East-like processes

Alessandra Faggionato

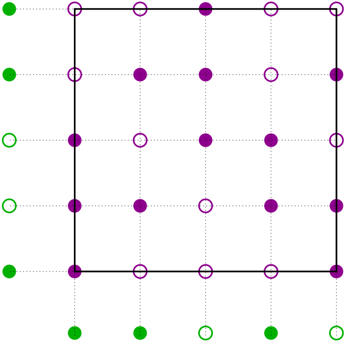
University La Sapienza - Rome

Joint work with P. Chleboun and F. Martinelli

d–dim East process

1. J.P. Garrahan, D. Chandler; *Coarse-grained microscopic model of glass formers.* PNAS **100**, 9710–4 (2003)
2. D. J. Ashton, L.O. Hedges, J.P. Garrahan; *Fast simulation of facilitated spin models.* Journal of Statistical Mechanics: Theory and Experiment P12010 (2005)
3. P. Chleboun, A. Faggionato, F. Martinelli; *Relaxation to equilibrium of generalized East processes on $\mathbb{Z}^d$: renormalization group analysis and energy-entropy competition.* http://arxiv.org/abs/1404.7257
4. P. Chleboun, A. Faggionato, F. Martinelli; *Dimensional effects on the relaxation process of East models: rigorous results.* Forthcoming.

d–dim East process on $\Lambda = [1, L]^d$



$\Lambda = [1, L]^d$

$\eta \in \{0, 1\}^\Lambda$

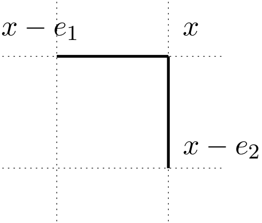
σ boundary condition

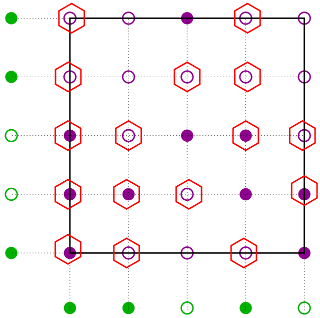
$\sigma \in \{0, 1\}^{\partial_E \Lambda}$

$\partial_E \Lambda$ East boundary

Constraint at x with b.c. σ

- $\mathcal{B}$ canonical basis of $\mathbb{R}^d$
- σ boundary condition, $\sigma \in \{0,1\}^{\partial_E \Lambda}$
- η satisfies constraint at $x \in \Lambda$ (with b.c. σ) if there is a vacancy at $x - e$ for some $e \in \mathcal{B}$.





sites x where the constraint is satisfied

East process on Λ with b.c. σ

- $q \in (0,1)$ parameter
- configuration $\eta \in \{0,1\}^\Lambda$

$\rightarrow$ for each site x, wait at x an exponential time of mean 1

$\rightarrow$ afterwards:

if constraint at x with b.c. σ is satisfied, refresh $\eta_{\mathbf{x}}$

according $(1-q)$–Bernoulli law: $\begin{cases} 1 & \text{prob. 1-q} \\ 0 & \text{prob. q} \end{cases}$

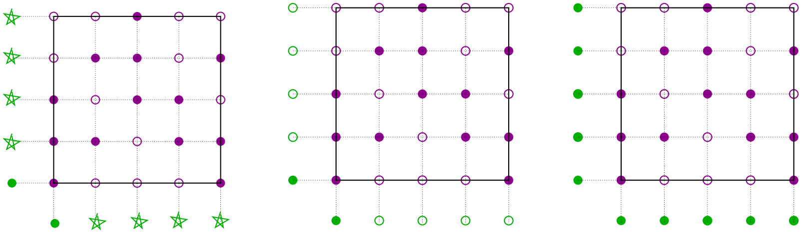
if constraint at x with b.c. σ is not satisfied, do nothing

$\rightarrow$ restart afresh

Ergodic boundary conditions

To have irreducible Markov chain:

$$\sigma_{(1,\dots,1)-e} = 0 \text{ for all } e \in \mathcal{B}$$



Ergodic b.c. Minimal b.c. Maximal b.c.

