Glassy dynamics of kinetically constrained models.

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(with A. Faggionato and F. Martinelli)

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Scope

• Kinetically constrained models (KCM):
  » Simple to define continuous time Markov process on $\Omega_A = \{0, 1\}^A$.
  » Simple stationary distribution (Bernoulli i.i.d).
  » However: Very interesting dynamics.
    • Particularly the large-scale dynamics (large systems, large times).

• Glassy effects arise at low temperature (high density):
  » Very slow relaxation to equilibrium (super Arrhenius).
  » Complex cooperative dynamics.
  » Dynamical heterogeneity and ageing.
  » Quantitative predictions about real glasses. [Keys, Garrahan, Chandler PNAS 2013]

• We will focus on:
  » Relaxation to equilibrium: Spectral gaps, mixing-times, local convergence...
  » Limiting dynamics on large scales (conjectures and videos).
Heuristics

• Motivation of KCM from glassy/amorphous systems
  » Disordered fluid like arrangement of particles
  » At high density the material is jammed – very slow dynamics!
    • Behaves like a ‘solid’ on experimentally relevant times scales,
    • but flow on longer time scales.

• Kinetically constrained models (KCM):
  » Coarse grained on a lattice (high density box -> 1).
  » The constraint mimics how the low density regions facilitate dynamics.
East Process: Definition

- 1D example the **East Process**:
  - \( q \in (0, 1) \) equilibrium density of (facilitating) zeros
  - Configurations: \( \sigma = (\sigma_x)_{x=1}^L, \sigma_x \in \{0, 1\}, \Omega_L = \{0, 1\}^L \)
  - Glauber dynamics with a *kinetic constraint*.
  - Zeros facilitating (mimic the *cage effect* in glasses).
  - Fixed zero at the origin: **Ergodic boundary condition**.

\[
\Lambda = \{1, 2, \ldots, L\}
\]

\[
\begin{array}{ccccccccccc}
0 & 1 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 1 \\
\sigma_1 & \sigma_2 & \cdots & & & & & & & \cdots & \sigma_L \\
\end{array}
\]
• Spin-flip dynamics:
  » Each site with rate 1 (indep.) attempts to update
  » then, iff $c_x(\sigma) = 1 - \sigma_{x-1} = 1$, toss a $p$-coin, refresh.

\[
\sigma_x = \begin{cases} 
1 \text{ with prob. } 1 - q \\
0 \text{ with prob. } q 
\end{cases}
\]

\[
\begin{array}{cccccccccccc}
0 & 1 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 1 \\
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**East Model: Definition**

- **Spin-flip dynamics**
  
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\end{cases}
\]

\[
\begin{array}{c}
0 \\
q \\
p = 1 - q
\end{array}
\]

\[
\begin{array}{cccccccccccc}
0 & 1 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 1 \\
\sigma_1 & \sigma_2 & \cdots & & \cdots & \sigma_L
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\begin{array}{cccccccc}
0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \\
\sigma_1 & \sigma_2 & \cdots & & & & & \sigma_L
\end{array}
Simple representation

- Vacancies (zeros) represented by articles black circles (particles).
East Model: Definition

- Graphical construction:
East Model: Definition

- Graphical construction:
East Model: Definition

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East Model: Definition

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East Model: Definition

- Graphical construction:
• Graphical construction:
East Model: Definition

- Graphical construction:
Dynamics

• Example jump chain (starting from all 1s):

[Source: Aldous, Diaconis JSP 107(5) (2002)]
If the lattice, $\Lambda$, is finite then we can define:

- Matrix of transition probabilities $P_t(\eta, \sigma)$ such that

$$\mathbb{E}_\eta[f(\eta_t)] = \sum_{\sigma \in \Omega} P_t(\eta, \sigma)f(\sigma) = P_t f(\eta)$$

- and

$$p_t(\sigma) = \sum_{\eta \in \Omega} p_0(\eta)P_t(\eta, \sigma) = p_0P_t(\sigma)$$

- Q-matrix of transition rates.
  - Rate to go from $\sigma$ to $\eta$: $Q(\sigma, \eta) \geq 0$, $\sigma \neq \eta$.
  - with diagonal $Q(\sigma, \sigma) = -\sum_{\eta \neq \sigma} Q(\sigma, \eta)$ then

$$P_t = e^{tQ}$$

$$\frac{d}{dt}P_t = P_t Q = HQP_t, \quad P_0 = I_d$$
Continuous time Markov processes

