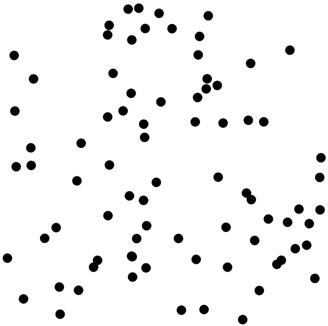
Thermodynamics of histories: some examples

Vivien Lecomte[1,2], Cécile Appert-Rolland[1], Estelle Pitard[3], Frédéric van Wijland[1,2]

[1]Laboratoire de Physique Théorique, Université d'Orsay
[2]Laboratoire Matière et Systèmes Complexes, Université Paris 7
[3]Laboratoire Colloïdes, Verres et Nanomatériaux, Université Montpellier 2

Nancy - 19th May 2006

Histories vs configurations



In equilibrium

- Boltzmann weight $P(\mathcal{C}) \propto e^{-\beta\mathcal{H}(\mathcal{C})}$
- time average from configurational average

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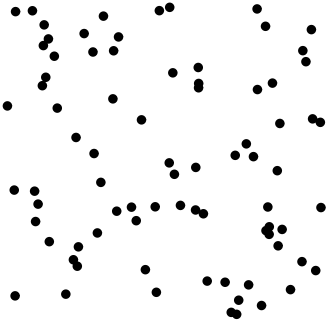

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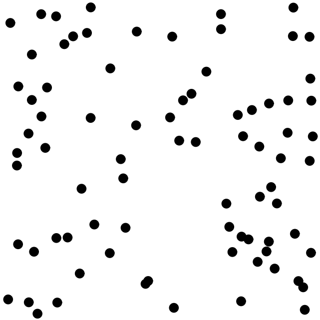

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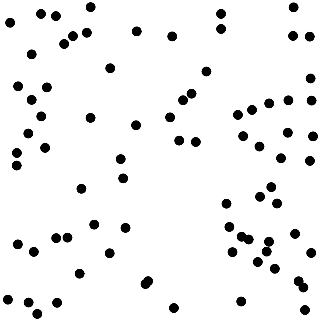

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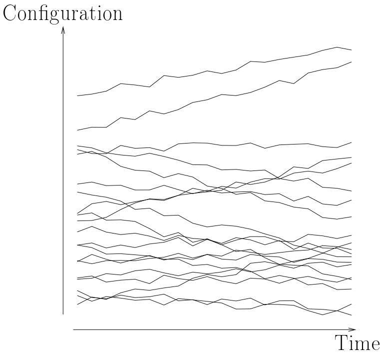

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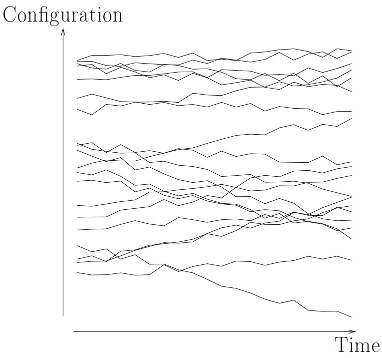

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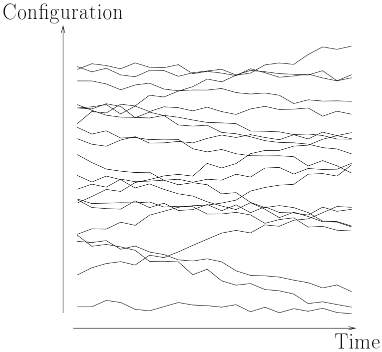

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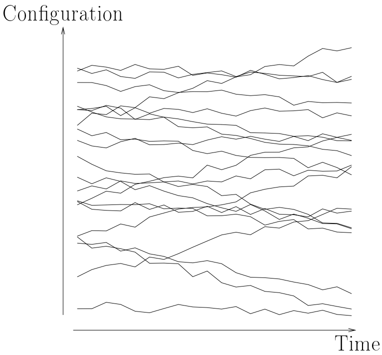
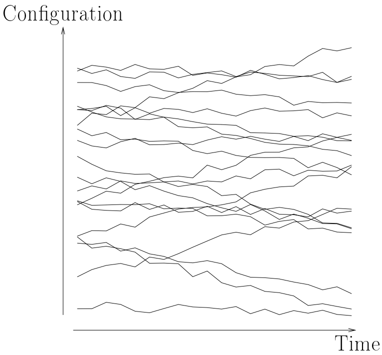


