Large deviations and heterogeneities in driven or non-driven kinetically constrained models

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with: J.P. Garrahan (Nottingham), R.L. Jack (Bath), V. Lecomte, K. van Duijvendijk, F. van Wijland (Paris), F. Turci (Montpellier)

Outline

- Introduction: what is a glassy system?
- Dynamic transition in Kinetically Constrained Models- large deviations
  - Phenomenology of kinetically constrained models (KCMs)
  - Relevant order parameters for space-time trajectories: activity K
  - We will show that in the stationary state, there is a coexistence between active and inactive trajectories.
  - These trajectories can be probed by tuning an external parameter s, or "chaoticity temperature".
  - Results: mean-field/ finite dimensions
- Driven KCMs, current heterogeneities and large deviations
  - A new dynamic phase transition for the integrated current Q
  - Fluctuations: large deviation function for the current
  - Link with microscopic spatial heterogeneities

Introduction

- What is a glassy phase?
- No static signature difference between fluid and glass
- No thermodynamical transition, no T_c
- How can one realize that a system is in a glassy state?
  - -either drive it out-of-equilibrium or investigate its relaxation properties
  - $\longrightarrow$ dramatic increase in viscosity, ageing.
- Importance of the dynamics and of spatio-temporal heterogeneitites (Fredrickson-Andersen 1984) $\longrightarrow$ Fluctuations!
- Models with
  - long-lived correlated spatial structures
  - slow, intermittent dynamics.
- Our choice: Kinetically Constrained Models (KCMs).

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
- 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.

$\downarrow\uparrow\downarrow \rightleftharpoons \downarrow\downarrow\downarrow$ is forbidden.

Mobile/blocked particles self-organize in space $\longrightarrow$ glassy, slow relaxation and dynamical correlation length ξ.

How to classify time-trajectories and their activity?

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

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 $C_0 \rightarrow C_1 \rightarrow .. \rightarrow C_t$.
- Master equation: $\frac{\partial P}{\partial t}(C,t) = \sum_{C'} W(C' \rightarrow C)P(C',t) - r(C)P(C,t)$, where $r(C) = \sum_{C' \neq C} W(C \rightarrow C')$
- Introduce s (analog of a temperature), conjugated to K:
- $\hat{P}(C,s,t) = \sum_K e^{-sK} P(C,K,t) \rightarrow$ new evolution equation
- Generating function of K: $Z_K(s,t) = \sum_C \hat{P}(C,s,t) =< e^{-sK} >$.
  For $t \rightarrow \infty$, $Z_K(s,t) \simeq e^{t\psi_K(s)}$.
  $\rightarrow \psi_K(s)$ is the large deviation function for the activity K.

Relevant order parameters for space-time trajectories

- Average activity: $\frac{<K>(s,t)}{Nt} \underset{t\to\infty}{=} -\frac{1}{N}\psi'_K(s)$.
- 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
- $\frac{<K>(s,t)}{Nt}$: mean activity/chaoticity.

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

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 $F_K(\rho, s)$ (ρ: density of mobile spins):

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

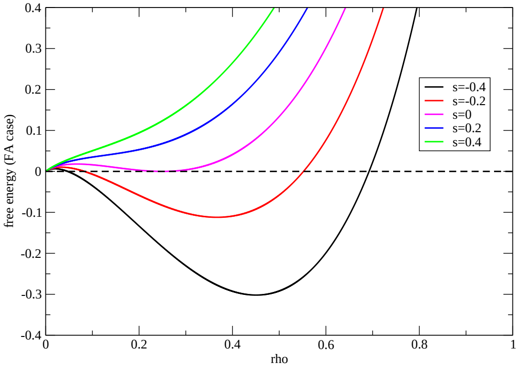
$$F_K(\rho, s) = -2\rho e^{-s}(\rho(1-\rho)kk')^{1/2} + k'\rho(1-\rho) + k\rho^2$$

- 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, $\rho_K(s) > 0$, $\psi_K(s)/N > 0$.

