Glass Transition and Kinetically Constrained Models

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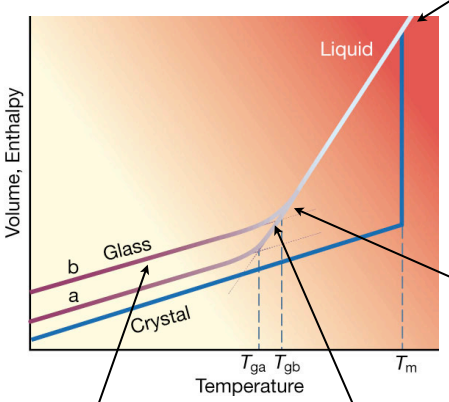
Review Talk (2/3) and some new results (1/3)

Collaborators: (expts-simults) Candelier, Dauchot, Harrowell, Reichman...
(analytical results) Cammarota.

What is the glass transition?



$\eta \propto 10^{-2} Pa \cdot s$

$D_{self} \propto 10^{-8} \frac{m^2}{s}$

$\eta \propto 10^{12} Pa \cdot s$

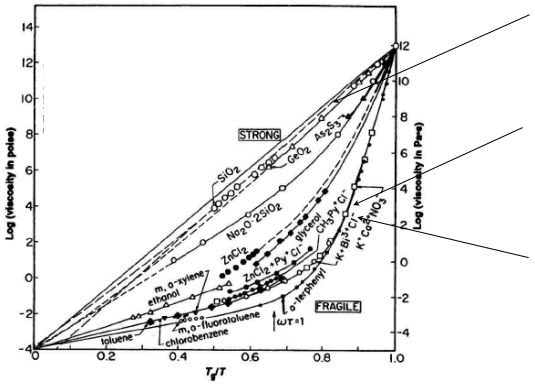
$D_{self} \propto 10^{-19} \frac{m^2}{s}$

A tiny molecule moves of few Angstroms in a second!

Amorphous rigid material: a glass

At Tg $\eta = 10^{12} Pa \cdot s$ by definition

The Angell plot



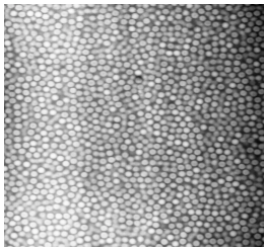
$$\eta \propto \exp\left(\frac{T_*}{T}\right)$$

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

$$\eta \propto \exp\left(D\left(\frac{T_*}{T}\right)^2\right)$$

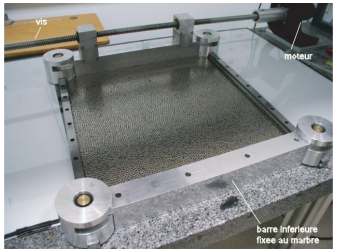
Many Glass Transitions

Colloids: Hard Spheres and Beyond



Weeks lab

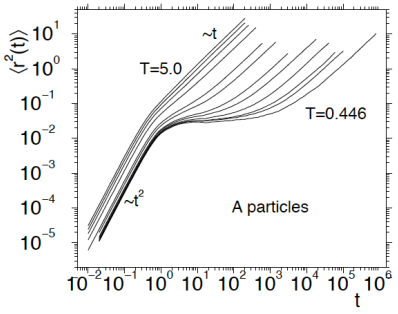
Glassy granular liquid under cyclic shear

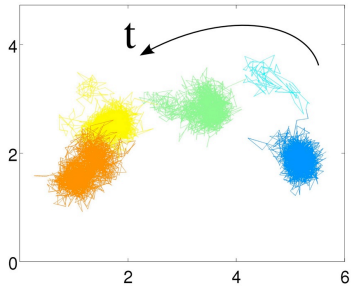


Dauchot lab

Even beyond physics: combinatorial optimization, error correcting codes,...

