Large deviations and heterogeneities in kinetically constrained models and glasses

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Outline

- Dynamic transition in KCMs- large deviations
  - Phenomenology of kinetically constrained models (KCMs)
  - Relevant order parameters for space-time trajectories
  - Results: mean-field/ finite dimensions
- Dynamic transitions in realistic glasses
- Driven KCMs, heterogeneities and large deviations

Phenomenology of KCMs

- Spin models on a lattice / lattice gases, designed to mimick steric effects in amorphous materials:
  - $s_i = 1$, $n_i = 1$: "mobile" particle - region of low density - fast dynamics
  - $s_i = -1$, $n_i = 0$: "blocked" particle - region of high density - slow dynamics
  - $H = \sum_i n_i \rightarrow < n >_{eq} = c = 1/(1 + e^{\beta}), \beta = 1/T$.
- Specific dynamical rules:

Fredrickson-Andersen (FA) model in 1 dimension: a spin can flip only if at least one of its nearest neighbours is in the mobile state.

"Dynamic heterogeneity" is put by hand.

Mobile/blocked particles self-organize in space $\rightarrow$ dynamical correlation length ξ.

(F. Ritort, P. Sollich, *Adv. Phys* **52**, 219 (2003).)

Phenomenology of KCMs

- In the FA model, configurations are split into 2 distinct partitions.
    - $\downarrow\uparrow\downarrow \rightleftharpoons \downarrow\downarrow\downarrow$ is forbidden
    - $n_i = 0$ for all i is a partition of its own.
    - all other configurations $(2^N - 1)$: "high-T" partition, active configurations.
    - $\rightarrow$ FA is reducible - "effectively" irreducible
    - $\rightarrow$ (even weak) reducibility is crucial in the study of phase-space trajectories.
- How to classify trajectories?
- Measure of activity?

Relevant order parameters for space-time trajectories

- Ruelle formalism: from deterministic dynamical systems to continous-time Markov dynamics
- Observable: Activity $K(t)$: number of flips between 0 and t, given a history $C_0 \to C_1 \to .. \to C_t$.
- Master equation: $\frac{\partial P}{\partial t}(C,t) = \sum_{C'} W(C' \to C)P(C',t) - r(C)P(C,t)$, where $r(C) = \sum_{C' \neq C} W(C \to C')$
- Introduce s (analog of a temperature), conjugated to K:
- $\hat{P}(C,s,t) = \sum_K e^{-sK} P(C,K,t) \to \partial_t \hat{P}(C,s,t) = \mathbb{W}_K \hat{P}(C,s,t)$, where $\mathbb{W}_K(s)(C,C') = e^{-s} W(C' \to C) - r(C)\delta_{C,C'}$.
- Generating function of K: $Z_K(s,t) = \sum_C \hat{P}(C,s,t) =< e^{-sK} >$.

  For $t \to \infty$, $Z_K(s,t) \simeq e^{t\psi_K(s)}$.

  $\to$ the large deviation function $\psi_K(s)$ is the largest eigenvalue of $\mathbb{W}_K(s)$.

Relevant order parameters for space-time trajectories

- Average activity: $\frac{<K>(s,t)}{Nt} \underset{t\to\infty}{=} -\frac{1}{N}\psi'_K(s)$.
  Average density of mobile particles at fixed s:
  $\rho_K(s) = \lim_{t\to\infty} \frac{1}{Z_K(s,t)} \sum_{\text{histories}} e^{-sK(\text{history})}\rho(t)$.
- Analogy with the canonical ensemble:

  - space of configurations, fixed β: $Z(\beta) = \sum_C e^{-\beta H} \simeq e^{-Nf(\beta)}, N \to \infty$.
  - space of trajectories, fixed s:
    $Z_K(s,t) = \sum_{C,K} e^{-sK} P(C,K,t) \simeq e^{-tf_K(s)}, t \to \infty$.
  - $f_K(s) = -\psi_K(s)$: free energy for trajectories
  - $\rho_K(s)$, $\frac{<K>(s,t)}{Nt}$: activity/chaoticity.

