Bootstrap percolation and Kinetically constrained models: critical time scales

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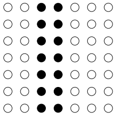
Bootstrap percolation

First example: 2-neighbour bootstrap on $\mathbb{Z}^2$

- At time $t = 0$ sites are i.i.d., empty with probability q, occupied with probability $1 - q$
- At time $t = 1$
  - each empty site remains empty
  - each occupied site is emptied iff it has at least 2 empty n.n.
- Iterate

$\Rightarrow$ *deterministic monotone dynamics*

$\Rightarrow$ $\exists$ *blocked clusters*



Critical density and Infection time

- *Will the whole lattice become empty?*

- $q_c := \inf\{q \in [0,1] : \mu_q(\text{origin is emptied eventually}) = 1\}$

- *How many steps are needed to empty the origin?*
- $\tau^{\text{BP}}(q) := \mu_q(\text{first time at which origin is empty})$

Critical density and Infection time

- *Will the whole lattice become empty?*

  $\rightarrow$ Yes (Van Enter '87)

- $q_c := \inf\{q \in [0,1] : \mu_q(\text{origin is emptied eventually}) = 1\}$

  $\rightarrow q_c = 0$

- *How many steps are needed to empty the origin?*

- $\tau^{\text{BP}}(q) := \mu_q(\text{first time at which origin is empty})$

$$\rightarrow \tau^{\text{BP}}(q) \sim \exp\left(\frac{\pi^2}{18q}(1+o(1))\right) \quad \text{for} \quad q \rightarrow 0$$

[Aizenmann-Lebowitz '88, Holroyd '02, ...]

The general framework: $\mathcal{U}$-bootstrap percolation

- Choose the update family, a finite collection $\mathcal{U} = \{U_1, \ldots, U_m\}$ of local neighbourhoods of the origin, i.e. $U_i \subset \mathbb{Z}^2 \setminus 0, \quad |U_i| < \infty$
- At time $t = 1$ site x is emptied iff at least one of the translated neighborhoods $U_i + x$ is completely empty
- Iterate

Example: 2-neighbour bootstrap percolation

$\mathcal{U}$ = collection of the sets containing 2 nearest neighb. of origin

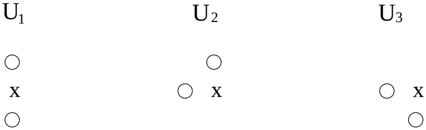
Some other examples

- r-neighbour bootstrap percolation:
  $\mathcal{U}$ = all the sets containing r nearest neighb. of origin

- East model $\mathcal{U} = \{U_1, U_2\}$ with $U_1 = (0, -1)$, $U_2 = (-1, 0)$

- North-East model $\mathcal{U} = \{U_1\}$ with $U_1 = \{(0, 1), (1, 0)\}$

- Duarte model $\mathcal{U} = \{U_1, U_2, U_3\}$



- q_c?
- Scaling of $\tau^{\mathrm{BP}}(q)$ for $q \downarrow q_c$?

Of course, answers depend on the choice of the rule $\mathcal{U}$

Three universality classes

- Supercritical models: $q_c = 0, \quad \tau^{\mathrm{BP}}(q) = 1/q^{\Theta(1)}$
- Critical models: $q_c = 0, \quad \tau^{\mathrm{BP}}(q) = \exp(1/q^{\Theta(1)})$
- Subcritical models: $q_c > 0$

[Bollobas, Smith, Uzzell '15, Balister, Bollobas, Przykucki, Smith '16]

Kinetically Constrained Models, a.k.a. KCM

Configurations : $\eta \in \{0,1\}^{\mathbb{Z}^2}$

Dynamics: continuous time Markov process of Glauber type, i.e. birth / death of particles

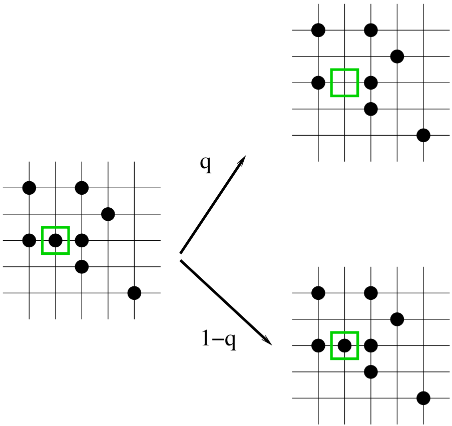
Fix an update family $\mathcal{U}$ and $q \in [0,1]$.