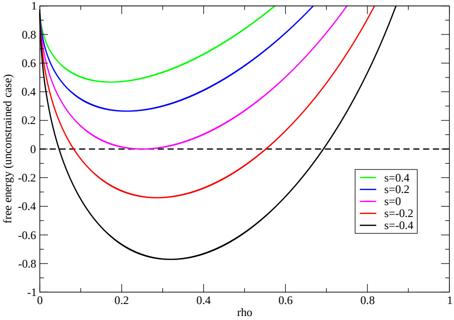
Results: Mean-Field FA

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



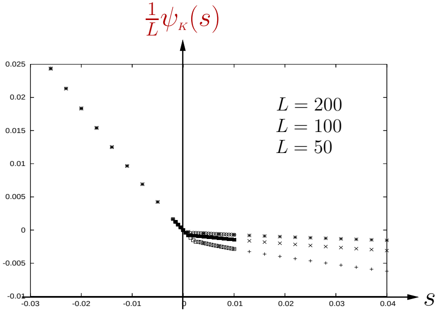
Results: Mean-Field unconstrained model

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



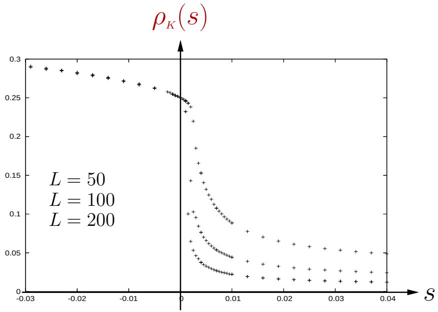
Results in finite dimensions

- Numerical solution using the algorithm of Giardina, Kurchan, Peliti for large deviation functions. (C. Giardinà, J. Kurchan, L. Peliti, *Phys. Rev. Lett.* **96**, 120603 (2006)).
- First-order phase transition for the FA model in 1d.



Results in finite dimensions

- $\rho_K(s)$ for the FA model in 1d. True also for particle systems!

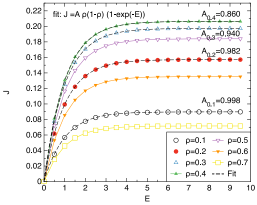


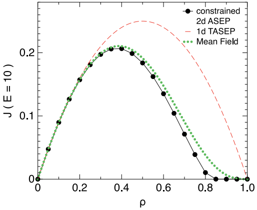
- *"Dynamic first-order transition in kinetically constrained models of glasses"*, J.P. Garrahan, R.L. Jack, V. Lecomte, E. Pitard, K. van Duijvendijk, F. van Wijland, *Phys. Rev. Lett. 98, 195702* (2007).
- *"First-order dynamical phase transition in models of glasses: an approach based on ensembles of histories"*, J.P. Garrahan, R.L. Jack, V. Lecomte, E. Pitard, K. van Duijvendijk, F. van Wijland, *J. Phys. A 42* (2009).

Driven KCMs, heterogeneities and large deviations

2d ASEP with kinetic constraints, a model of particles at fixed density ρ on a 2d square lattice (model introduced by M. Sellitto, 2008).

- Dynamical constraint: *A particle can hop to an empty neighbouring site if it has at most 2 occupied neighbouring sites, before and after the move*
- Asymmetric Exclusion Process: Driving field $\vec{E}$ in the horizontal direction.



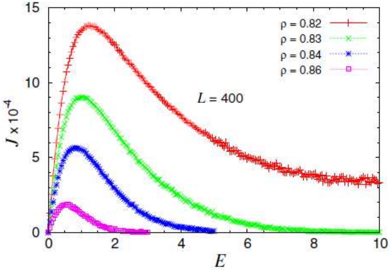


For low densities ρ,

- the current J is an increasing function of E
- J is well approximated by a mean-field argument: $J = (1 - e^{-E})\rho(1 - \rho)(1 - \rho^3)^2$

Driven KCMs, current heterogeneities and large deviations

The dynamical constraints induce a new transport regime.



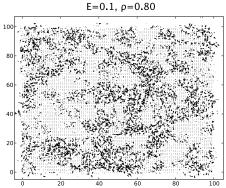
For large densities, $\rho > \rho_c \simeq 0.78$,

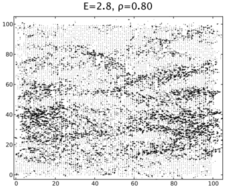
- $E < E_{max}$: shear-thinning, the current J grows with E
- $E > E_{max}$: shear-thickening, J decreases with E

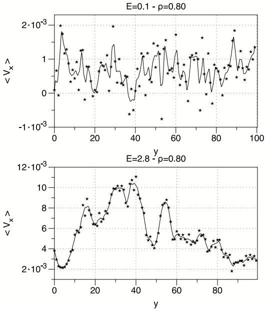
Driven KCMs, current heterogeneities and large deviations

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

→ very different density profiles for small and large driving fields.