Energy

- Hamiltonian $\mathcal{H}(\eta) = \sharp\{$ vacancies in η $\}$
- $q = \frac{e^{-\beta}}{1+e^{-\beta}}$, β inverse temperature.
- $\pi = \prod_{x\in\Lambda} \pi_x$, π_x is the $(1-q)$–Bernoulli probability for η_x
- π is reversible
- π Gibbs distribution associated to $\mathcal{H}$ and β
- $\beta \approx \log \frac{1}{q}$, Fabio's $\theta_q = \log_2 \frac{1}{q} \approx \frac{\beta}{\log 2}$

Relaxation times

$T^{\sigma}_{\rm rel}(L)$: relaxation time for East model on $[1,L]^d$ with b.c. σ
It is the minimal positive eigenvalue of sign–inverted Markov generator.

$$T^{\max}_{\rm rel}(L) \leq T^{\sigma}_{\rm rel}(L) \leq T^{\min}_{\rm rel}(L)$$

$$T^{\max}_{\rm rel}(L)\,,\; T^{\min}_{\rm rel}(L) \nearrow \;\text{ as } L \nearrow \infty$$

$$T_{\rm rel}(\mathbb{Z}^d) = \lim_{L\to\infty} T^{\max}_{\rm rel}(L)$$

East process, $d = 1$

$\Lambda = [1, L]$

Theorem

Set $n = \lceil \log_2 L \rceil$. *Then as* $q \searrow 0$

$$T_{\rm rel}^{\rm East}(L;q) \asymp \begin{cases} e^{\beta n} \times n! 2^{-\binom{n}{2}}, & L \leq 1/q\,, \\ e^{\beta^2/2\log 2} & L \geq 1/q\,. \end{cases}$$

- $1/q$ is the mean inter–vacancy distance at equilibrium
- n represents the minimal energy barrier between the ground state and the set of configurations with a vacancy at L.
- $e^{\beta n}$ energetic factor, $n!2^{-\binom{n}{2}}$ entropic factor
- $T_{\rm rel}^{\rm East}(\mathbb{Z};q) \asymp e^{\beta^2/2\log 2}$

Dimensional effects in the relaxation process

$d \geq 2$. Physics literature: relaxation process is quasi one dimensional, in particular

$$T_{\mathrm{rel}}(\mathbb{Z}^d; q) \asymp T_{\mathrm{rel}}^{\mathrm{East}}(L_c; q)$$

$L_c = (1/q)^{1/d}$ mean inter–vacancy distance at equilibrium

As a consequence,

$$T_{\mathrm{rel}}(\mathbb{Z}^d; q) \asymp e^{\beta^2 \left(\frac{2d-1}{2d^2 \log 2}\right)}$$

Note: $T_{\mathrm{rel}}^{\mathrm{East}}(L_c; q) \asymp e^{\beta^2/d \log 2}$ by using the incorrect formula for $T_{\mathrm{rel}}^{\mathrm{East}}(\cdot; q)$ with no entropy factor

Dimensional effects in the relaxation process

The previous asymptotic is indeed not correct: the relaxation is faster for $d \geq 2$. Indeed:

Theorem

As $q \searrow 0$

$$T_{\mathrm{rel}}(\mathbb{Z}^d; q) = e^{\frac{\beta^2}{2d \log 2}(1+o(1))}$$

In particular

$$T_{\mathrm{rel}}(\mathbb{Z}^d; q) = T_{\mathrm{rel}}^{\mathrm{East}}(\mathbb{Z}; q)^{\frac{1}{d}(1+o(1))}$$

Moreover the $o(1)$ *correction is* $O(\beta^{-1/2})$ *and* $\Omega\left(\beta^{-1}\log\beta\right)$

- $f = O(g)$: $|f| \leq C|g|$ for some constant C
- $f = \Omega(g)$: $\limsup |f|/|g| > 0$

Fast simulation

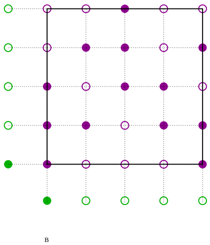
- D. J. Ashton, L.O. Hedges, J.P. Garrahan; *Fast simulation of facilitated spin models*. Journal of Statistical Mechanics: Theory and Experiment P12010 (2005)
- The authors apply Novotny's algorithm Monte Carlo with absorbing Markov chains (MCAMC) to simulate kinetically constrained models of glasses (Fredrickson–Andersen model and the East model in arbitrary dimensions).
- Simulations suggest that $T_{\mathrm{rel}}(\mathbb{Z}^d; q) = e^{b\frac{\beta^2}{d}(1+o(1))}$, $b \approx 0.8$
- $T_{\mathrm{rel}}(\mathbb{Z}^d; q) = e^{\frac{\beta^2}{2d\log 2}(1+o(1))} \implies b = \frac{1}{2\log 2} = 0.721347520..$

Finite volume relaxation times

Strong dependence on the boundary condition !

