Bootstrap percolation and Kinetically constrained models: time and length scales

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Liquid/glass transition

"The deepest and most interesting unsolved problem in solid state theory is probably the theory of the nature of glass and the glass transition." [Nobel prize P.W. Anderson]

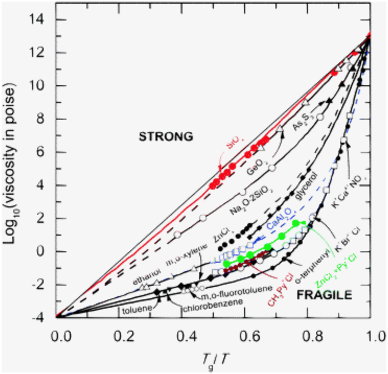
Glasses display properties of both liquids and solids

How can you manufacture a glass?

- Take a liquid and cool it rapidly in order to prevent nucleation of the ordered crystal structure;
- relaxation times increase dramatically, the liquid falls out of equilibrium and enters a metastable phase;
- the molecules move slower and slower:
  your liquid is now a thick syrup..
- finally the liquid freezes in a structureless solid:
  here is your glass.

Key features of liquid/glass transition

- huge divergence of timescales;
- no significant structural changes;
- cooperative relaxation;
- dynamical heterogeneities: non trivial spatio-temporal fluctuations, coexistence of frozen and mobile regions;
- rich phenomenology: anomalous transport properties, aging, rejuvenation, ...
- a similar jamming transition: grains in powders, emulsions, foams, colloidal suspensions, ...



Strong supercooled liquids: *Arrhenius* $\tau \sim \exp(\Delta E/T)$

Fragile supercooled liquids: *superArrhenius* $\tau \sim \exp(c/T^2), \dots$

Friedrickson Andersen model on $\mathbb{Z}^2$

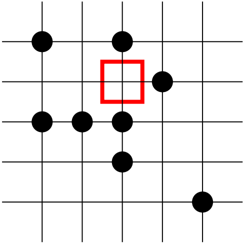
Configurations : $\eta = \{\eta_i\}_{i\in\mathbb{Z}^2}$ with $\eta_i \in \{0,1\}$

Glauber dynamics = Birth and death of particles on $\mathbb{Z}^2$

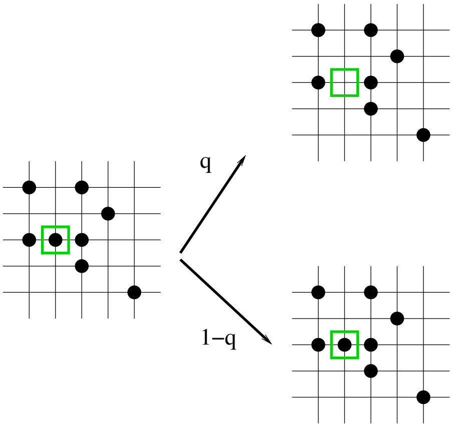
Kinetic constraint = at least 2 empty nearest neighbours

If constraint satisfied: $1 \to 0$ rate q, $0 \to 1$ rate $1-q$

The kinetic constraint

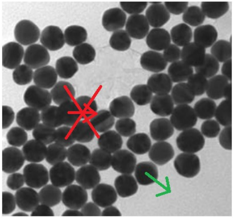


The kinetic constraint



Ideas behind KCSM

- Free volume shrinks when temperature is lowered;
- molecules should escape the "cage" formed by neighbours;
- local constraints act cooperatively;
- blocked structures may percolate $\rightarrow$ time scales diverge



Other examples

- Friedrickson Andersen k-facilitated models (FA-kf) on Z^d: at least k empty nearest neighbours

- East : *at least one* empty site among $\{x - \vec{e}_1, \ldots, x - \vec{e}_d\}$

The general framework

- Choose your favorite lattice;
- Choose a collection of finite neighborhoods of 0: $\{C_1, \ldots, C_m\}$ with $C_i \subset \mathbb{Z}^d \setminus 0$
- Constraint at x: at least one of the $C_i + x$ completely empty

KCSM: properties

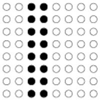
- Constraint at x does not depend on η_x
  $\rightarrow$ detailed balance w.r.t. product measure

$$\mu(\eta) = \prod_{i \in \mathbb{Z}^2} q^{1-\eta_i}(1-q)^{\eta_i}$$

- μ is not the unique invariant measure

- Blocked clusters, blocked configurations

Example of blocked cluster for FA-2f and for North-East



Main issues, main obstacles

→ Does convergence to equilibrium at large time occurs?

→ Is there a critical vacancy density below which blocked clusters percolate and relaxation is prevented?