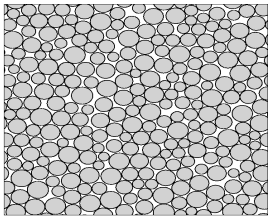
How particles move



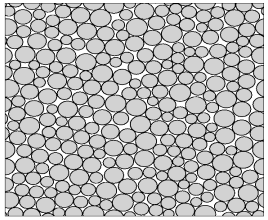


- Particles oscillate for a long time around amorphous positions.
- The particles arrangements are amorphous.

No simple static correlations...



Liquid

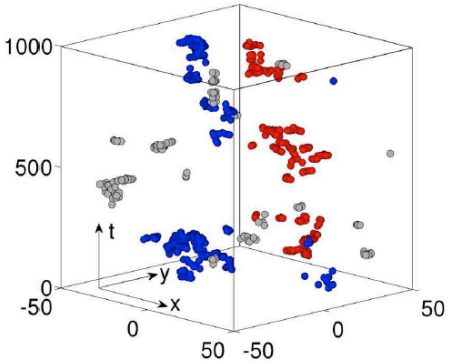


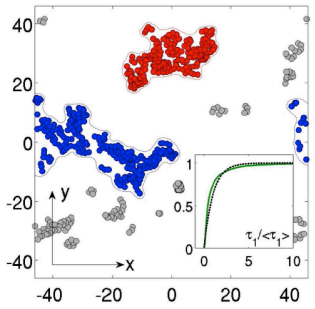
Glass

Krauth 2000

(Simple) Static correlation functions are featureless!

... but dynamical correlations!





Particle motions leading to structural relaxation are correlated

Measurements by 4-points dynamical correlation functions

...;Candelier, Widmer-Cooper et al. (GB) 2009

KCM: physical assumptions

- Particle mobility is sparse

  Most atomic motions are small amplitude vibrations and not diffusion steps.

- Static correlations do not play a role for dynamics

- Facilitation

  A region of jammed atoms can become unjammed only when is adjacent to a region that is already unjammed.

Fredrickson, Andersen (84)...Harrowell; Garrahan, Chandler...

Models

- Lattice "spins" models with stochastic dynamics
- $n_i = 0, 1$ 0 is a Facilitating region, 1 is a jammed region
- Trivial Hamiltonian: $H = -\sum_i n_i$
- Dynamic constraints on the rates:

$$n_i = 0 \to 1 \quad f(\mathbf{n}) \frac{e^{\beta}}{1 + e^{\beta}}$$

$$n_i = 1 \to 0 \quad f(\mathbf{n}) \frac{1}{1 + e^{\beta}}$$

Detailed Balance

$$\frac{P(1)}{P(0)} = e^{\beta}$$

- $f(\mathbf{n}) = 0, 1$ depends on the configuration $\mathbf{n}$ of a finite neighborhood of i but not on $n_i$itself.

- Fredrickson-Andersen Models

$f(\mathbf{n}) = 1$ if at least m neighbors of i are empty,
$f(\mathbf{n}) = 0$ otherwise

$1 \leq m \leq d$ for d-dimensional hypercubic lattices

1-FA in d=1 $11111111110111111111101111111111$

$..11011.. \rightarrow ..11001.. \rightarrow ..11101..$

Many other models:

- Oriented Models: East Model, North-East model, Spiral Model ...
- Kinetically Constrained Lattice Gases: Kob-Andersen model,...

Outcome I: Slow dynamics

- Arrhenius: $\tau \propto \exp\left(\frac{T_*}{T}\right)$ 1-FA
- Super-Arrhenius:

$\tau \propto \exp\left(\left(\frac{T_*}{T}\right)^2\right)$ East Model *(Evans-Sollich '99)*

$\tau \propto \exp\left(\exp\left(\frac{T_*}{T}\right)\right)$ 2D 2-FA and KA *(Reiter '91; Toninelli, GB, Fisher '04)*