Where dynamics matters

- out of equilibrium systems

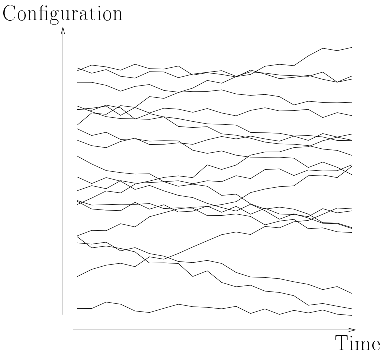
Histories vs configurations



Where dynamics matters

- out of equilibrium systems
- glassy dynamics
- evolution driven by rare events

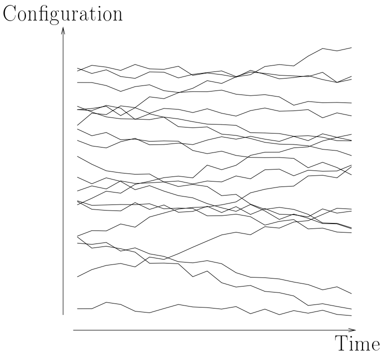
Histories vs configurations



Historical background

- Ruelle's thermodynamic formalism: deterministic dynamics

Histories vs configurations



Historical background

- Ruelle's thermodynamic formalism: deterministic dynamics
- Pierre Gaspard: *discrete* time stochastic dynamics
- our contribution: *continuous* time stochastic dynamics

Contents

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Dynamical partition function

Motivation

- Thermodynamics of configurations

$$Z(\beta, N) = \sum_{\mathcal{C}} \mathrm{e}^{-\beta\,\mathcal{H}(\mathcal{C})} = \mathrm{e}^{N\,f(\beta)} \qquad \text{(large } N\text{)}$$

Dynamical partition function

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Conjugate variables

- μ conjugated to number of particles
- s conjugated to Kologorov-Sinai entropy

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Breaking of analyticity

- $f(\beta)$ not analytic in $\beta_c \leftrightarrow$ (configurational) phase transition
- $f_{\text{dyn}}(s)$ not analytic in $s_c \leftrightarrow$ “phases” in space of histories

System with Markovian dynamics: results

$$\partial_t P(\mathcal{C},t) = \sum_{\mathcal{C}'} \Big[\underbrace{W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}',t)}_{\text{gain term}} - \underbrace{W(\mathcal{C} \to \mathcal{C}') P(\mathcal{C},t)}_{\text{loss term}} \Big]$$

Advantages of the Markov approach

- $f_{\rm dyn}(s)$ is the largest eigenvalue of $\mathbb{W}_+$, of eigenvector $|\Pi_+\rangle$
- $\rightarrow$ exact results, numerical approach

Dynamical state observable

$\mathcal{O}_+(s) \equiv$ mean value in the state $|\Pi_+\rangle$

$$\mathcal{O}_+(s) = \begin{cases} \text{typical value of } \mathcal{O} \text{ in } \textbf{highly chaotic} \text{ histories} & (s \to \infty) \\ \text{typical value of } \mathcal{O} \text{ in } \textbf{steady state} & (s \simeq 0) \\ \text{typical value of } \mathcal{O} \text{ in } \textbf{lowly chaotic} \text{ histories} & (s \to -\infty) \end{cases}$$

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The Ising ferromagnet (1)

Equilibrium

- N spins $\{\sigma_i\}$ of total magnetisation $M = \sum_i \sigma_i$
- Hamiltonian (infinite range interaction)

$$H\big(\{\sigma_i\}\big) = -\frac{1}{2N}\sum_{i,j}\sigma_i\sigma_j$$

Phase transition

- high temperature (disordered) phase: $\beta < 1 \quad \Rightarrow \quad m = 0$
- low temperature (ordered) phase: $\beta > 1 \quad \Rightarrow \quad m = \pm m_0$
- m_0 solution of: $\tanh m_0 = \beta \tanh m_0$

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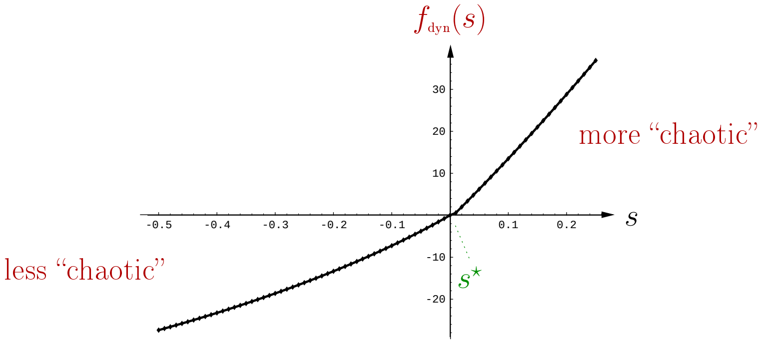
The Ising ferromagnet (2)

Dynamics

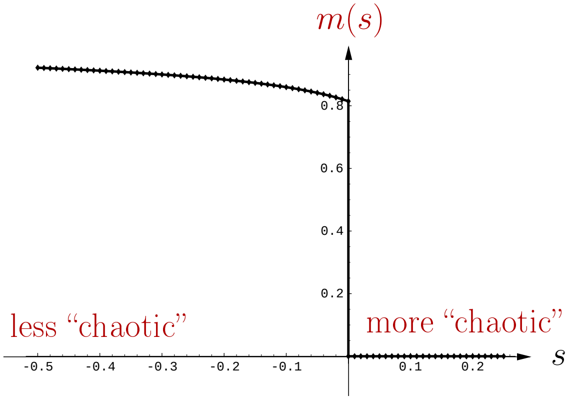
transition rates

$$W(\sigma_i \to -\sigma_i) = \mathrm{e}^{-\beta\sigma_i M/N}$$



Dynamical phase transition at $s = s^\star$.