Active phase: $< K > (s,t)/(Nt) > 0$, $\rho_K(s) > 0$: $s < 0$.
Inactive phase: $< K > (s,t)/(Nt) = 0$, $\rho_K(s) = 0$: $s > 0$.

Results: Mean-Field FA

- $W_i(0 \to 1) = k' \frac{n}{N}$, $W_i(1 \to 0) = k \frac{n-1}{N}$, $n = \sum_i n_i$.
- The result is a variational principle for $\psi_K(s)$, involving a Landau-Ginzburg free energy $F_K(\rho, s)$:

$\frac{1}{N} f_K(s) = -\frac{1}{N}\psi_K(s) = \min_\rho F_K(\rho, s)$, with

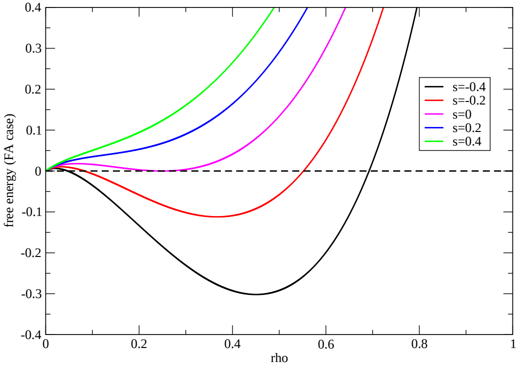
$$F_K(\rho, s) = -2\rho e^{-s}(\rho(1-\rho)kk')^{1/2} + k'\rho(1-\rho) + k\rho^2$$

- Minima of $F_K(\rho, s)$ at fixed s:

  - $s > 0$: inactive phase, $\rho_K(s) = 0$, $\psi_K(s)/N = 0$.
  - $s = 0$: coexistence $\rho_K(0) = 0$ and $\rho_K(0) = \rho^*$, $\psi_K(0) = 0$, $\to$ first order phase transition.
  - $s < 0$: active phase, $\rho_K(s) > 0$, $\psi_K(s)/N > 0$.

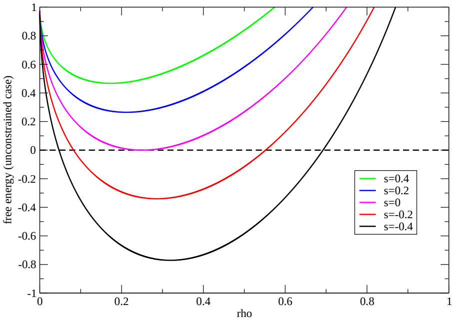
Results: Mean-Field FA

- $F_K(\rho, s)$ for different values of s:



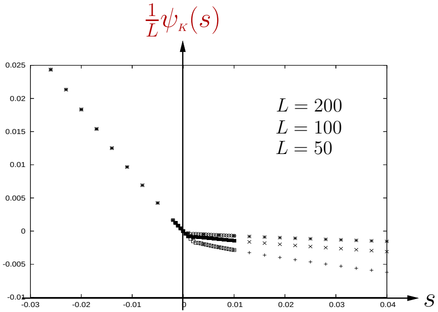
Results: Mean-Field unconstrained model

- One removes the constraints: $W_i(0 \to 1) = k'$, $W_i(1 \to 0) = k$, for all i
- $F_K(\rho, s) = -2e^{-s}(\rho(1-\rho)kk')^{1/2} + k'(1-\rho) + k\rho$
- No phase transition



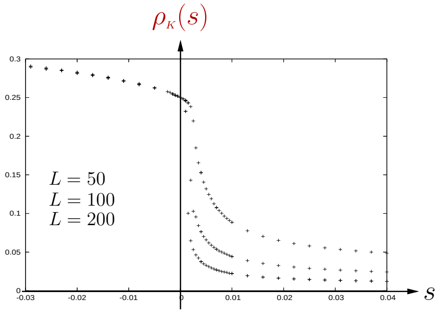
Results in finite dimensions

- Numerical solution using the algorithm of Giardina, Kurchan, Peliti for large deviation functions.
- First-order phase transition for the FA model in 1d.



