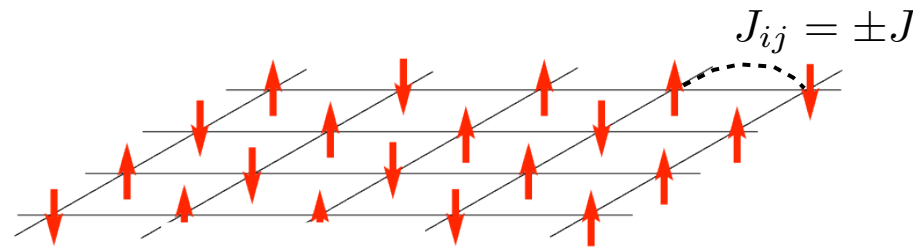
- Nothing in the structure factor $\langle \rho(x)\rho(y) \rangle_c$



T=314K, 255K,
200K

Tg=240K

- Lesson from spin glasses

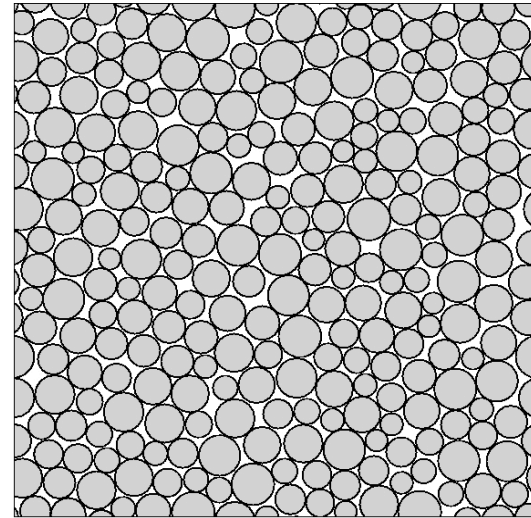
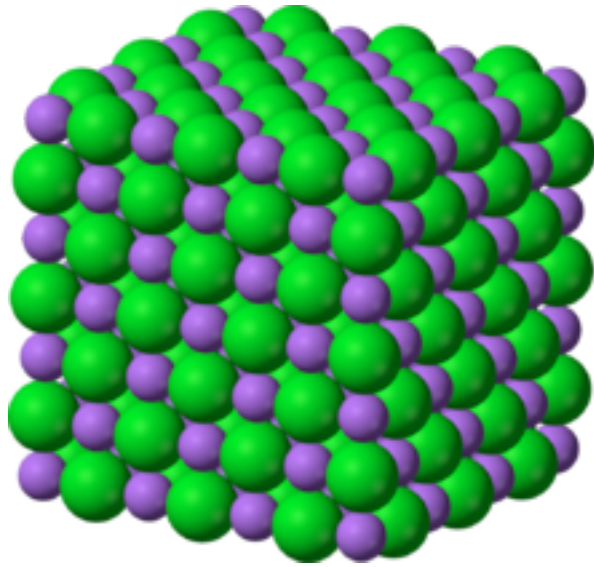


$$\langle S_x S_y \rangle_c \propto \epsilon_{xy} e^{-x/\xi}$$

$$\epsilon_{xy} = \pm \epsilon_0 \quad \longrightarrow \quad |\langle S_x S_y \rangle_c|^2 \propto \epsilon_0^2 e^{-2x/\xi}$$

Dasgupta et al. ('91): nothing in $\langle \rho(x)\rho(y) \rangle_c^2$

Unveiling Order in Disordered/Glassy systems



Problem: no guideline from the type of symmetry breaking and the order parameter

Are these strings “ordered” and how much?

123456789012345678901234567890

Are these strings “ordered” and how much?

123456789012345678901234567890

1234678912343456456712343456

Are these strings “ordered” and how much?

123456789012345678901234567890

1234678912343456456712343456

Are these strings “ordered” and how much?