Each site for which the $\mathcal{U}$ bootstrap constraint is satisfied is updated to empty at rate q and to occupied at rate $1-q$.

KCM are a stochastic version version of BP:

- $\Rightarrow$ non monotone dynamics ;
- $\Rightarrow$ reversible w.r.t. product measure at density $1 - q$;
- $\Rightarrow$ blocked clusters for BP $\leftrightarrow$ blocked clusters for KCM;
- $\Rightarrow$ empty sites needed to update $\rightarrow$ slowing down when $q \downarrow 0$

2-neighbour KCM



Origins of KCM

KCM introduced by physicists in the '80's to model the liquid/glass transition

- understanding this transition is a major open problem in condensed matter physics;
- sharp divergence of timescales;
- no significant structural changes.

KCM:

$\Rightarrow$ constraints mimic *cage effect*:
if temperature is lowered free volume shrinks, $q \leftrightarrow e^{-1/T}$

$\Rightarrow$ trivial equilibrium, sharp divergence of timescales when $q \downarrow 0$, glassy dynamics (aging, heterogeneities, . . .)

Why are KCM mathematically challenging?

- KCM dynamics is not attractive: more empty sites can have unpredictable consequences
- Coupling arguments and censoring arguments fail
- $\exists$ blocked clusters $\rightarrow$ relaxation not uniform on initial condition $\rightarrow$ worst case analysis is too rough
- Coercive inequalities (e.g. Log-Sobolev) anomalous

$\rightarrow$ new tools are needed

KCM: time scales

$\tau^{\mathrm{KCM}}(q) := \mathbb{E}_{\mu_q}($ first time at which origin is emptied $)$

- How does τ^{KCM} diverge when $q \downarrow q_c$?
- How does it compare with τ^{BP}, the infection time of the corresponding bootstrap process?

An (easy) lower bound

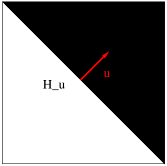
$$\tau^{\mathrm{KCM}} \geq c\,\tau^{\mathrm{BP}}$$

General, but it does not always capture the correct behavior

How can you identify the universality class of $\mathcal{U}$?

We need the notion of stable and unstable directions

- Fix a direction $\vec{u}$
- Start from a configuration which is
  - completely empty on the half plane perpendicular to $\vec{u}$ in the negative direction (H_u)
  - filled otherwise
- Run the bootstrap dynamics



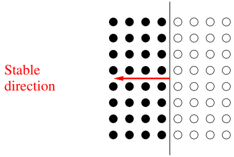
$$\vec{u} \text{ is } \begin{cases} \text{stable} & \text{if no other site can be emptied} \\ \text{unstable} & \text{otherwise} \end{cases}$$

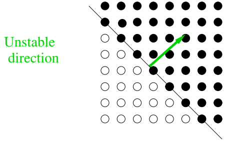
Stable and unstable directions: examples

Of course, the stability of a direction depends on $\mathcal{U}$

Ex. East model:

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



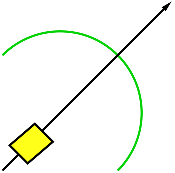


Instead :

- both directions are unstable for 1-neighbour bootstrap
- both directions are stable for North East

Supercritical universality class

$\mathcal{U}$ is supercritical iff there exists an open semicircle $\mathcal{C}$ which does not contain stable directions



$\Rightarrow$ exists a finite empty droplet from which we can empty the line bisecting $\mathcal{C}$

