

Finite size scaling of the dynamical free-energy in the interfacial regime of a kinetically constrained model

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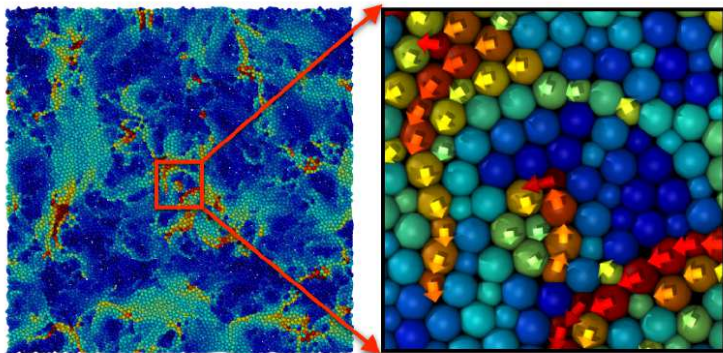
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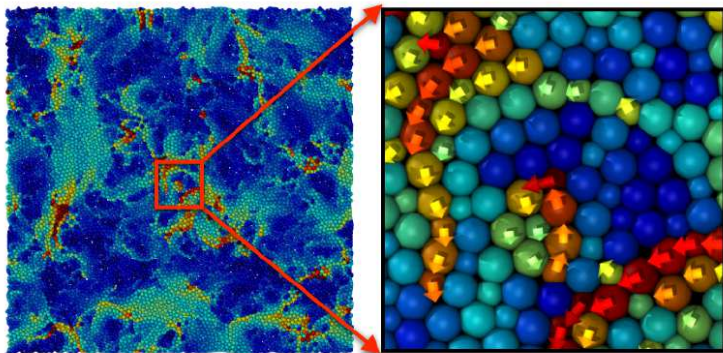
ITP Leuven – 21th November 2012

Dynamical excitations in glass-forming liquids



From: Keys *et. al* PRX **1** 021013 (2011)

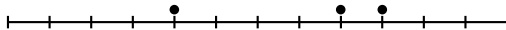
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Can we model this simply?

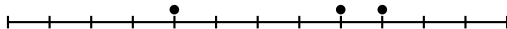
Example 0: (in 1D for simplicity)



Independent sites

- L sites $\mathbf{n} = \{n_i\}$ with $\begin{cases} n_i = 0 & \text{unexcited site} \\ n_i = 1 & \text{excited site} \bullet \end{cases}$

Example 0: (in 1D for simplicity)

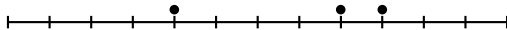


Independent sites

- L sites $\mathbf{n} = \{n_i\}$ with

{	$n_i = 0$	unexcited site
}	$n_i = 1$	excited site •
- Transition rates in each site:
 - excitation with rate $W(0_i \rightarrow 1_i) = c$
 - unexcitation with rate $W(1_i \rightarrow 0_i) = 1 - c$

Example 0: (in 1D for simplicity)



Independent sites

Unconstrained model

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- Transition rates in each site:
 - excitation with rate $W(0_i \rightarrow 1_i) = c$
 - unexcitation with rate $W(1_i \rightarrow 0_i) = 1 - c$

Equilibrium distribution: $P_{\text{eq}}(\mathbf{n}) = \prod_i c^{n_i} (1 - c)^{1 - n_i}$

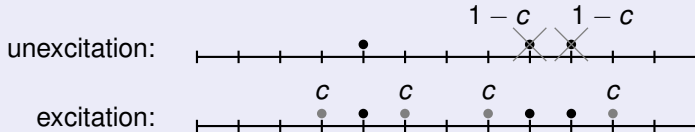
Mean density of excited sites: $\langle n \rangle = \frac{1}{L} \sum_i \langle n_i \rangle = c$

Kinetically constrained models (KCM)

Constrained dynamics: changes occur only around excited sites.

Fredrickson Andersen model in 1D

at least one neighbor of i must be excited to allow i to change

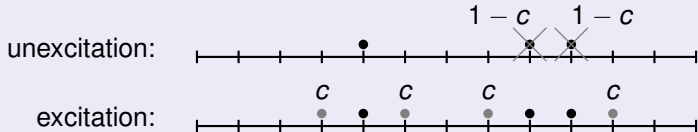


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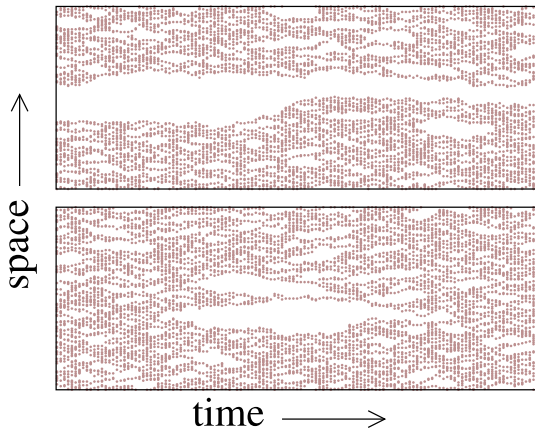
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- *same* equilibrium distribution $P_{\text{eq}}(\mathbf{n})$ with&without the constraint
- BUT: ageing, super-Arrhenius slowing down, dynamical heterogeneity

→ static free-energy landscape not useful
 → need for a dynamical description

Space-time “bubbles” of inactivity



From: Merolle, Garrahan and Chandler, PNAS **102**, 10837 (2005)

Questions

Active and inactive histories
having a probability of the same order



Coexistence of **dynamical** phases?

- How to describe a **dynamical** 1st order phase transition?
- Dynamical Landau free-energy landscape?