123456789012345678901234567890

1234678912343456456712343456

648565584507346374650734655845

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123456789012345678901234567890

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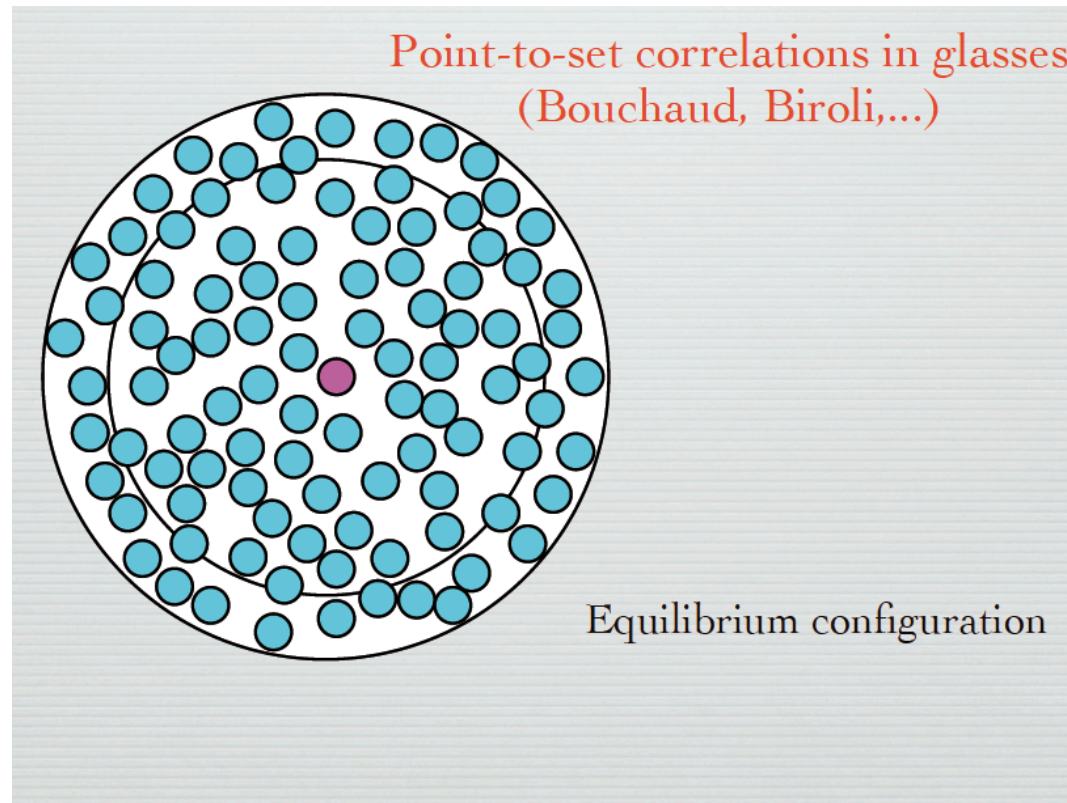
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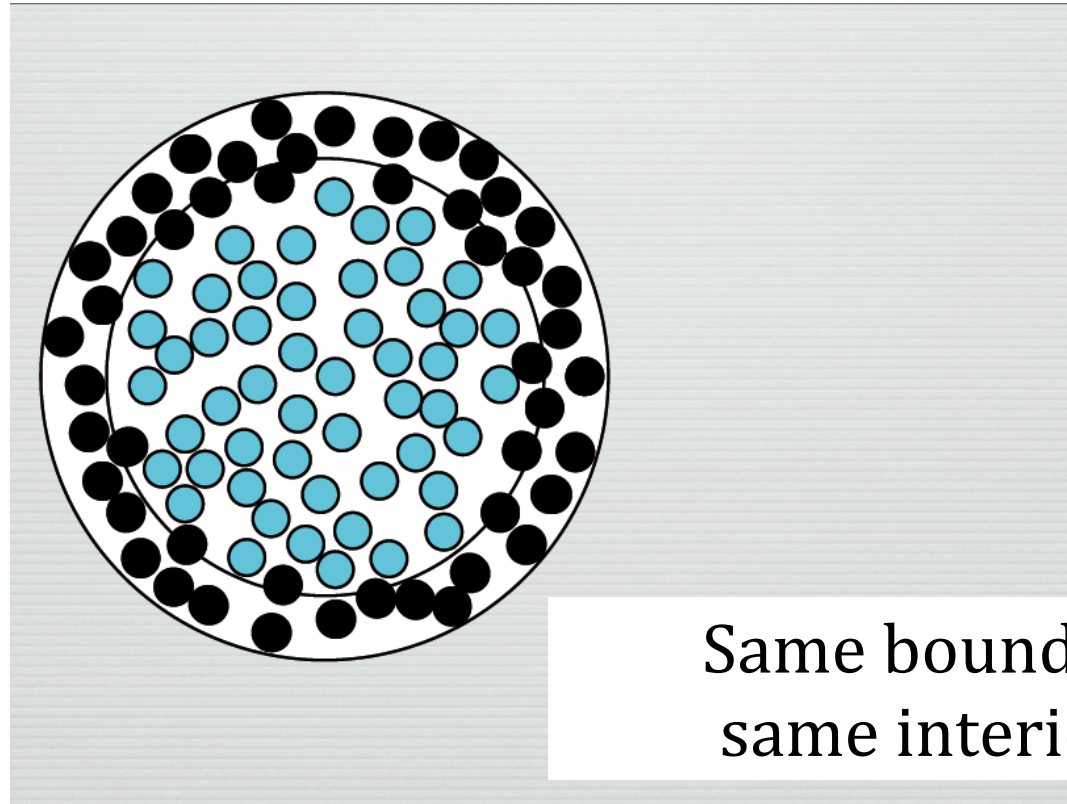
Order: predictability - low entropy

