Non-equilibrium dynamics of Kinetically Constrained Models

Paul Chleboun
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SMFP - Heraclion
• Kinetically constrained models (KCM)
  » Motivation
  » Definition

• Results
  » In one dimension
    • There is timescale separation at low temperature.
    • Precise bounds on characteristic times.
  » Higher dimensions
    • Non trivial dependence on the boundary conditions.
    • Detailed results on the relaxation to equilibrium.

• Open problems
  » Shape limits and cut-off in higher dimensions.
Motivation

- Motivation
  - Kinetically constrained models (KCM).
    - Glassy effects arise at low temperature:
      - Featureless stationary distribution (i.i.d).
      - Slow relaxation (super Arrhenius).
      - Complex out-of-equilibrium dynamics;
      - Dynamical heterogeneity and ageing.
      - Quantitative predictions about real glasses [Keys, Garrahan, Chandler PNAS 2013]
  - KCM challenging mathematically.
    - Hardness of constraints and not monotone/attractive.
  - Attracted interest in different communities:
    - Physics, probability and combinatorics.
  - Open problems
    - Mixing of North-East model
    - Shape limit theorems
    - Scaling limits
1D example the **East Process**:

- \( q \in (0, 1) \) equilibrium density of (facilitating) zeros
  \[
  q = \frac{e^{-\beta}}{1 + e^{-\beta}}, \quad \beta = \frac{1}{\text{Temp}}.
  \]

- Configurations: \( \sigma = (\sigma_x)^L_{x=1} \), \( \sigma_x \in \{0, 1\} \)
- Glauber dynamics with a **kinetic constraint**.
- Zeros facilitating (mimic **cage effect** in glasses).
- Fixed zero at the origin: **Ergodic boundary condition**

\[
\begin{array}{ccccccc}
0 & 1 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 1 \\
\sigma_1 & \sigma_2 & \cdots & \cdots & \cdots & \sigma_L
\end{array}
\]
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.

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

\[0 \ 1 \ 1 \ 0 \ 1 \ 0 \ 1 \ 1 \ 1 \ 0 \ 0 \ 1\]

$\sigma_1 \ \sigma_2 \ \cdots \ \cdots \ \sigma_L$
东模型：定义

- Spin-flip dynamics
  - 每个站点以率 1（独立）尝试更新
  - 然后，如果 $c_x(\sigma) = 1 - \sigma_{x-1} = 1$，掷一个 $p$-硬币，刷新。

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

$$
\begin{array}{c}
0 \\
q = 1 - p \\
\sigma_1 \quad \sigma_2 \quad \cdots \\
\end{array}
\quad \begin{array}{c}
1 \\
p \\
\sigma_L
\end{array}
$$
• 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.

$$\sigma_x = \begin{cases} 
1 & \text{with prob. } 1 - q \\
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\end{cases}$$

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• 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.

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

\[
\begin{array}{cccccccccc}
0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\
\sigma_1 & \sigma_2 & \cdots & & & & & \cdots & \sigma_L
\end{array}
\]
East Model: Equilibrium

- Trivial equilibrium:
  - \( q \in (0, 1) \) equilibrium density of (facilitating) zeros

\[
q = \frac{1}{e^\beta + 1}, \quad \beta = \frac{1}{\text{Temp.}}
\]

- \( \pi \): product Bernoulli(1-q) measure on \( \{0, 1\}^L \) is reversible (dynamics satisfy detailed balance with respect to \( \pi \))

\[
\pi[\eta] \propto e^{-\beta H(\eta)}
\]

Where \( H(\eta) = -\sum_{x=1}^{L} \eta(x) \)

- If \( L < 1/q \) the ground state is the filled configuration.
• Simple representation
East model: Dynamics

[Source: Aldous, Diaconis JSP 107(5) (2002)]
East model: Observations

“Up hill” for small q
Two adjacent ‘domains’ of 1s:

As long as the intermediate 0 does not flip, the second domain evolves independently of the first as an East process on $L'$ sites.

If the \textbf{persistence time} of 0 is large enough then the second block has to equilibrate.

Gives rise to a hierarchical evolution...
Dynamics: Characteristic times

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

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

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

\[
T_{\text{mix}}(L) := \inf \left\{ t > 0 : \sup_{\eta} |P_t(\eta, \cdot) - \pi|_{TV} \leq 1/4 \right\}
\]

\[
|\mu - \nu|_{TV} = \max_{A \subset \Omega} |\mu(A) - \nu(A)|
\]

\[
= \frac{1}{2} \sum_{\sigma \in \Omega} |\mu(\sigma) - \nu(\sigma)|
\]
Dynamics: Characteristic times

- Relaxation time: $T_{\text{rel}}(L)$
- Mixing time: $T_{\text{mix}}(L)$
- 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: $T_{\text{hit}}(L)$
  - All increasing in $L$.

**Theorem 1** [with Faggionato, Martinelli (2014)]

For any $L = O(1/q)$

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

- All characteristic times are equiv. at low temperature (the ratios are bounded by constants even at equilibrium scale).
Energy barrier

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

[Chung, Diaconis, Graham, *Adv. in App. Math* (‘01)]
East model: Dynamics small $q$

“Up hill”
East model: Result (fixed L)

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

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

Domain length $6 \in C_3$

\[
\begin{array}{cccccccccccc}
0 & 1 & 1 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 1 \\
\end{array}
\]

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

East model: Result (fixed L)

- On fixed system sizes low temperature limit:
  - Energy barrier dominates

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

- Gives rise to ageing and hierarchical coalescence.