- If the lattice, $\Lambda$, is infinite then $\Omega_{\Lambda}$ is no longer countable:
  - Analogue of the transition matrix is the semigroup $P_t$ s.t.
    \[ \mathbb{E}_\eta[f(\eta_t)] = P_t f(\eta), \quad p_t = p_0 P_t. \]
  - Analogue of the $Q$-matrix is the generator.
    - For $f$ depending only on the configuration at finitely many sites
      \[ \mathcal{L} f(\sigma) = \sum_{\eta \neq \sigma} Q(\sigma, \eta) (f(\eta) - f(\sigma)) \]
      \[ \mathcal{L} f = \lim_{t \to 0} \frac{P_t f - f}{t} \]
    - Module domains of definition these behave as you would expect from countable state Markov process...
      - E.g. forward and backward equation...
East Model: Definition

• Spin-flip dynamics
  » Each site with rate 1 (indep.) tries to update
  » then, iff \( c_x(\sigma) = 1 - \sigma_{x-1} = 1 \), toss a \( p \)-coin, refresh.
  » Long hand...

\[
\mathcal{L} f(\eta) = \sum_{x \in \Lambda} c_x(\eta) [q\eta_x + (1-q)(1-\eta_x)] (f(\eta^x) - f(\eta))
\]
East Model: Definition

• Spin-flip dynamics
  » Each site with rate 1 (indep.) tries to update
  » then, iff \( c_x(\sigma) = 1 - \sigma_{x-1} = 1 \), toss a p-coin, refresh.
  » More compact notation...

\[
\mathcal{L} f(\eta) = \sum_{x \in \Lambda} c_x(\eta) \left( \pi_x(f) - f \right)(\eta)
\]

» Where \( \pi_x(f)(\eta) \) means fix \( \eta \) out side of site \( x \), and average at site \( x \) with respect to the Bernoulli(1-q) dist.
Stationary distribution

• Trivial equilibrium:
  » \( q \in (0, 1) \) equilibrium density of (facilitating) zeros
  » \( \pi : \) product Bernoulli(1-\( q \)) measure on \( \{0, 1\}^L \) is reversible (dynamics satisfy detailed balance with respect to \( \pi \))
    • i.e on a finite lattice
      \[
      \pi(\eta)Q(\eta, \sigma) = \pi(\sigma)Q(\sigma, \eta)
      \]
    • Forward and backward trajectories started from \( \pi \) have the same distribution.
    • The generator is self-adjoint in \( L^2(\pi) \).
  
  » If \( L << 1/q \) the ground state is the filled configuration.
Motivation

• Glassy effects arise at small $q$ (low temperature):
  » Extremely slow relaxation (super Arrhenius).
  » Complex out-of-equilibrium dynamics (cooperative dynamics).
  » Dynamical heterogeneity and ageing.
  » Simple stationary distribution (Bernoulli i.i.d).

• KCM are very challenging mathematically.
  » Hardness of constraints and not monotone/attractive.
  » Many powerful tools do not hold; FKG inequalities, monotone coupling, censoring … not available.

• Many interesting open problems.
Equilibration for low temperature \((q \downarrow 0)\)

- Let \(L_c = 1/q\) be the equilibrium length scale

<table>
<thead>
<tr>
<th>Four interesting regimes</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. (L = O(1)) (finite scale)</td>
</tr>
<tr>
<td>2. (L \sim L_c^\gamma) with (\gamma \in (0, 1)) (mesoscopic scale)</td>
</tr>
<tr>
<td>3. (L \propto L_c) (equilibrium scale)</td>
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<tr>
<td>4. (L \geq L_c) (comparable with infinite system)</td>
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</tbody>
</table>

» Significant contribution to (2).

» Greatly improved bounds in (4).

» Aldous and Diaconis suggest a nice conjecture for (3), still open!
Dynamics: Characteristic times

- **Mixing time:** $T_{\text{mix}}(L)$
- **Relaxation time:** $T_{\text{rel}}(L)$
- **Hitting time:** $T_{\text{hit}}(L)$
Dynamics: Characteristic times

• **Mixing time:** \( T_{\text{mix}}(L) \)
• **Relaxation time:** \( T_{\text{rel}}(L) \)
• **Hitting time:** \( T_{\text{hit}}(L) \)

\[
\| P - Q \|_{TV} = \max_{A \subseteq \Omega} |P(A) - Q(A)|
= \frac{1}{2} \sum_{\sigma \in \Omega} |P(\sigma) - Q(\sigma)|
\]
Dynamics: Characteristic times

• **Mixing time:** $T_{\text{mix}}(L)$
• **Relaxation time:** $T_{\text{rel}}(L)$
• **Hitting time:** $T_{\text{hit}}(L)$

$$d_L(t) := \sup_{\eta} ||P_t(\eta, \cdot) - \pi||_{TV}$$
Dynamics: Characteristic times