Biroli, Bouchaud 2004...
Kurchan, Levine, 2010...

Consider all possible spherical regions inside the particle configuration



Consider all possible spherical regions inside the particle configuration

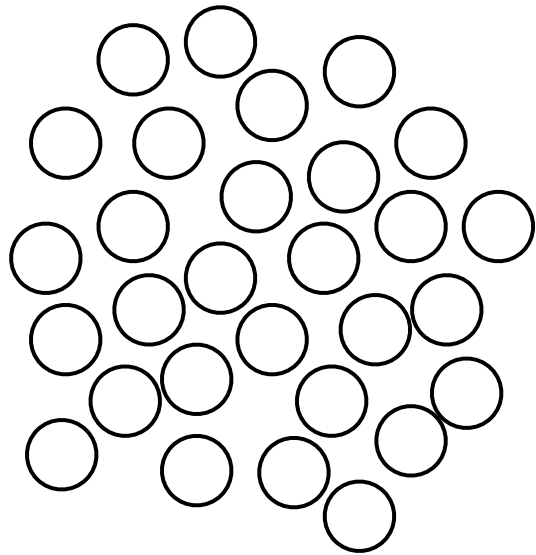


Same boundary
same interior?

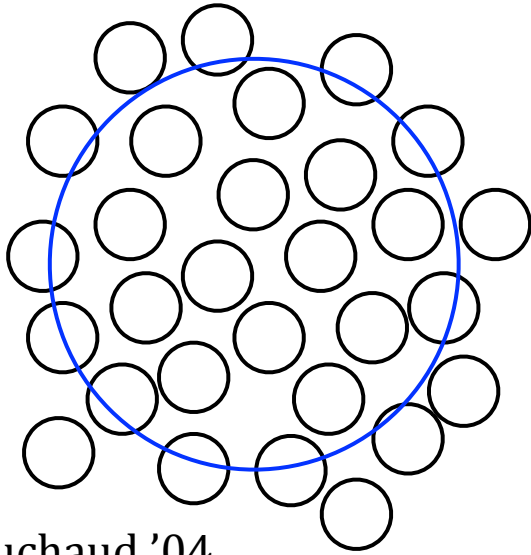
If yes (to same extent) for radii less than L then the system is ordered on the length-scale L

L: point-to-set length-scale

In practice...