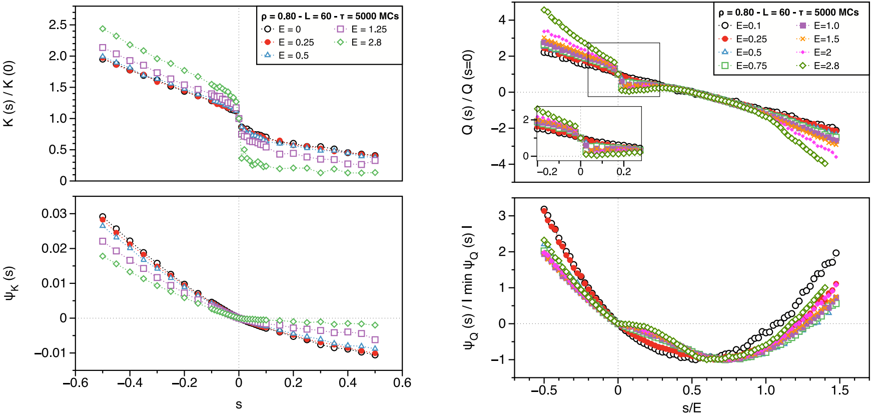




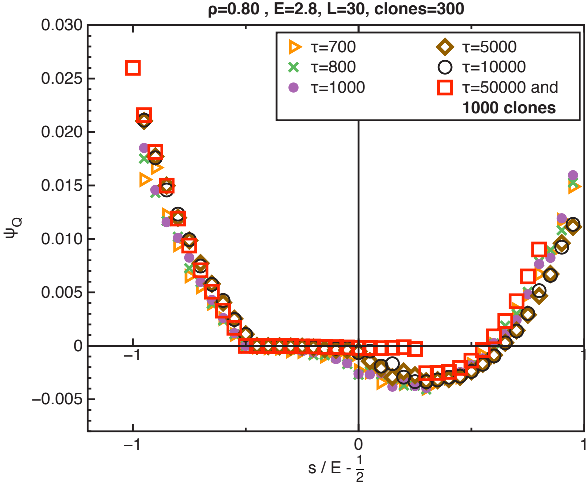


Large deviation functions for the activity $K(t)$ and the integrated current $Q(t)$: $Q(t) = \int_0^t J(t')dt'$.

- 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). Absent for ASEP without constraints!



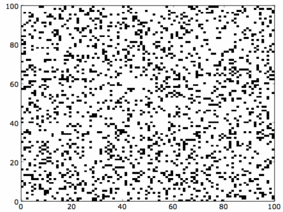
Large deviation functions for the integrated current $Q(t)$:
Fluctuation theorem $P(Q)/P(-Q) = e^{Q}$ implies $\psi_Q(s) = \psi_Q(E - s)$.

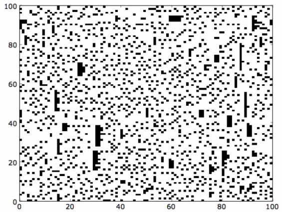


Dynamical blocking walls -1

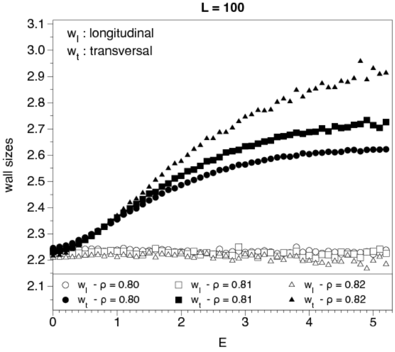
Dense domain walls play the role of kinetic traps at large fields.

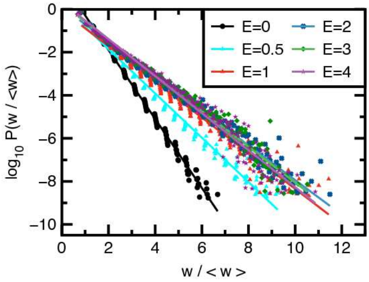
- At small E, voids are random.
- At large E, voids organize into domain walls transverse to the field.



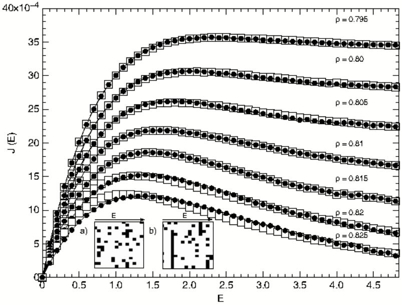


Dynamical blocking walls -2





Dynamical blocking walls -3

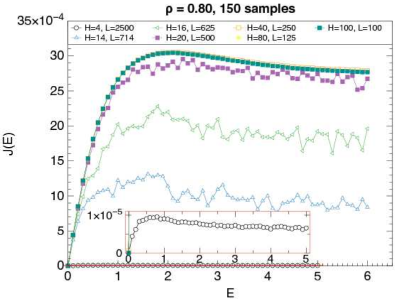


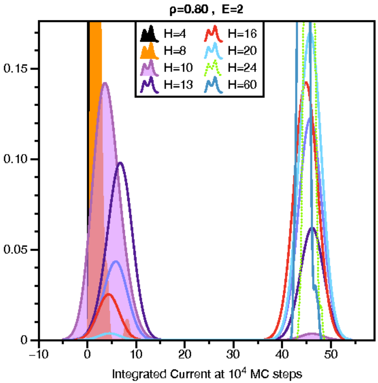
Phenomenological fit of $J(E)$ on the basis of the effective blocking effect of the walls:
$J(E) \simeq A(1 - e^{-E})(1 - \alpha < w >)$.