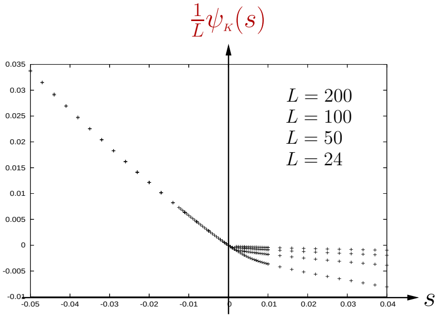
Results in finite dimensions

- $\rho_K(s)$ for the FA model in 1d.



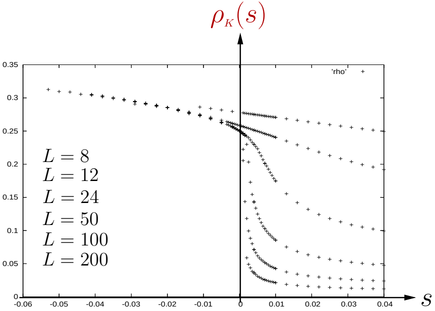
Results in finite dimensions

- First-order phase transition for the East model.



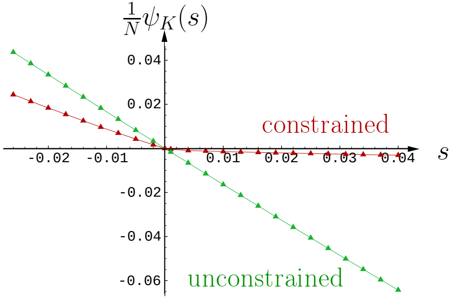
Results in finite dimensions

- $\rho_K(s)$ for the East model.



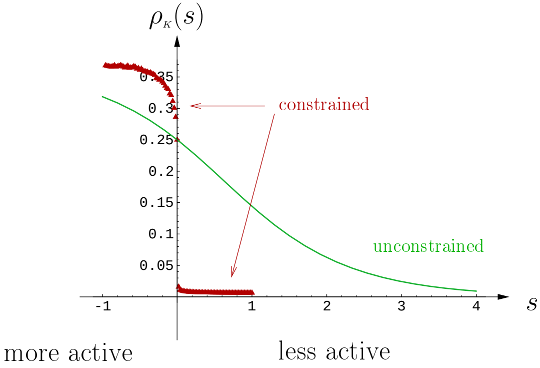
Results in finite dimensions

- Comparison between 1d FA model and unconstrained model $A \xrightarrow{k} \emptyset$, $\emptyset \xrightarrow{k'} A$.



Results in finite dimensions

- $\rho_K(s)$ for the 1d FA model and $A \xrightarrow{k} \emptyset$, $\emptyset \xrightarrow{k'} A$.

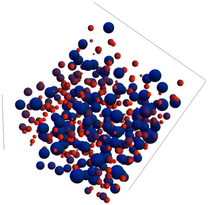


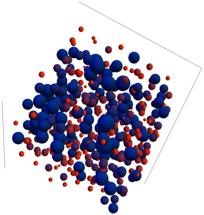
Conclusions

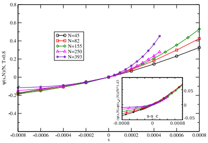
- Large deviation functions of generating functions in trajectories space provide useful order parameters that probe active/inactive phases. s plays the role of a "chaoticity" temperature.
- KCMs which are (even weakly) reducible show a first-order phase transition at $s = 0$. In a real system, coexistence between inactive and active states induce the slowing down of the dynamics. Configurations where the number of spins in the mobile phase is subextensive are responsible for the slow dynamics.
- Possible link between ξ -dynamical correlation length- and moments of $K(t)$.
- Need fot studies of more realistic (particles) glassy systems in trajectory space.