→ How does relaxation time diverge when we approach this critical density?

- KCSM dynamics is not monotone
- Coupling arguments and censoring not available
- Blocked configurations → relaxation not uniform on the initial condition, worst case analysis too rough
- Coercive inequalities (e.g. Log-Sobolev) anomalous

$\mathcal{U}$-bootstrap percolation

Influence classes: $\mathcal{U} = \{C_1, \ldots, C_m\}$, $C_i \subset \mathbb{Z}^d$, $0 \notin \cup_{i=1}^m C_i$.
Initial configuration $\eta \in \{0,1\}^{\mathbb{Z}^d}$.

A deterministic discrete time process:

- empty sites remain empty forever;
- site v is emptied at time t if the translated at v of (at least) one the influence classes C_i is completely empty at $t-1$, i.e. if the same constraint as for KCSM is satisfied

Equivalent formulation:

- A_t set of empty sites at time t
- $A_0 := \{x \in \mathbb{Z}^d : \eta(x) = 0\}$
- $A_{t+1} := A_t \cup \{v \in \mathbb{Z}^d : v + C \subset A_t \text{ for some } C \in \mathcal{U}\}$

Dynamics is monotone

Critical probability

Fix $q \in (0,1)$ and pick η random with law $\mu =$ Bernoulli distribution with $\mu(\eta_x = 0) = q$.

Does the final set of empty sites cover the lattice?
Which are the finite size effects ?

Consider the process on the torus $\mathbb{Z}_n^d$.

$$q_c(n, \mathcal{U}) := \inf\{q \in [0,1] : \mu(\cup_{t \geq 0} A_t = \mathbb{Z}_n^d) \geq 1/2\}$$

How does $q_c(n, \mathcal{U})$ depend on $\mathcal{U}$? How does it scale for $n \to \infty$?

KCSM and $\mathcal{U}$-bootstrap

Final set of 1's for bootstrap $\leftrightarrow$ blocked particles for KCSM

- μ is mixing for a KCSM iff $q > q_c := \liminf_{n\to\infty} q_c(n,\mathcal{U})$
- How fast do we converge to μ? Exponentially
  $\forall q > q_c, \ \ \exists T_{rel}(q) < \infty$ s.t.
  $\mu(fP_tg) - \mu(f)\mu(g) \le C_{f,g} \exp(-t/T_{rel}(q)), \ \ \forall f,g \in L^2(\mu)$
- How does T_{rel} (=inverse of spectral gap) diverge as $q \downarrow q_c$?
  Set $L_c(q) := \min\{n : q_c(n,\mathcal{U}) = q\}$. Then

$$L_c \le T_{rel} \le e^{L_c^d}$$

[Cancrini, Martinelli, Roberto, C.T. '08]

Relaxation time for FA-kf model, $k \leq d$

$q_c = \liminf_{n\to\infty} q_c(n, \mathcal{U}) = 0$ [Van Enter '87, Schonmann '90]

$$\exists \lambda(d,k) > 0 \text{ s.t.} \quad L_c = \exp_{k-1}\left(\frac{\lambda(d,k)+o(1)}{q^{1/(d-k+1)}}\right)$$

[Aizenmann, Lebowitz '88, Cerf,Manzo '02, Balogh, ..., Bollobas, Duminil-Copin,Morris '12]

Theorem (Martinelli, C.T. '16)

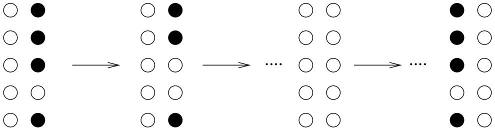
- *For the FA-2f model there exists $\alpha, c > 0$ s.t.*

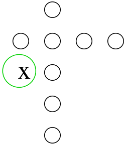
$$\exp(c/q^{1/(d-1)}) \leq T_{rel} \leq \exp\left(\log(1/q)^{\alpha}/q^{1/(d-1)}\right)$$

- *For the FA-kf model for any $k \geq 3$ there exists c, c' s.t.*

$$\exp_{k-1}\left(\frac{c}{q^{1/(d-k+1)}}\right) \leq T_{rel} \leq \exp_{k-1}\left(\frac{c'}{q^{1/(d-k+1)}}\right)$$

FA-2f Dominant relaxation mechanism

1) 

2) 

3) Set $\ell_q := 1/q \log 1/q$.

μ(a segment of length ℓ_q contains at least one vacancy) ~ 1

$FA-2f$ $d=2$, *strategy of the proof*

$$T_{rel} := \inf\{\lambda : Var(f) \le \lambda \mu(f, -\mathcal{L}f)\} \quad \forall f \text{ local}$$

$$\mu(f, -\mathcal{L}f) = \sum_{x \in \mathbb{Z}^2} \mu(c_x Var_x(f))$$

c_x= indicator function that x has ≥ 2 empty nearest neighb.