- Longer length scales entropy reduces the activation time
East model: Result (fixed L)

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

\[ c(n)e^{\beta n} \leq T_{\text{rel}}(L) \leq c'(n)e^{\beta n} \quad \text{where} \quad n = \lceil \log_2 L \rceil \]

• Gives rise to ageing and hierarchical coalescence.

• Longer length scales entropy reduces the activation time
• Low temperature dynamics (super Arrhenius)
  » Separation of timescales up to the equilibrium length scale

**Theorem** [with Faggionato, Martinelli]

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

$$T_{\text{rel}}(L) = e^{\beta[(1-\frac{\gamma}{2})n + \gamma \log_2 n] + O(1)} \quad \text{where} \quad n = \lfloor \log_2 L \rfloor.$$

• Corrected a prediction in the physics literature.

[East model: Result]

Higher dimensional ‘East’

- Model:
  - D-dim Lattice (e.g. in 2D): $\Lambda_L = \{1, 2, \ldots, L\}^D$
  - State space: $\Omega_L = \{0, 1\}^{\Lambda_L}$
  - Configurations: $\sigma = (\sigma_x)_{x \in \Lambda_L}$

![Diagram of a 2D lattice with configurations]
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.
Higher dimensional ‘East’

- Ergodic boundary conditions:
  - Constraint at site $x \in \Lambda_L$:
    \[ c_x(\sigma) = 1 \{ \sigma_{x-e_i} = 0 \text{ for at least one } i \in \{1, \ldots, d\} \} \]

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<th>Maximal:</th>
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<td>1 1 1 1 1</td>
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</tbody>
</table>
Higher dimensional ‘East’

- Minimal (small $q$)
- Maximal (small $q$)

- Videos?
Higher dimensional ‘East’: Results

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

Theorem [with Faggionato, Martinelli]

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

If \( L \) is fixed as \( q \searrow 0 \) then \( T_{\text{rel}}^{\min}(L) \simeq e^{\beta n} \)
where \( \|\Lambda_L\|_1 + 1 \in (2^{n-1}, 2^n] \).

» 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

• Interesting and highly non trivial dependence on boundary conditions:
  » For maximal boundary conditions the relaxation time is significantly reduced by entropic effects (number of path through configuration space)

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<tr>
<td>If $L \to \infty$ as $q \searrow 0$ then $T_{\text{rel}}^{\text{max}}(L) = e^{\left(\beta n - d \frac{n^2}{2}\right)}(1+o(1)).$</td>
<td></td>
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<tr>
<td>Extra entropic reduction</td>
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» Relaxation time on infinite lattice: Confirm prediction in physics literature (and corrected the constants)

$$T_{\text{rel}}^{\text{D-dim}}(\infty) = T_{\text{rel}}^{\text{EAST}}(\infty) \frac{1}{D} (1+o(1))$$
• 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:

» Usual approach fails since the log-Sobolev constant grows like $L^d$.

» Approach: a zero creates a wave of equilibrium in front of it before it moves too far away.
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:

  » Starting from all ones in the upper quadrant

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

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

• In particular, mixing time should satisfy

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

with a cut-off.
Open problems and conjectures

• 2D East:
Another higher dimensional KCM

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

• Stationary distribution
  » Constraint at \( x \) does not depend on configuration at \( x \)
  \[ \Rightarrow \pi : \text{product Bernoulli}(1-q) \text{ reversible stat. distribution} \]

• Directed percolation on infinite lattice:

\[
\begin{array}{cccc}
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 1 \\
1 & 1 & 1 & 0 \\
1 & 0 & 0 & 0 \\
\vdots
\end{array}
\]

\[ q_c = \inf\{ q \in [0, 1] : \text{starting from } \pi, \mathbb{Z}^2 \text{ is emptied with prob. } 1 \} \]
North-East Results

• Relaxation time:

\[ q_c = \inf\{q \in [0, 1] : \text{starting from } \pi, \mathbb{Z}^2 \text{ is emptied with prob. 1}\} \]

• \( q > q_c \), then \( T_{\text{rel}}(\Lambda_L) \leq T_{\text{rel}}(\mathbb{Z}^2) < \infty \)

• \( q \leq q_c \), then \( e^{cL} \leq T_{\text{rel}}(\Lambda_L) \leq e^{c'L} L \)

[N. Cancrini, F. Martinelli, C. Roberto, C. Toninelli (2008)]


For \( q > q_c \) (finite relaxation time),

\[ CL \leq T_{\text{mix}}(\Lambda_L) \leq C'L \log L. \]
Pictures

Videos if time
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.
• Results:
  » with F. Martinelli
    • Mixing time bounds for oriented kinetically constrained spin models,
  » with A. Faggionato, F. Martinelli
    • Time scale separation and dynamic heterogeneity in the low temperature East model,
    • Time scale separation in the low temperature East model: Rigorous results,
    • Relaxation to equilibrium of generalized east processes on \( \mathbb{Z}^d \),
      Accepted Annals of Probab., (2015)
    • The influence of dimension on the relaxation process of East-like models,
      EPL 107(3) 36002, (2014)
    • Mixing time and local exponential ergodicity of the East-like process in \( \mathbb{Z}^d \),

• Tools:
  » Potential theory and electrical network techniques
  » Algorithmic construction of an small bottleneck
  » Renormalization group analysis via coarse-grained dynamics
  » Comparison with East process on a spanning tree