- **Mixing time:** $T_{\text{mix}}(L)$
- **Relaxation time:** $T_{\text{rel}}(L)$
- **Hitting time:** $T_{\text{hit}}(L)$

\[ T_{\text{mix}}(L) := \inf \{ t > 0 : d_L(t) \leq 1/4 \} \]

\[ d_L(t) := \sup_\eta \| P_t(\eta, \cdot) - \pi \|_{\text{TV}} \]
Dynamics: Characteristic times

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• **Mixing time:** $T_{\text{mix}}(L)$

• **Relaxation time:** $T_{\text{rel}}(L)$

• **Hitting time:** $T_{\text{hit}}(L)$

» Zero is always an eigenvalue of $-\mathcal{L}_L$ others are non-negative.

» If lattice is finite then there is a unique smallest non-zero eigenvalue of $-\mathcal{L}_L$ called the spectral gap (Perron–Frobenius!).
Dynamics: Characteristic times

- **Mixing time:** $T_{\text{mix}}(L)$
- **Relaxation time:** $T_{\text{rel}}(L)$
- **Hitting time:** $T_{\text{hit}}(L)$

» Min-max principle for eigenvalues gives variation principle:

$$\text{gap}(\mathcal{L}_L) := \inf_{\substack{f: \Omega \to \mathbb{R} \\ f \text{ non constant}}} \frac{\langle f, -\mathcal{L}_L f \rangle_\pi}{\text{Var}_\pi(f)} , \quad \text{where} \quad \langle f, g \rangle_\pi = \int fg d\pi = \pi(fg)$$

» Might be zero if the lattice is infinite. For the East process it isn’t!
Dynamics: Characteristic times

- **Mixing time:** $T_{\text{mix}}(L)$
- **Relaxation time:** $T_{\text{rel}}(L)$
- **Hitting time:** $T_{\text{hit}}(L)$

\[ T_{\text{rel}}(L) := 1/\text{gap}(\mathcal{L}_L) \]

\textbf{Min-max principle for eigenvalues gives variation principle:}

\[
\text{gap}(\mathcal{L}_L) = \inf_{f: \Omega \to \mathbb{R} \atop f \text{ non-constant}} \frac{\langle f, -\mathcal{L}_L f \rangle_{\pi}}{\text{Var}_\pi(f)}, \quad \text{where} \quad \langle f, g \rangle_{\pi} = \int f g \, d\pi = \pi(fg)
\]
Dynamics: Characteristic times

- **Mixing time:** $T_{\text{mix}}(L)$
- **Relaxation time:** $T_{\text{rel}}(L)$
- **Hitting time:** $T_{\text{hit}}(L)$

For reversible dynamics spectral decomposition gives:

\[
T_{\text{rel}}(L) := \frac{1}{\text{gap}(\mathcal{L}_L)}
\]

For reversible dynamics spectral decomposition gives:

\[
\lim_{t \to \infty} \frac{-1}{t} \log d_L(t) = \text{gap}(\mathcal{L}_L)
\]

Asymptotic decay rate
Dynamics: Characteristic times

- **Mixing time:** $T_{\text{mix}}(L)$
- **Relaxation time:** $T_{\text{rel}}(L)$
- **Hitting time:** $T_{\text{hit}}(L)$

$$T_{\text{rel}}(L) := 1 / \text{gap}(\mathcal{L}_L)$$

» Contraction of the variance:

$$\text{Var}_\pi(P_t f(\eta)) \leq e^{-\frac{2t}{T_{\text{rel}}}} \text{Var}_\pi(f)$$
Dynamics: Characteristic times

- **Mixing time:** $T_{\text{mix}}(L)$
- **Relaxation time:** $T_{\text{rel}}(L)$
- **Hitting time:** $T_{\text{hit}}(L)$

\[ T_{\text{hit}}(L) = \mathbb{E}_{10}[\tau_L] \]

\[ \tau_L = \inf\{t \geq 0 : \sigma_L(t) = 1\} \]
Dynamics: Characteristic times

- Relaxation time: $T_{\text{rel}}(L)$
- Mixing time: $T_{\text{mix}}(L)$
- Hitting time: $T_{\text{hit}}(L)$

\[
T_{\text{rel}}(L) \leq T_{\text{rel}}(L + 1) \leq T_{\text{rel}}(\infty) < \infty \quad \text{for each } q \in (0, 1).
\]

and on $\mathbb{Z}$,

\[
T_{\text{rel}}(\infty) \simeq \exp \left[ \frac{\log(1/q)^2}{2 \log 2} \right] \quad \text{as } \quad q \searrow 0.
\]