Magnetization



Example II: the contact process

Dynamics (infinite range interaction)

- N sites $\{n_i\}$ with $n_i = 1$ or 0
- Total number of particles $n = \sum_i n_i$
- Transition rates:

$$W(n_i \to 1 - n_i) = \begin{cases} \lambda \frac{n}{N} & \text{if} \quad n_i = 0 \\ 1 & \text{if} \quad n_i = 1 \end{cases}$$

Collective variable: n

Transition rates:

$$W(n \to n \pm 1) = \begin{cases} (N - n)\lambda \frac{n}{N} \\ n \end{cases}$$

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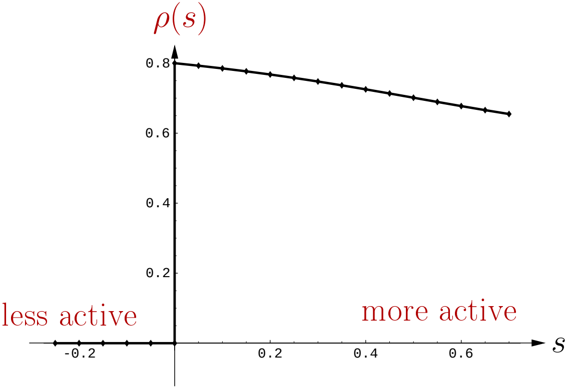
Density

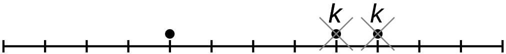


Example III: a kinetically constrained model

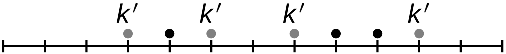
Dynamics (Fredrickson Andersen model)

- L sites $\{n_i\}$ with $n_i = 1$ or 0 in one dimension
- Constraint: at least one neighbor is alive to allow a move
- Transition rates:
  - annihilation with rate k
  - creation with rate k'

annihilation:



creation:



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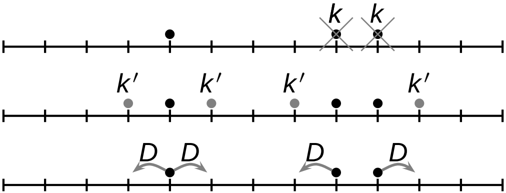
  - creation with rate k'
  - diffusion with rate D (not constrained)

annihilation:

creation:

diffusion:



Example III: a kinetically constrained model

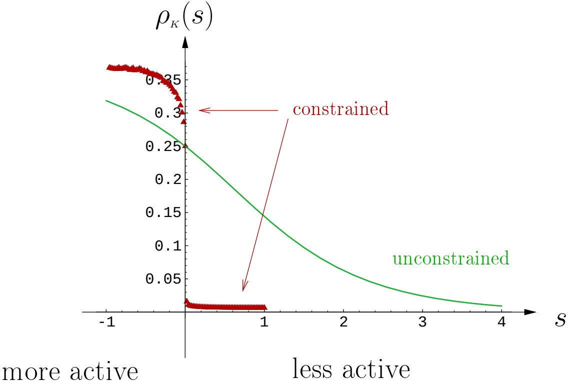
Comparison with the unconstrained model

- Same equilibrium distribution
- Slow decay in the constrained model

Numerical simulation

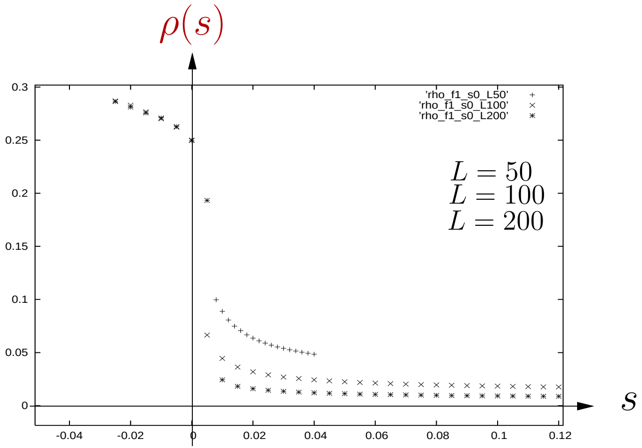
- Generalization of [Giardinà, Kurchan, Peliti]'s algorithm
- Biased rates to explore fixed-s dynamics
- Direct measurement of $\rho(s)$

Dynamical phase transition



Comparison between constrained and unconstrained model

Dynamical phase transition



Large size scaling

Summary

- Thermodynamic formalism $\Leftrightarrow$ large time limit
- Dynamical free energy f_{dyn} $\rightarrow$ *dynamical phase transition*
- Dynamical order parameter $m(s)$

Perspective

- Other kinds of phase transition
- Caracterization of glassy dynamics

References:

- *Chaotic properties of systems with Markov dynamics*, PRL '05
- `cond-mat/next-week`