$\Rightarrow q_c = 0$

[Bollobas, Smith, Uzzell '15]

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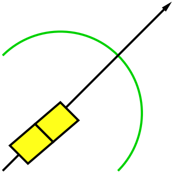

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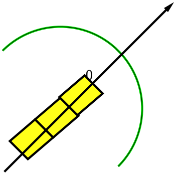


$\Rightarrow$ exists a finite empty droplet from which we can empty the line bisecting $\mathcal{C}$

$\Rightarrow q_c = 0$

$\Rightarrow \tau^{\text{BP}} \sim$ distance of origin from empty droplet $\sim 1/q^{\Theta(1)}$

[Bollobas, Smith, Uzzell '15]

Examples of supercritical rules

1-neighbour

East

For East and 1-neighbour: droplet = single empty site

Supercritical KCM: a refined classification

We say that supercritical model is

- rooted if it has at least 2 non opposite stable directions
- unrooted otherwise

Examples
- East model is rooted
- 1-neighbour model is unrooted

Supercritical KCM : results

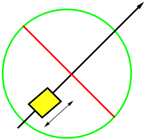
Theorem 1. [Martinelli, Morris, C.T. '17]

(i) for all supercritical unrooted models $\tau^{\mathrm{KCM}} = 1/q^{\Theta(1)}$

(ii) for all supercritical rooted models $\tau^{\mathrm{KCM}} = 1/q^{\Theta(\log(1/q))}$

Thus for rooted models: $\tau^{\mathrm{KCM}}(q) \gg \tau^{\mathrm{BP}}(q)$. Why? $\ldots$

Unrooted KCM:

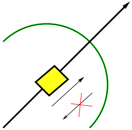


- empty droplet, D, can move back and forth
- D behaves roughly as a random walk of rate $q^{|D|}$
- distance of origin to first empty droplet $\sim 1/q^{|D|}$

$$\Longrightarrow \tau^{\mathrm{KCM}} \sim 1/q^{c}$$

Heuristic for supercritical rooted KCM

Rooted KCM:



- empty droplet moves only in one direction
- $\rightarrow$ logarithmic energy barriers (L.Marêché '17):

to create new droplet at distance $n \sim 1/q^c$ we have to go through a configuration with $\log n$ empty sites

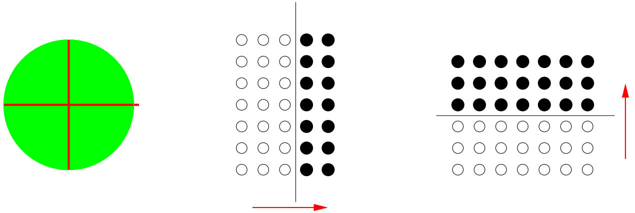
$$\Longrightarrow \tau^{\text{KCM}} \sim 1/q^{c|\log q|}$$

Critical universality class

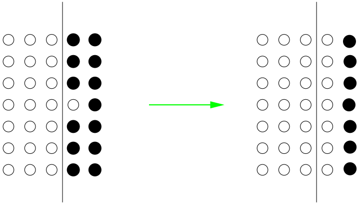
A KCM is critical if

- it is not supercritical
- and there exist an open semicircle $\mathcal{C}$ with only a finite number of stable directions

Example 2-neighbour model



2-neighbour model



- 1 site is sufficient to unblock $\vec{e}_1$
  $\rightarrow$ $\vec{e}_1$ is stable with *difficulty* 1
- A column of size $1/q \log(1/q)$ is a *droplet*:
  if it is empty it can (typically) empty the next column

$\mathcal{U}$-bootstrap: the general critical case

- Difficulty of direction $\vec{u}$:
  $d(\vec{u})$ = minimal number of empty sites to unstabilize $\vec{u}$

- Difficulty of a model :
  $\alpha = \min_{\mathcal{C}} \max_{\vec{u} \in \mathcal{C}} d(\vec{u})$