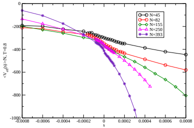
with: J.P. Garrahan (Nottingham), R.L. Jack (Bath), V. Lecomte, K. van Duijvendijk, F. van Wijland (Paris), PRL (2007), J. Phys. A (2009)

Dynamic transitions in realistic glasses









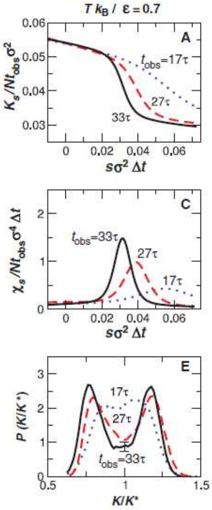
- Cloning algorithm for a generalized activity, LJ mixture $K(t) = \int_0^t V_{eff}(t')dt'$ where $Veff = \sum_i \left[\frac{\beta}{4} F_i^2 + \frac{1}{2}\nabla F_i\right]$ with V. Lecomte, F. van Wijland.
- Prob to stay in the same configuration between t and $t + dt \sim exp(-\beta V_{eff} dt)$

  Two phases:

  Small K: energy basins, "inactive"

  Large K: local maxima, "active"
- Link between dynamic phases and energy landscape?

Dynamic transition in realistic glasses

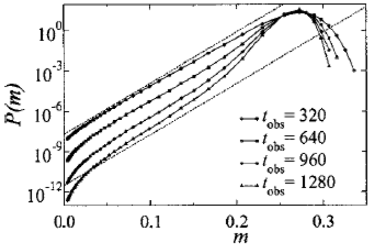


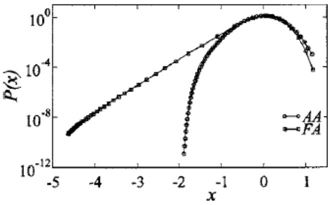
- Transition path-sampling in the s-ensemble.

  (Hedges, Jack, Garrahan, Chandler, Science (2009)).

- Activity:
  $K(t) = \Delta t \sum_{t=0}^{t_{obs}} \sum_{i=1}^{N} [\vec{r}_i(t+\Delta t) - \vec{r}_i(t)]^2$
  Δt: time to move a distance $\sim$ molecular diameter.

Dynamic transition in realistic glasses





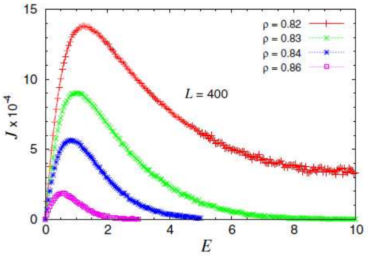
- Experimental challenge: measure $P(K)$. (for KCMs: Jack, Garrahan, Chandler, JCP (2006)).

- Particle tracking?
- Importance of finite-size effects
- Experimental parameter for s?

Driven KCMs, heterogeneities and large deviations

2d ASEP with kinetic constraints, (with F. Turci, EPL (2011))

- A particle can hop to an empty neighbouring site if it has at most 2 occupied neighbouring sites, efore and after the move.
- Driving field $\vec{E}$



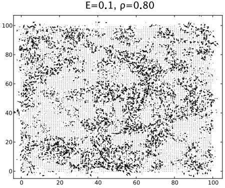
Pour $\rho > \rho_c$,

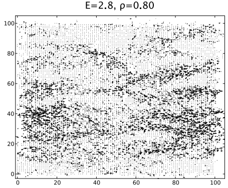
- $E < E_{max}$: shear-thinning, the current J grows with E
- $E > E_{max}$: shear-thickening, J decreases with E

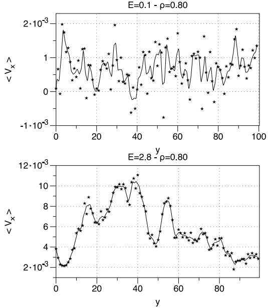
Driven KCMs, heterogeneities and large deviations

Microscopic analysis: transient shear-banding at large fields, localization of the current.