Activity of histories: order parameter

Activity K = number of events = (# excitations) + (# unexcitations)

(Dynamical) canonical ensemble

- β conjugated to energy (statics)
- s conjugated to activity K (dynamics)

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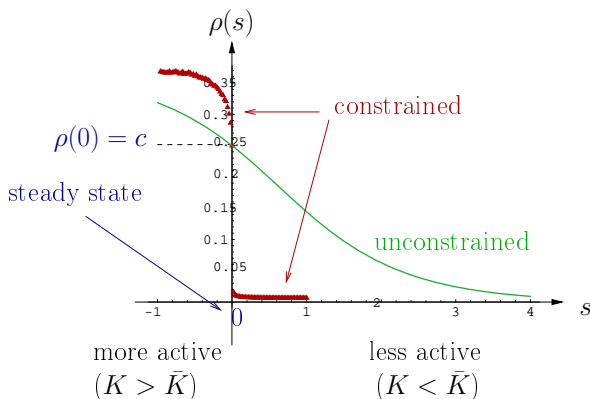
(Dynamical) canonical ensemble

- β conjugated to energy (statics)
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s -ensemble: $\left\{ \begin{array}{l} s < 0 : \text{more active histories ("large" activity } K > \bar{K}) \\ s = 0 : \text{equilibrium state (equilib. activity } K = \bar{K}) \\ s > 0 : \text{less active histories ("small" activity } K < \bar{K}) \end{array} \right.$

Dynamical phase transition: FA model ($d=1$)

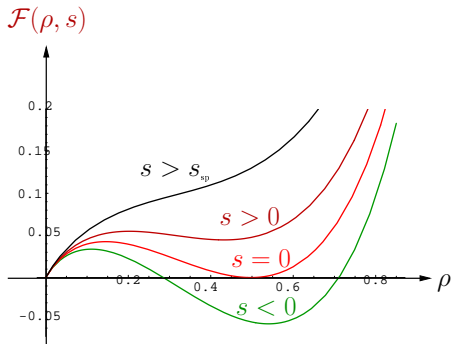
Density of excitations $\rho(s)$ depending on histories.



Comparison between **constrained** and **unconstrained** dynamics

Dynamical Landau free-energy landscape $\mathcal{F}(\rho, s)$

$$\text{Prob}_{[0,t]}(\rho, \mathbf{s}) \sim e^{-tL\mathcal{F}(\rho, \mathbf{s})} \quad \text{in the } \mathbf{s}\text{-ensemble}$$



Dynamical free energy:

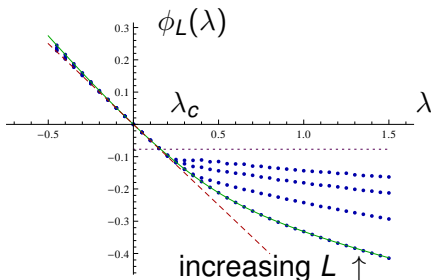
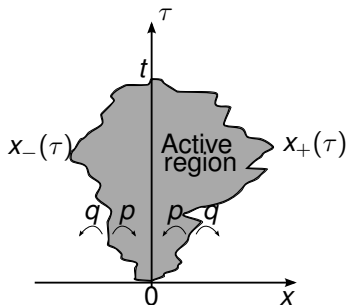
$$\psi(\mathbf{s}) = \min_{\rho} \mathcal{F}(\rho, \mathbf{s})$$

reached at $\rho = \rho(\mathbf{s})$

Scaling of the free energy in the interfacial regime

Finite-size scaling of the free energy ψ : $\phi_L(\lambda) = \psi\left(\frac{\lambda}{L}\right)$

$$s = \frac{\lambda}{L}$$



Interfacial model

Surface tension Σ



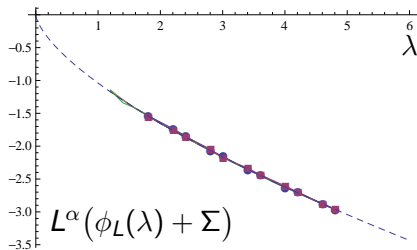
finite-size scaling

$$\phi_L(\lambda) = -\Sigma - A\left(\frac{\lambda}{L}\right)^{\frac{2}{3}}$$

Scaling function

Finite-size scaling of the free energy f : $\phi_L(\lambda) = f\left(\frac{\lambda}{L}\right)$

$$s = \frac{\lambda}{L}$$



Summary and outlook

- **Correspondence** $\left\{ \begin{array}{l} \text{finite-size scaling} \\ \text{of dyn. free-energy } \psi(s) \end{array} \right\} \longleftrightarrow \left\{ \begin{array}{l} \text{geometrical features} \\ \text{of active excitations} \end{array} \right\}$:

$$\underbrace{\phi_L(\lambda)}_{\substack{\text{finite-size} \\ \phi_L(\lambda) = f\left(\frac{\lambda}{L}\right)}} = \underbrace{-\Sigma}_{\substack{\text{surface tension} \\ \text{(excitations} \\ \text{are bubbles)}}} - \underbrace{A\left(\frac{\lambda}{L}\right)^\alpha}_{\substack{\alpha = \frac{2}{3} \\ \text{(boundaries are} \\ \text{Brownian)}}}$$

- Questions:

- ★ How to link $\left\{ \begin{array}{l} \text{the } (s > 0) \text{ bubbles of excitation to} \\ \text{the } (s = 0) \text{ bubbles of inactivity} \end{array} \right\}$?
- ★ How to write the **correspondence** in more realistic models?
- ★ Link dynamical phase transition and glassy features.

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J. Stat. Phys. **147** 1 (2012) – arXiv:1111.6394

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