- $T_{\mathrm{rel}}^{\min}(L;q)$

$$\begin{cases} \text{it scales as the relaxation time of 1d East model } T_{\mathrm{rel}}^{\mathrm{East}}(L;q) \\ \text{the slowest mode occurs along the coordinate axes} \\ \text{it is } d\text{–independent} \end{cases}$$



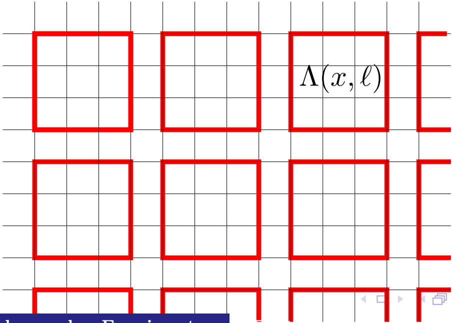
- $T_{\mathrm{rel}}^{\max}(L;q)$ much shorter and is d–dependent

Renormalization group analysis behind $T_{\mathrm{rel}}(\mathbb{Z}^d; q)$

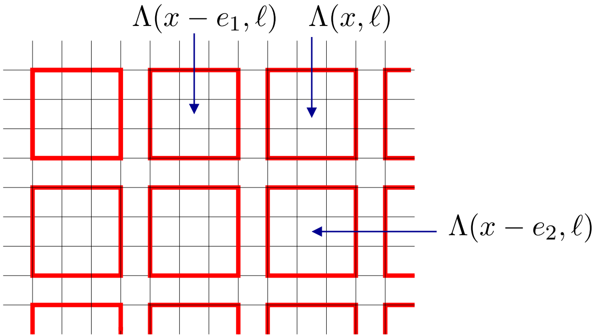
Given positive integer ℓ and $x \in \mathbb{Z}^d$, set $\Lambda(x,\ell) = \ell x + [0, \ell-1]^d$
Partition $\mathbb{Z}^d$ in boxes $\Lambda(x,\ell)$, $x \in \mathbb{Z}^d$

Block dynamics on $\{0,1\}^{\mathbb{Z}^d}$:

- For each $x \in \mathbb{Z}^d$ wait an exponential time of mean 1
- Afterwards, if the constraint is satisfied, update $\eta_{\Lambda(x,\ell)}$ by sampling it according to a $(1-q)$–Bernoulli probability
- Start afresh



The (almost correct) constraint



- **Constraint at x: η has at least a vacancy in $\Lambda(x - e_1, \ell)$ or $\Lambda(x - e_2, \ell)$**
- $\pi\left(\exists \text{vacancy in } \Lambda(y, \ell)\right) = 1 - (1 - q)^{\ell^d} =: q_*$
- $T_{\text{rel}}^{\text{block}}(\mathbb{Z}^d; q) = T_{\text{rel}}(\mathbb{Z}^d; q_*)$

Back to d–dim East process

- $\eta_{\Lambda(x,\ell)}$ does not take a mean 1 exponential time to equilibrate, it takes $T^{\sigma}_{\mathrm{rel}}(\ell;q)$, σ suitable
- Then, one would expect,

$$T_{\mathrm{rel}}(\mathbb{Z}^d;q) \sim T^{\sigma}_{\mathrm{rel}}(\ell;q)\, T^{\mathrm{block}}_{\mathrm{rel}}(\mathbb{Z}^d;q) = T^{\sigma}_{\mathrm{rel}}(\ell;q)\, T_{\mathrm{rel}}(\mathbb{Z}^d;q_*)$$

- Rigorous result:

$$T_{\mathrm{rel}}(\mathbb{Z}^d;q) \le T^{\min}_{\mathrm{rel}}(3\ell;q)\, T_{\mathrm{rel}}(\mathbb{Z}^d;q_*) \tag{1}$$

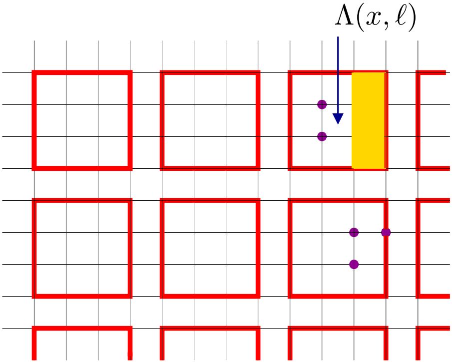
- Using (1) and knowing

$$\begin{cases} T^{\min}_{\mathrm{rel}}(3\ell;q) \approx T^{\mathrm{East}}_{\mathrm{rel}}(3\ell;q)\,, \\ T_{\mathrm{rel}}(\mathbb{Z}^d;q_*) \le T_{\mathrm{rel}}(\mathbb{Z};q_*)\,, \end{cases}$$

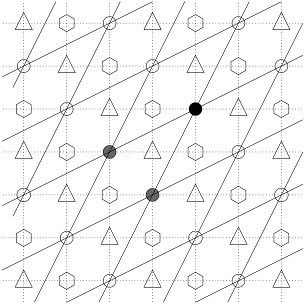
one has iterative procedure leading the correct asymptotic of $T_{\mathrm{rel}}(\mathbb{Z}^d;q)$