$\Rightarrow$ the size of the minimal empty droplet is $\sim 1/q^{\alpha}$

$\Rightarrow$ $\tau^{\mathrm{BP}}(q) \sim e^{1/q^{\alpha} \log(1/q)^{\Theta(1)}}$ = mean distance from origin to nearest empty droplet

$\Rightarrow$ $q_c = 0$

Critical KCM

We introduce a new key quantity the *bilateral difficulty* :

$\beta = \min_{\mathcal{C}} \max_{\vec{u}\in\mathcal{C}} \max\{d(\vec{u}), d(-\vec{u})\}$

Theorem 2. [Martinelli, Morris, C.T. '18]

Let $\gamma = \min(2\alpha, \beta)$. Then

$$\tau^{\mathrm{KCM}}(q) \le e^{1/q^{\gamma}|\log q|^{\Theta(1)}}$$

Critical KCM

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Conjecture

The upper bound is tight.

Conjecture proven for

- $\alpha = \beta$, just use general bound $\tau^{\mathrm{KCM}} \geq c\tau^{\mathrm{BP}}$
- Duarte model (hard!) [L.Marêché, F.Martinelli, C.T '18]
- work in progress for general cases ...

The case of the Duarte model

- Constraint: *at least 2 empty among S , W, and N neighb.*
- $\vec{e}_1, \pm\vec{e}_2$ have difficulty $= 1$;
- all other stable directions have difficulty $= \infty$

$\rightarrow$ $\alpha = 1$ and $\beta = \infty$

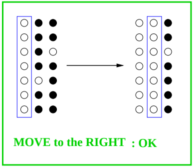
$\rightarrow$ $\gamma = \min(2\alpha, \beta) = 2$

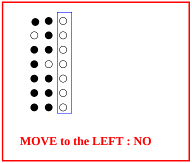
Theorem 3. [Marêché, Martinelli, C.T. '18]

For Duarte model it holds $\tau^{\mathrm{KCM}} = \exp\left(\frac{c|\log q|^4}{q^2}\right)$

Thus $\tau^{\mathrm{KCM}} \gg \exp\frac{c|\log q|^2}{q} = \tau^{\mathrm{BP}}$. Why? ...

Duarte model: heuristic





- Droplet: empty column of size $\ell = \frac{|\log q|}{q}$
- Droplets evolve East-like: we can tipically create/destroy a droplet to the right of an existing droplet
- Density of droplets is $q_{eff} = q^\ell = \exp -\frac{|\log(q)|^2}{q}$
- Droplets also occasionally move up (or down) if they find an empty site above (resp. below) the next column

Heuristic for Duarte model: KCM vs BP

$L=$ distance from the origin to the nearest droplet on the left

- L is typically $1/q_{eff}$
- due to the East like dynamics of droplets we must overcome a logarithmic energy barrier to empty the origin, i.e. create $\log_2 L$ simultaneous droplets

$$\Longrightarrow \tau^{\mathrm{KCM}} \sim \frac{1}{q_{eff}^{c|\log_2 q_{eff}|}} = \exp \frac{c|\log q|^4}{q^2}$$

$$\tau^{\mathrm{BP}} = \text{number of moves in the shortest path} \sim \exp \frac{c|\log q|^2}{q}$$

$$\Longrightarrow \tau^{\mathrm{KCM}} \gg \tau^{\mathrm{BP}}$$

Turning heuristics into a proof: the key difficulties

- the droplets evolve only if the environment is "good"
- the environment evolves
- no monotonicity, no coupling arguments
- the droplet is not a "rigid" object
- how can we get the lower bound on τ^{KCM}?
  couldn't there be a relaxation mechanism faster than the East-like motion of droplets?

Summary

- KCM are the stochastic counterpart of bootstrap percolation;
- times for KCM may diverge very differently from those of bootstrap due to the occurrence of *energy barriers*;
- a refined classification of update rules needed to capture the universality classes of KCM

Thanks for your attention

many thanks to the organisers

and very happy birthday Anton!