→ dense domain walls play the role of kinetic traps.

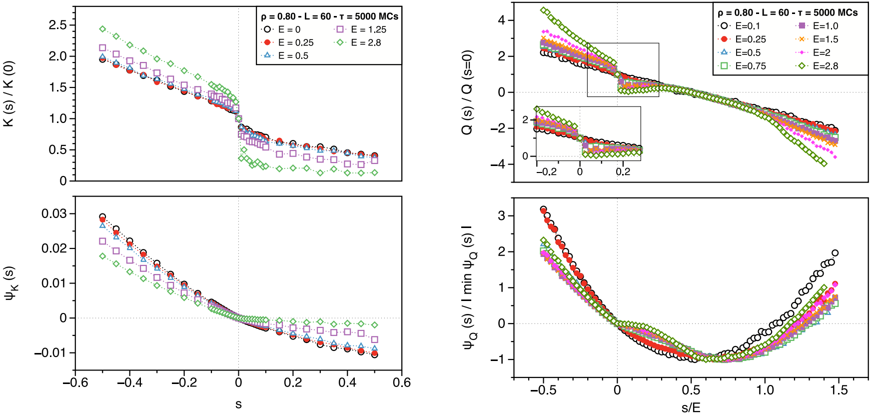






Large deviation functions for the activity $K(t)$ and the integrated current $Q(t)$:

- For K, the first-order transition persists like for unforced KCMs.
- For Q, there is a first-order transition only at large fields (coexistence of histories with large current and histories with no current).
- $\rightarrow$ Link between current heterogeneities and singularity in the large deviation function.



(with F. Turci)

Results in finite dimensions

- Numerical solution using the algorithm of Giardina, Kurchan, Peliti (discrete time Markov processes) for large deviation functions.
- $P(C,t) = \sum_{C'} W(C \to C')P(C', t-1)$
- solution at fixed C_0:

$$P(C,t) = \sum_{C_1,\ldots,C_{t-1}} W(C_0 \to C_1)\ldots W(C_{t-1} \to C)$$

- One looks for the large deviation function of an additive observable $A = \alpha(C_0 \to C_1) + \cdots + \alpha(C_{t-1} \to C_t)$.
$< e^{-sA} > \simeq e^{t\psi_\alpha(s)}$, $t \to \infty$

Results in finite dimensions

- Defining $W_\alpha(s)(C \to C') = W(C \to C') e^{-s\alpha(C \to C')}$,

$$< e^{-sA} >= \sum_{C_1,\dots,C_t} \prod_{i=0}^{t-1} W_\alpha(s)(C_i \to C_{i+1})$$

- but $W_\alpha(s)$ is not a stochastic matrix.
- Introducing $Y(C) = \sum_{C'} W_\alpha(s)(C \to C')$, and $W'_\alpha(s)(C \to C') = \frac{W_\alpha(s)(C \to C')}{Y(C)}$, $W'_\alpha(s)$ is stochastic.

$$< e^{-sA} >= \sum_{C_1,\dots,C_t} \prod_{i=0}^{t-1} W'_\alpha(s)(C_i \to C_{i+1}) Y(C_i)$$

Results in finite dimensions

- One performs the dynamics of N copies ($N \gg 1$) of the system:
  - each copy in configuration C is cloned with probability $Y(C)$
  - stochastic evolution with $W'_\alpha(s)(C \to C')$
  - the number of copies is sent back uniformly to N, with ratio X_t
- $\psi_\alpha(s) = -\lim_{t\to\infty} \frac{1}{t} \ln(X_1 \ldots X_t)$
- (C. Giardinà, J. Kurchan, L. Peliti, *Phys. Rev. Lett.* **96**, 120603 (2006)).