• *"Large deviations and heterogeneities in a driven kinetically constrained model"*, F. Turci, E. Pitard, *Europhys. Lett. 94, 10003* (2011).

Size effects -1

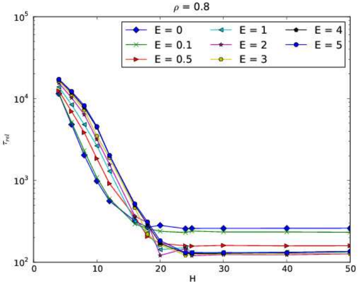
H: vertical confinement length.





Size effects -2

$\xi(\rho, E)$: dynamical correlation length.



For $E = 0$,

$\xi(\rho) \propto exp(exp(C/(1-\rho)))$. (Toninelli, Biroli, Fisher, 2004.)

$\rightarrow$ Determination of $\xi(\rho, E)$: dynamical correlation length in the presence of an external field E.

F. Turci, M. Sellitto, E. Pitard, in preparation

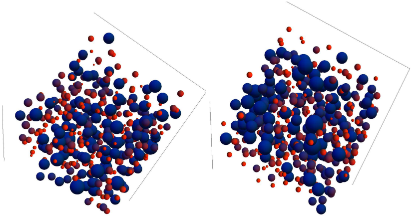
Conclusions

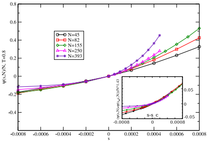
- Large deviation functions of generating functions in trajectories space provide useful order parameters that probe active/inactive phases or large current/small current phases according to the observable. s plays the role of a "chaoticity" temperature.
- KCMs show a first-order phase transition at $s = 0$. In a real system, there is coexistence between 2 different dynamical phases.
- How to probe these two phases experimentally?
- Link between transport properties, microscopic lengths between defects and dynamical correlation lengths?
- Dynamic transitions and phase coexistence in realistic (Lennard-Jones) glasses $\longrightarrow$ new perspectives

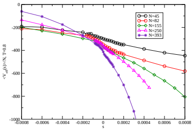
  L. Hedges, R.L. Jack, J-P. Garrahan, D.C. Chandler, Science, 323, 1309 (2009).

  E. Pitard, V. Lecomte, F. van Wijland, Europhys. Lett. 96 56002 (2011).

Dynamic transitions in realistic glasses







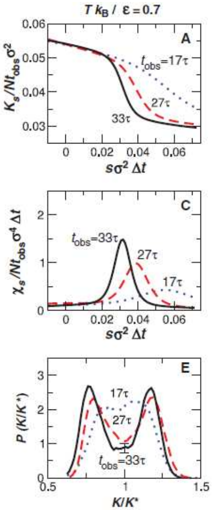
- Cloning algorithm for a generalized activity, LJ mixture $K(t) = \int_0^t V_{eff}(t')dt'$ where $Veff = \sum_i \left[\frac{\beta}{4} F_i^2 + \frac{1}{2} \nabla F_i\right]$ with V. Lecomte, F. van Wijland.
- Prob to stay in the same configuration between t and $t + dt \sim exp(-\beta V_{eff} dt)$

  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.

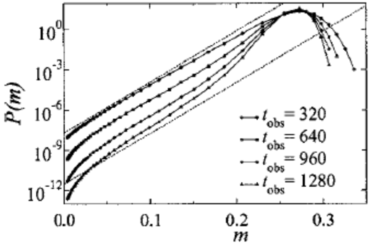
  (Hedges, Jack, Garrahan, Chandler, Science (2009)).

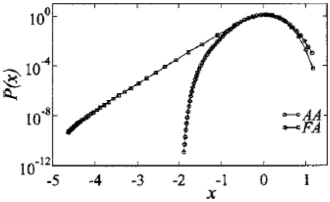
- Activity:

  $K(t) = \Delta t \sum_{t=0}^{t_{obs}} \sum_{i=1}^{N} [\vec{r}_i(t + \Delta t) - \vec{r}_i(t)]^2$

  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?

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:

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

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

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)).