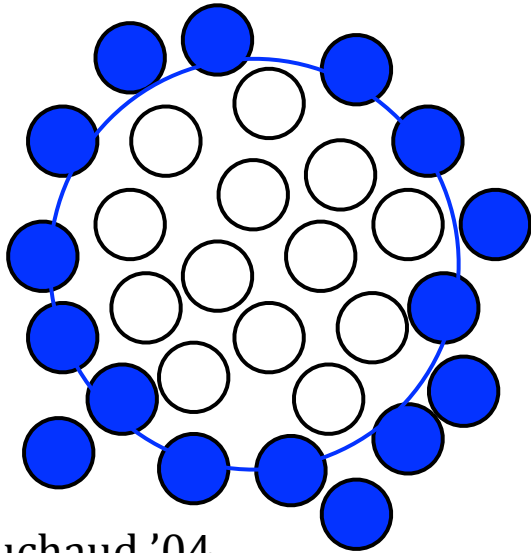


In practice...



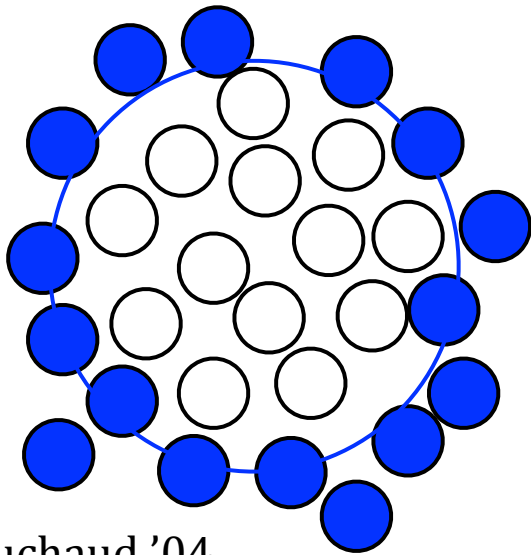
Biroli, Bouchaud '04

In practice...



Biroli, Bouchaud '04

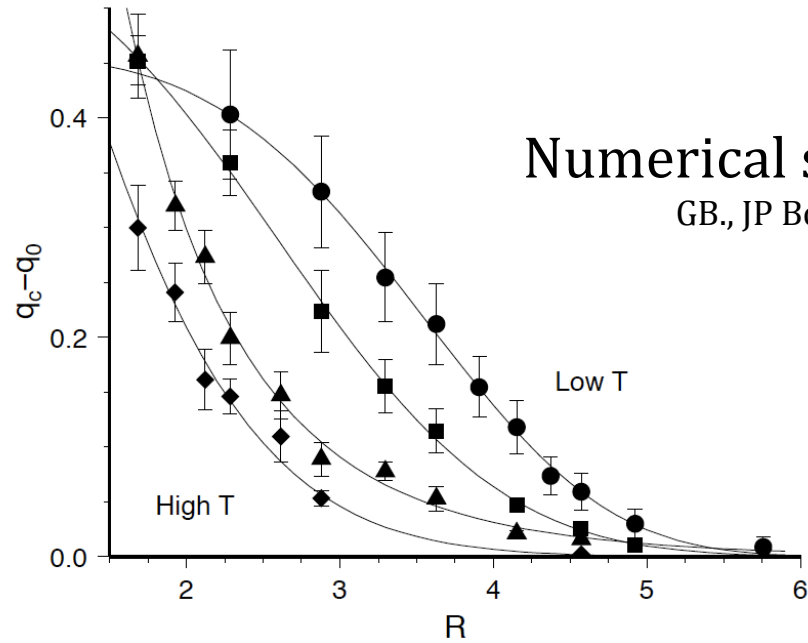
In practice...



Measure the overlap (at the center) between two equilibrated configurations with the same amorphous boundary condition

Biroli, Bouchaud '04

Numerical simulations



Numerical simulation of soft spheres mixture

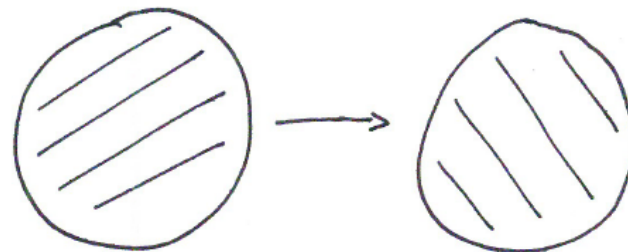
GB., JP Bouchaud, A. Cavagna, T.S. Grigera, P. Verrocchio,
Nature Physics, 2007.