Problem with the suggested constraint

In the d–dim East process vacancies inside $\Lambda(x - e_1, \ell)$ or $\Lambda(x - e_2, \ell)$ could not be enough to allow equilibration inside $\Lambda(x, \ell)$



Correct constraint: Knight block process



- Vertexes correspond to $x \in \mathbb{Z}^d$, parametrizing $\Lambda(x, \ell)$
- Knight block process $\sim$ three independent copies of the previously defined block dynamics

Persistence times

- East process in $\mathbb{Z}_+^d$, minimal boundary condition, starting from the configuration with no vacancies
- $T(x;q)$: **Persistence time** at $x \in \mathbb{Z}_+^d$. $T(x;q)$ is the mean time it takes to create a vacancy at x.
- $L_c = (1/q)^{1/d}$
- For simplicity, we restrict to $|x| = O(L_c)$ or $|x| = O(1)$
- If process was quasi one-dimensional, $T(x;q)$ would be almost a function of $\|x\|_1 := \sum_{i=1}^d |x_i|$.

Persistence times

Theorem

1. *Let* $v_* = (dL_c, 0, \dots, 0)$ *and* $v^* = (L_c, L_c, \dots, L_c)$. *Then, as* $q \downarrow 0$,

$$T(v_*; q) \asymp T_{\rm rel}^{\rm East}(L_c; q) \asymp T_{\rm rel}^{\rm East}(\mathbb{Z}; q)^{(2d-1)/d^2}, \qquad (2)$$

$$T(v^*; q) \asymp T_{\rm rel}(\mathbb{Z}^d; q) \asymp T_{\rm rel}^{\rm East}(\mathbb{Z}; q)^{1/d}. \qquad (3)$$

   In particular, $T(v^*; q) \ll T(v_*; q)$.

2. *Fix* $n \in \mathbb{N}$ *and let* $x \in \mathbb{Z}^d_+$ *be such that* $\|x\|_1 \in [2^{n-1}, 2^n)$. *Then, as* $q \downarrow 0$,

$$T(x; q) = e^{n\beta + O_n(1)}. \qquad (4)$$

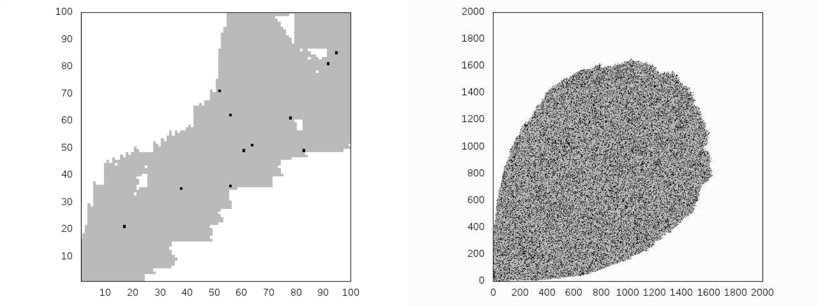


Figure: A snapshot of a simulation of the East-like process with minimal boundary conditions and initial condition constantly identically equal to 1. White dots are vertices that have never been updated, grey dots correspond to vertices that have been updated at least once and the black dots are the vacancies present in the snapshot. (A) $q = 0.002,\ t = 3 \times 10^{12}$; (B) $q = 0.25,\ t = 9 \times 10^{3}$.

Further techniques

- Bottleneck
  1. $A \subset \{0,1\}^\Lambda$, $\Lambda = [1, L]^d$.
  2. $\partial A := \{\eta \in A \ : \ \text{East process can jump from } \eta \text{ to } A^c\}$
  3. Bottleneck inequality

$$T_{\rm rel}^{\max}(L) \geq L^{-d} \frac{\pi(A)\pi(A^c)}{\pi(\partial A)}.$$

  4. Deterministic algorithm to build the optimal bottleneck leading to the lower bound of $T_{\rm rel}^{\max}(L)$
- The bottleneck inequality is used also to bound from below the persistence times
- Electrical networks method to bound from above the persistence times

Electrical networks

- d–dim East process on $\Lambda = [1, L]^d$ with b.c. σ
- $\mathcal{K}^\sigma(\eta, \eta')$ probability rate for a jump $\eta \to \eta'$
- $C^\sigma(\eta, \eta') = \pi(\eta)\mathcal{K}^\sigma(\eta, \eta')$ conductance associated to the edge (η, η')
- Resistor network on $\{0, 1\}^\Lambda$
- $B_x = \{\eta : \eta_x = 0\}$
- $R^\sigma_{\mathbb{1}, B_x}$ resistance between $\mathbb{1}$ and B_x

If $L \leq L_c$ then

$$T^\sigma(x; q) \sim R^\sigma_{\mathbb{1}, B_x}$$

Hierarchical analysis