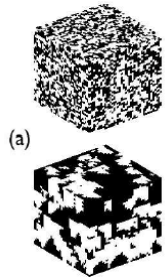
- Finite temperature glass transitions

$$\tau \propto \exp\left(D\frac{T_c^\mu}{(T-T_c)^\mu}\right)$$

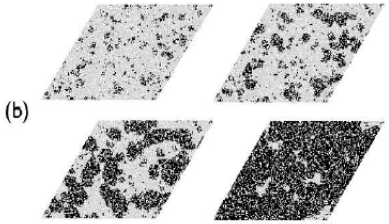
Spiral model *(Toninelli, GB, Fisher '07-'08)*

Outcome II: dynamical correlations

Spatial distribution of local persistence (white if no change between 0 and t; black otherwise)



3D North-East-Front Model



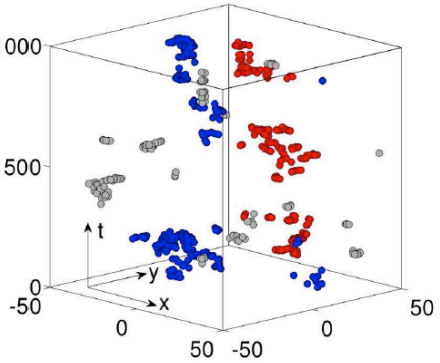
2D Kob-Andersen Model

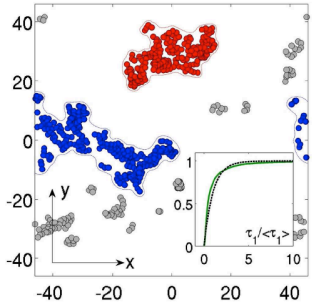
From Berthier-Garrahan '05

Scaling laws for the growth of the dynamic correlation length

That's the end of the review part. Much more in Garrahan, Sollich, Toninelli chapter's of "Dynamical heterogeneity in glasses, colloids and granular media", Oxford Univ. Press 2011 and arxiv 1009.6113

Does facilitation exist?





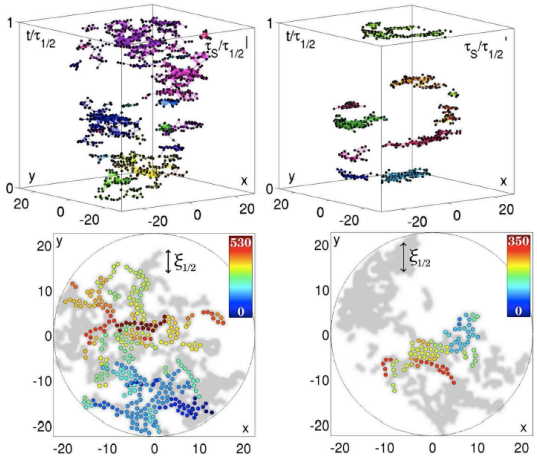
Yes! Both in simulations of supercooled liquids and experiments of granular systems close to jamming

Candelier, Widmer-Cooper et al. (GB) 2009
Candelier, Dauchot, Biroli 2008

Is facilitation like in the models?

Only one (negative) test from experiments on granular systems close to jamming

Candelier, Dauchot, Biroli 2010

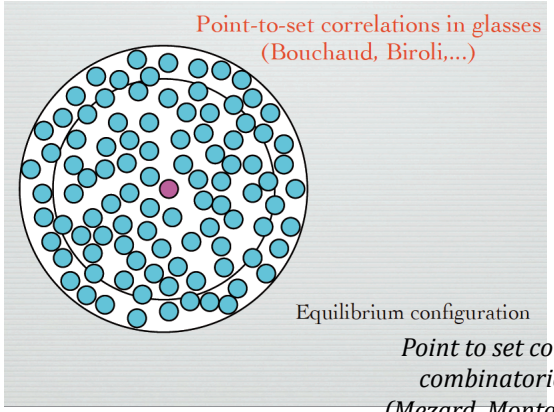


Kinetic constraints are more violated close to the jamming transition.

Facilitation plays a lesser role close to the jamming transition.

Amorphous boundary conditions and static length-scales

Recently, a lot of studies to check the growth of static order in super-cooled liquids.