State of the art on the point-to-set length

- Very challenging computational problem: we need smart ways to equilibrate! (swap particles, “density annealing”, parallel tempering)
- After 8 years still moderate temperatures only have been investigated: the point-to set length grows when temperature is lowered and reaches values of 4-5 inter-particle distances

Binder, Kob, Parisi; Berthier, Kob; Kack, Fullerton; Reichman et al., Sausset, Tarjus, ...

- The point-to-set length plays an important role in the theory of the glass transition: it allowed us to go beyond mean-field theory and it is related to the growth of the relaxation time



$$\tau \simeq \tau_0 e^{L^\psi / T}$$

Cooperative motion

Franz; Dzero, Schmalian, Wolynes; Biroli, Bouchaud; Cammarota, Gradenigo, Biroli; ...

Is it the most general length?

- It must diverge if the relaxation time diverges.

Rigorous bound $L \geq c(T \log \tau)^{1/d}$
(Montanari-Semerjian '06)

- It is obtained from a N-point correlation function with N arbitrary large, that should be able to capture any kind of translational order.

Caveat (that can be fixed): it only probes translational orders and not, e.g. orientational.

- Other static lengths introduced in the literature but more ad-hoc: related to orientational order, plastic modes and local preferred structures

Tanaka et al. Procaccia et al. ; Royal et al. ; Tarjus et al.

Application: Reconstruction in computer science

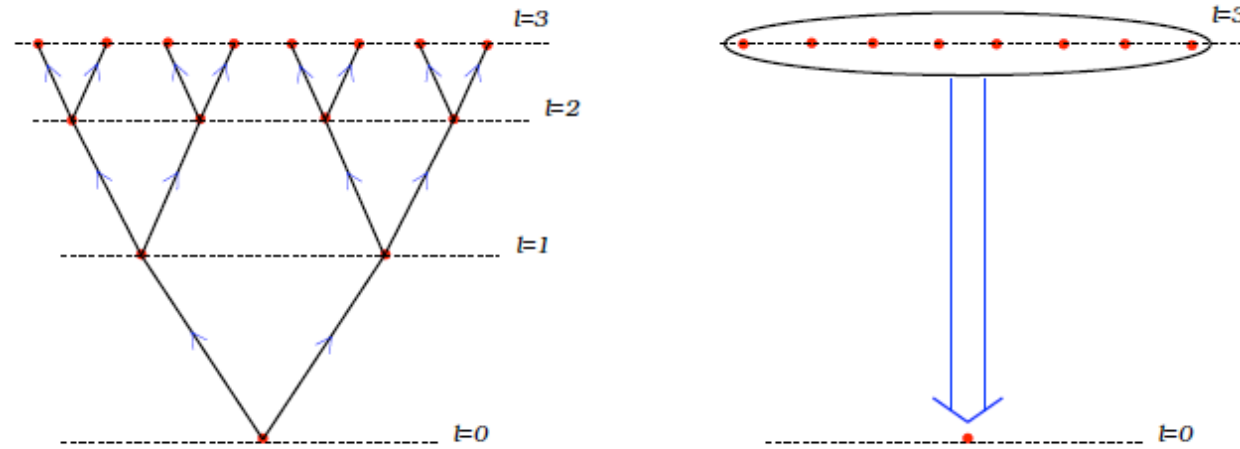


FIG. 1: Left: Broadcast on a tree. The signal is sent from the root. Each edge is a noisy communication channel broadcasting upwards. Right: The reconstruction problem asks to find what signal was sent from the root, given the signals received on the leaves

(Mezard-Montanari '05)

- Several applications and spin-offs: compressed sensing (Krzakala, Mezard, Zdeborova), probing the multiplicity of solutions in optimization problems

Conclusion

- Point-to-set length: the hidden static length-scale of super-cooled liquids
- A generic tool to unveil “hidden order”
- Applications to other physical problems (jamming,...) and beyond physics (computer science, optimization problems)