[N. Cancrini, F. Martinelli, C. Roberto, C. Toninelli, PTRF (2008)]
Dynamics: Characteristic times

- Relaxation time: \( T_{\text{rel}}(L) \)
- Mixing time: \( T_{\text{mix}}(L) \)
- Hitting time: \( T_{\text{hit}}(L) \)


All increasing in \( L \), and for any \( L = O(1/q) \)

\[
\frac{T_{\text{mix}}(L)}{T_{\text{rel}}(L)}, \frac{T_{\text{hit}}(L)}{T_{\text{rel}}(L)} \rightarrow 1 \quad \text{as} \quad q \searrow 0.
\]

> All characteristic times are equiv. at low temperature (the ratios are bounded by constants even at equilibrium scale).
Dynamics: Characteristic times

- Relaxation time: $T_{\text{rel}}(L)$
- Mixing time: $T_{\text{mix}}(L)$
- Hitting time: $T_{\text{hit}}(L)$


All increasing in $L$, and for any $L = O(1/q)$

$$T_{\text{mix}}(L)/T_{\text{rel}}(L), T_{\text{hit}}(L)/T_{\text{rel}}(L) \to 1 \quad \text{as} \quad q \searrow 0.$$  

» Up to the typical stationary separation of zeros $L_c = 1/q$, we can look at which ever is most convenient.
East model: Combinatorics

- Energy barrier at low temperature (low $q$)

  » Has to create at least $n$ more simultaneous zeros.
  
  $$L \in [2^{n-1} + 1, 2^n]$$
  
  » Activation time: $t_n = (1/q)^n$.
East model: Dynamics small $q$

“Up hill”
• Energy barrier at low temperature (low $q$)

$$L \in [2^{n-1} + 1, 2^n]$$

» Has to create at least $n$ more simultaneous zeros.

[Chung, Diaconis, Graham, Adv. in App. Math (‘01)]

» Activation time: $t_n = (1/q)^n$.

» Metastability: Actual final excursion is on a much shorter timescale.

» If $L \gg 1$ actual time reduced by an entropic factor.
• On fixed system sizes as $q \to 0$.
  
  » Energy barrier dominates

$$c(n)q^{-n} \leq T_{\text{rel}}(L) \leq c'(n)q^{-n} \quad \text{where} \quad n = \lfloor \log_2 L \rfloor$$

» Clear separation of timescales.

$$C_n = [2^{n-1} + 1, 2^n] \quad \text{for} \ n \geq 1$$

East model: Result (fixed L)

• On fixed system sizes low temperature limit:
  
  » Energy barrier dominates

\[
c(n)q^{-n} \leq T_{\text{rel}}(L) \leq c'(n)q^{-n} \quad \text{where} \quad n = \lfloor \log_2 L \rfloor
\]

• Gives rise to ageing and hierarchical coalescence.

\[
t_n^\pm = (1/q)^{n(1 \pm \varepsilon)}
\]

• Longer length scales entropy reduces the activation time

• On fixed system sizes low temperature limit:
  » Energy barrier dominates

\[ c(n)q^{-n} \leq T_{\text{rel}}(L) \leq c'(n)q^{-n} \quad \text{where} \quad n = \lfloor \log_2 L \rfloor \]

• Gives rise to ageing and hierarchical coalescence.

\[ t_{n}^{\pm} = \left( \frac{1}{q} \right)^{n(1 \pm \epsilon)} \]

• Longer length scales entropy reduces the activation time
• Still separation of time scales?
Low temperature dynamics (super Arrhenius)

- Separation of timescales up to the equilibrium length scale:


If $L = 1/q^\gamma$ with $\gamma \in (0, 1]$ then

$$T_{\text{rel}}(L) = e^{\left[(1 - \frac{\gamma}{2})n + \gamma \log_2 n\right] \theta_q + O(1)}$$

where

$$\theta_q = \ln(1/q),$$

$$n = \lfloor \log_2 L \rfloor.$$

- Corrected a prediction in the physics literature.
- Gives rise to a detailed picture of the limiting dynamics.
D. Chandler and J. Garranhan suggested a more realistic model of glassy dynamics involving a D-dimensional analogue of the East process.  

We call the corresponding process the East-like process.

New and interesting features in higher dimensions!
Higher dimensional ‘East’

- Model:
  - Constraint at site $x \in \Lambda_L$:
    \[ c_x(\sigma) = 1 \{\sigma_{x-e_i} = 0 \text{ for at least one } i \in \{1, \ldots, d\} \} \]
  - The same spin flip dynamics under this constraint.