Var_x=local variance at x

We want to prove $T_{rel} \le \exp(c|\log q|/q)$, i.e. that $\forall f$ it holds

$$Var(f) \le \exp(c|\log q|/q) \sum_{x \in \mathbb{Z}^2} \mu(c_x Var_x(f))$$

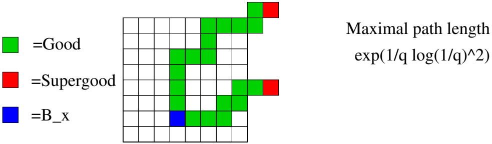
Step 1: a key constrained Poincaré inequality

Renormalize on $L \times L$ boxes with $L = 1/q \log 1/q$.

- a box is good if it contains at least one empty site on each column and on each line $\to \mu(\text{good}) \sim 1$
- a box is super good if it is good and contains at least one empty column and one empty row
  $\to \mu(\text{supergood}) \sim exp(-1/q \log(1/q)^2) \ll 1$

$$Var(f) \leq \sum_{x \in \mathbb{Z}^2(L)} \mu(\kappa_x Var_{B_x})$$

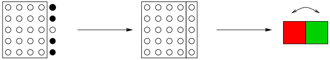
κ_x= indicator function of



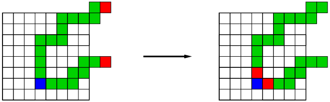
Very flexible tool

Step 2: construct allowed paths

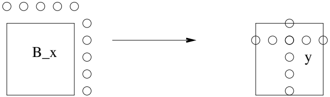
Swap neighbouring good and supergood boxes



Bring two supergood boxes near B_x



For any $\omega \in \{0,1\}^{B_x}$ and $y \in B_x$ we can now bring an empty row and column near $y \in B_x$: the constraint at y is now satisfied



Step 3: canonical paths for reversible Markov chains

Key ingredient: the whole path is constructed by "shifting" an empty column of height $L = 1/q \log 1/q$

Our constrained Poincaré inequality + canonical paths for reversible Markov chains

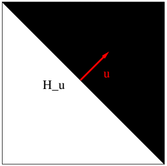
$$\rightarrow T_{rel} \leq \exp(c/q(\log(1/q))^2)$$

(= length of the path $\times$ congestion constant)

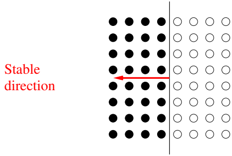
Changing the notion of Good, Supergood, L, and the oriented neighborhood of B_x we cover other models..all critical models?

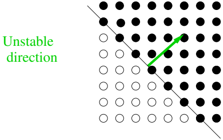
A universality result for cellular automata in $\mathbb{Z}^2$

Take $u \in S^1$, let $H_u := \{x \in \mathbb{Z}^2 :< x, u >< 0\}$.
u is a stable direction if starting from η empty on H_u and filled on $\mathbb{Z}^2 \setminus H_u$ no other site can be emptied.



Ex. East: $\vec{u} = -\vec{e}_1$ is stable; $\vec{u} = \vec{e}_1 + \vec{e}_2$ is unstable

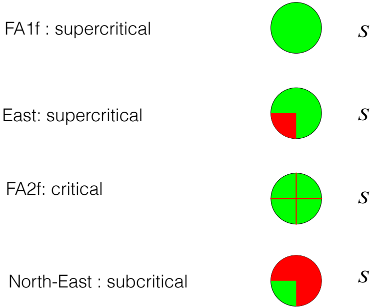




Classification of cellular automata in $\mathbb{Z}^2$

- supercritical if $\exists$ open semicircle without stable directions;
- critical if every open semicircle has a stable direction and $\exists$ a semicircle with a finite number of stable directions
- subcritical otherwise

Red= stable direction; Green= unstable direction



A universality result for cellular automata in $\mathbb{Z}^2$

Theorem [Bollobas, Smith, Uzzell '15 + Bollobas, Duminil-Copin, Morris, Smith '16 + Balister, Bollobas, Przykucki, Smith '16]

- Supercritical models: $q_c(n,\mathcal{U}) = (1/n)^{\Theta(1)}$
- Critical models: $\exists \alpha(\mathcal{U}) > 0$ s.t. $q_c(n,\mathcal{U}) = \Theta\left(1/\log n\right)^{\alpha}$
- Subcritical models: $\liminf_{n\to\infty} q_c(n,\mathcal{U}) > 0$