Two equivalent definitions

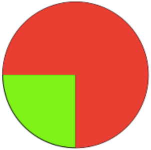
$\mathcal{U}$ is subcritical iff it is neather supercritical nor critical

or

$\mathcal{U}$ is subcritical iff each open semicircle contains infinite stable directions

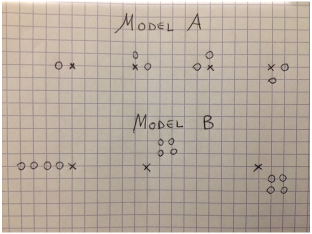
$\Rightarrow$ $q_c > 0$: blocked clusters percolate at $q < q_c$

Example: North East model



Given a KCM, how can we guess its scaling?

- If I give you a rule, can you guess its scaling?
- Sharp divergence: numerics often cannot give clear cut answer



Try to guess:

is model A superArrhenius or Arrhenius? And model B? Is B faster or slower than A?

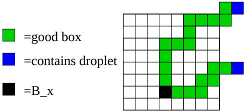
2-neighbour KCM: more on the proof

- First step: upper bound infection time with relaxation time

$$\tau \leq \frac{T_{rel}}{q} = \frac{1}{q} \inf\Big(\lambda : \ \mathrm{Var}(f) \leq \lambda \sum_x \mu_q(c_x \ \mathrm{Var}_x(f)) \ \forall f\Big)$$

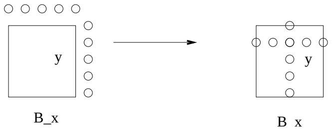
$c_x = 1_{x \text{ has at least 2 empty neighbours}}$

- Second step: an auxiliary long range *block* dynamics
  - blocks are $\ell \times \ell$ boxes, $\ell = 1/q \log(1/q)$
  - put equilibrium on box B_x at rate 1 iff it belongs to a good cluster with two droplets at distance at most $L = \exp(1/q \log(1/q)^2)$



2-neighbour KCM: more on the proof

- Third step : we establish a new long range Poincaré inequality that yields $T_{rel}^{aux} = O(1)$
- Fourth step : canonical path techniques for reversible Markov chains
  - We construct an allowed path to bring the droplets near B_x
  - We move the droplets inside B_x near any site $y \in B_x$: flip at y is now allowed $\rightarrow$ we "reconstruct" the update of block B_x via allowed elementary moves



$\rightarrow \tau^{\text{2-neighb. KCM}} \leq$ length of path $\times$ congestion $= \exp\left(c/q(\log 1/q)^2\right)$

k-neighbour model on $\mathbb{Z}^d$, $k \in [2, d]$

$q_c = 0$, blocked clusters do not percolate [Schonmann '90]

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

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

Theorem (Martinelli, C.T. '16)

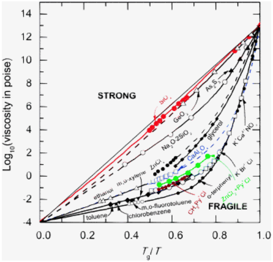
- *2-neighbour KCM:*

$$\exp(c/q^{1/(d-1)}) \leq \tau^{KCM}(q) \leq \exp\left(\log(1/q)^c / q^{1/(d-1)}\right)$$

- *k-neighbour KCM:*

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

Liquid/glass transition



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

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

$$q \leftrightarrow e^{-1/T}$$

- $\Rightarrow$ supercritical unrooted models $\leftrightarrow$ strong liquids
- $\Rightarrow$ supercritical rooted models $\leftrightarrow$ fragile liquids

A general constrained Poincare inequality

$$\Omega = S^{\mathbb{Z}^2}$$

$$\mu = \prod_x \mu_x$$

A_x event on quadrant with bottom left corner x

If $\sup_{x \in \mathbb{Z}^2} (1 - \mu(A_x))|Supp(A_x)| \leq 1/4$

$$Var_\mu(f) \leq 4 \sum_x \mu(c_x Var_{\mu_x}(f))$$

where $c_x = 1_{A_x}$