<table>
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<th>Minimal:</th>
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<tr>
<td>1 1 1 1 0</td>
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</tbody>
</table>
Higher dimensional ‘East’

- Minimal (small \( q \))
- Maximal (smaller \( q \))
Higher dimensional ‘East’: Results

• Highly non trivial dependence on boundary conditions:
  » The relaxation time is given by the slowest mode...
  » For minimal boundary conditions slowest mode is along the axes;
• Along the axes the dynamics are exactly that of the 1D-East


• If $L \to \infty$ as $q \searrow 0$ then $T_{\text{rel}}^{\text{min}}(L) \simeq T_{\text{rel}}^{\text{EAST}}(L)$.

» Can also bound the asymptotic of the hitting times first time to flip to zero at $x$ starting from all ones.
Higher dimensional ‘East’: Results

- Highly non trivial dependence on boundary conditions:
  - Max boundary conditions the relaxation time is significantly reduced by further entropic effects


If \( L \to \infty \) as \( q \searrow 0 \) then
\[
T_{rel}^{\text{max}}(L) = e^{\left(n\theta_q - d\frac{n^2}{2}\right)}(1+o(1)).
\]
where \( L \in (2^{n-1}, 2^n] \)

- Relaxation time on infinite lattice: Confirm prediction in physics literature (and corrected certain constants).

\[
T_{rel}^{\text{D-dim}}(\infty) = T_{rel}^{\text{max}}(L \ge q/D) = T_{rel}^{\text{EAST}}(\infty) \frac{1}{D}(1+o(1)).
\]
• Convergence to equilibrium.


If the initial distribution \( \nu \) contains ‘some’ zeros then

\[
\sup_x \left| \mathbb{E}_\nu [\eta_t (x)] - p \right| \leq e^{-\lambda t^{1/2d}}
\]


\[
C(q) L \leq T_{\text{mix}} (L) \leq C(q)’ L.
\]

• Proof:
  » Technically difficult, the log-Sobolev constant decays like \( L^{-d} \).
  » Approach: a zero creates a wave of equilibrium in front of it before it moves too far away.
Higher dimensional ‘East’: Results

• Proof techniques:
  » Potential theory and electrical network techniques.
  » Algorithmic construction of a small bottleneck.
  » Comparison with East process on a spanning tree.
  » Auxiliary block dynamics.

• Relaxation time on the infinite lattice is not given by minimal boundary conditions at the equilibrium scales.
  » Novel renormalization group analysis via coarse-grained dynamics.
Open problems and conjectures

• Influence region:

\[ R_t = \{ \text{Sites which have flipped at least once by time } t \} \]

• Limit shape for the influence region:

\[ \frac{R_t}{t} \to S \subset \mathbb{R}^d \]

[G. Kordzakhia and S.P. Lalley. (2006)]

• In particular, mixing time should satisfy

\[ T_{\text{mix}}(\Lambda_L) \approx cL \]

with a cut-off....
Mixing times and relaxation

- What is Cut-off... coined by P. Diaconis (in early 90s)

For $\epsilon < 1/4$, 

$$\lim_{n \to \infty} d_n ((1 - \epsilon)T_{mix}(n)) = 1$$

$$\lim_{n \to \infty} d_n ((1 + \epsilon)T_{mix}(n)) = 0$$

[Adapted from Levin, Peres, Wilmer (2009)]

- Detailed information about convergence.
- Very useful for simulations.
Open problems and conjectures

• Known in 1D – East, front satisfies a CLT.

Let $X(\eta_t)$ denote the right most 0 in $\eta$ at time $t$.

Then $\frac{1}{t} X(\eta_t) \rightarrow \nu_{\infty}$, and the distribution behind the front converges to the equilibrium distribution $\pi$.

[O. Blondel, (2013)]
[Ganguly, Lubetzky, Martinelli, (2015)]

• In higher dimensions starting from all ones in the upper quadrant...
Open problems

• Influence region:
  \[ R_t = \{ \text{Sites which have flipped at least once by time } t \} \]

• Limit shape, starting from all ones in the upper quadrant
  \[ \frac{R_t}{t} \to S \subset \mathbb{R}^d \]

• In particular, mixing time should satisfy
  \[ T_{\text{mix}}(\Lambda_L) \approx cL \]
  with a cut-off.
Summary

• KCM have rich and complex ‘glassy’ behaviour.
• Mathematically they are very challenging and there are many open questions.
• Numerical simulations can be very instructive, but can be misleading due to huge timescales.
• Rigorous analysis is contributing to a deeper understanding of the complexity of “glassy dynamics”.

Thank you.