$\to L_c(q) = 1/q^{\Theta(1)}$ for supercritical models
$\to L_c = \Theta(\exp(1/q^{\alpha}))$ for critical models

$L_c(q)$ determined by the action of the cellular automata on discrete half planes

Supecritical models the key mechanism

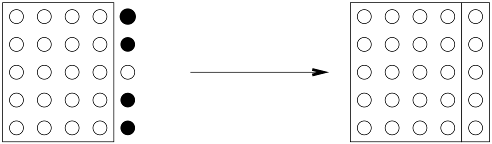
Supercritical models:

- there is a finite empty droplet $D \subset Z^d$ from which we can empty an infinite half line
- if $n \gg 1/q^{|D|}$ we will typically droplets to empty all $\mathbb{Z}_n^d$
- Ex. East: a single empty site is a droplet

Critical models the key mechanism

Critical models:

- we can expand a finite empty droplet one step further iff we find a group of α empty sites on its boundary
- if we have an empty droplet of size $\gg 1/q^{\alpha}$ we will typically be able to continue untill emptying all $\mathbb{Z}_n^d$.
- Ex. FA-2f: a rectangle of empty sites can be expanded if there is at least one empty on the next column



Supercritical KCSM on $\mathbb{Z}^2$

Theorema [Martinelli, Morris, C.T. '16]

A refined classification : a supercritical model is rooted if there are two non opposite stable directions. It is unrooted otherwise.

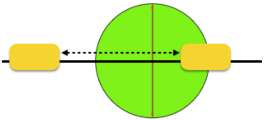
- for all supercritical unrooted models $T_{rel} = 1/q^{\Theta(1)}$
- for all supercritical rooted models $T_{rel} = 1/q^{\Theta(\log(1/q))}$

$$L_c = \frac{1}{q}^{\Theta(1)}$$

$\rightarrow$ unrooted models $\exists \alpha$ s.t. $T_{rel} = O(L_c^\alpha)$

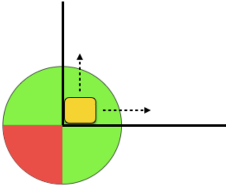
$\rightarrow$ rooted models $\exists \alpha$ s.t. $T_{rel} \geq L_c^{\alpha \log L_c}$

Intuition behind the unrooted result



- ∃ *empty droplet* can be *shifted* back and forth along a line: from the droplet one can empty the entire line
- FA-1 f is unrooted, empty droplet = a single empty site
- scaling proven via renormalization to FA1f model in $d = 1$ and using the polynomial result for FA1f [Cancrini, Martinelli, Roberto, Toninelli '08]

Intuition behind the rooted result



- from any finite empty region we can empty only a cone.
- lower bound: logarithmic energy barriers
  - start from a single droplet
  - to create a new droplet at distance ℓ you necessarily go through a configuration with $c \log \ell$ simultaneous empty sites
  - $\rightarrow$ time $1/q^{c \log 1/q}$
- upper bound: renormalisation to East in $d = 1$ model and using $T_{rel}^{East} = 1/q^{c \log 1/q}$ [Aldous, Diaconis '02, Cancrini, Martinelli, Roberto, Toninelli '08, Chleboun, Faggionato,Martinelli '15]

Critical KCSM on $\mathbb{Z}^2$

$\alpha(\vec{u})$ = difficulty of direction $\vec{u}$= minimal number of empty site to be added to H_u in order to grow the empty set H_u of one step in the $\vec{u}$ direction

$$\alpha := \min_{C} \max_{\vec{u} \in C} \alpha(\vec{u})$$

$$\rightarrow L_c = \Theta(\exp(c/q^{\alpha}))$$

Conjecture

[Martinelli, Morris ,C.T.] A refined classification: a critical model is α -rooted if there are two non opposite stable directions of difficulty $> \alpha$. It is α-unrooted otherwise. Then

- for α- unrooted models $T_{rel} = O(\exp(c/q^{\alpha}|\log(1/q)|)$
- for α-rooted models $T_{rel} \geq \exp(c/q^{\beta}), \;\; \beta > \alpha$

Summary

- KCSM are stochastic models for liquid/glass transition
- intimate relation to bootstrap percolation
- ergodicity for KCSM = percolation cellular automata
- $T_{rel} = 1/\text{gap} < \infty$ in the ergodic regime and $T_{rel} > L_c$
- universality results for bootstrap percolation in $d = 2$
- due to logarithmic barriers sometimes $T_{rel} \gg L_c$
- a refined classification of the influence classes, conjecture on the universal behavior for supercritical / critical KCSM
- a new toolbox to upper bound T_{rel}
  - scaling for FA-kf on $\mathbb{Z}^d$
  - scaling for all critical/supercritical models in $d = 2$ hopefully ...