Point to set correlations also in combinatorial optimization (Mezard, Montanari, Semerjian,...)

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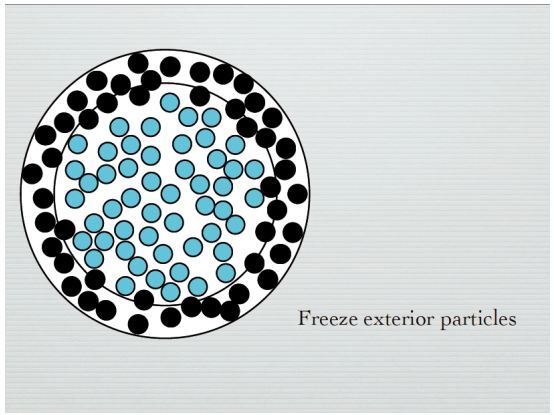

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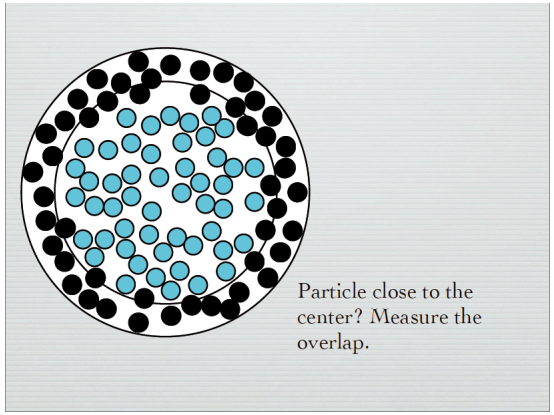


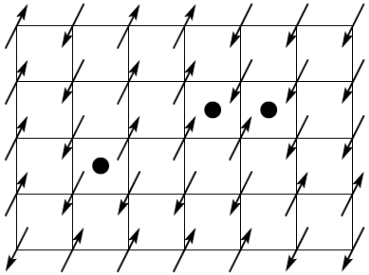
Effect of amorphous boundary conditions on static and dynamic properties within the KCM's scenario

Jack and Garrahan '05:

Focus on a model whose dynamics is effectively described by KCMs, e.g. the square plaquette model

$$H = -\frac{1}{2}\sum_{xy} \sigma_{x,y}\sigma_{x,y+1}\sigma_{x+1,y}\sigma_{x+1,y+1}$$

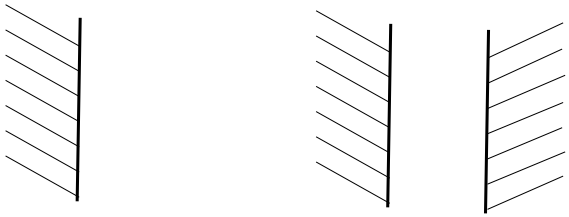
$$p_{x,y} = \sigma_{x,y}\sigma_{x,y+1}\sigma_{x+1,y}\sigma_{x+1,y+1}$$



Amorphous boundary conditions around the cavity affect the dynamical properties on a length $\xi_d \propto e^{\frac{1}{T}}$ and the static properties (the overlap) on a length $\xi_s \propto e^{\frac{1}{2T}}$

Other geometries

Cammarota, Biroli 2011



One wall ‘Sandwich’ Pinned particles

<u>Statics not affected at all</u>: cavity and infinite geometries are very different!

Dynamics affected (slowed down) by ABCs on a length-scale $\xi_d \propto e^{\frac{1}{T}}$

- Are these results general within the KCM’s scenario?
- If yes (likely), they will provide a smoking gun test-comparison with respect to other theories/scenarii.

Conclusion

- KCMs display a phenomenology very similar to liquids approaching the glass and jamming transitions.
- Their behavior is very rich: dynamical transitions, diverging dynamical correlation length and time scales, aging,...
- They provide a framework to understand many concepts and phenomena related to glassy behaviors and test new theoretical ideas.
- Whether they provide the correct theoretical framework to explain the glass transition is not clear: work in progress!