Bootstrap percolation and Kinetically constrained models: critical time scales

Cristina Toninelli

Laboratoire de Probabilités et Modèles Aléatoires

European Research Council
Established by the European Commission

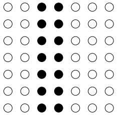
Collaborators: Laure Marêché, Fabio Martinelli, Rob Morris

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

- At time $t = 0$ sites of $\mathbb{Z}^2$ are i.i.d., empty with prob q, occupied with prob $1 - q$
- At time $t = 1$ empty sites remain empty and occupied sites with at least 2 empty nearest neighbours are emptied
- Iterate

$\Rightarrow$ *deterministic monotone dynamics*

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



Critical density and Infection time

- *Will the whole lattice become empty eventually?*

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

- *How many steps does it take to empty the origin?*
- $\tau(q) := \mu_q(\text{first time at which origin is empty})$

Critical density and Infection time

- *Will the whole lattice become empty eventually?*
  $\rightarrow$ 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 does it take to empty the origin?*

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

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

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

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

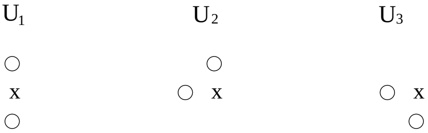
- Choose the update family, a finite collection $\mathcal{U} = \{U_1, \ldots, U_m\}$ of local neighbourhoods of the origin, i.e. $U_i \subset \mathbb{Z}^2 \setminus 0, \quad |U_i| < \infty$
- At time $t = 1$ site x is emptied iff at least one of the translated neighborhoods $U_i + x$ is completely empty
- 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 $\mathcal{U} = \{U_1, U_2, U_3\}$



Universality classes

- q_c?
- Scaling of $\tau(q)$ for $q \downarrow q_c$?

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

Three universality classes

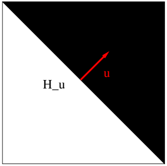
- Supercritical models: $q_c = 0, \quad \tau(q) = 1/q^{\Theta(1)}$
- Critical models: $q_c = 0, \quad \tau(q) = \exp(1/q^{\Theta(1)})$
- Subcritical models: $q_c > 0$

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

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



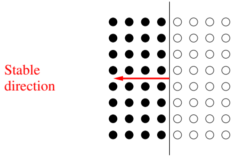
$$\vec{u} \text{ is } \begin{cases} \text{stable} & \text{if no other site can be emptied} \\ \text{unstable} & \text{otherwise} \end{cases}$$

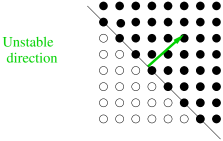
Stable and unstable directions: examples

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

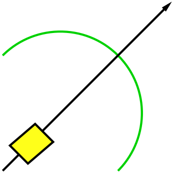




Instead :

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

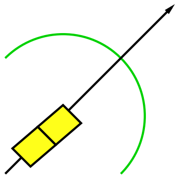
$\mathcal{U}$ is supercritical iff there exists an open semicircle $\mathcal{C}$ which does not contain stable directions



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

Supercritical universality class

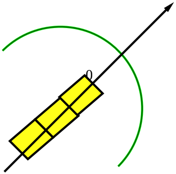
$\mathcal{U}$ is supercritical iff there exists an open semicircle $\mathcal{C}$ which does not contain stable directions



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

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 $\mathcal{C}$

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

$\Rightarrow q_c = 0$

Examples of supercritical models

1-neighbour

East

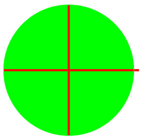
For East and 1-neighbour: droplet = single empty site

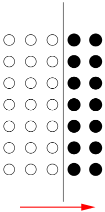
Critical universality class

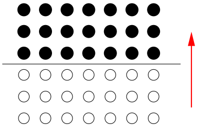
$\mathcal{U}$ is critical iff

1) it is not supercritical
2) $\exists$ open semicircle $\mathcal{C}$ with only a finite number of stable directions

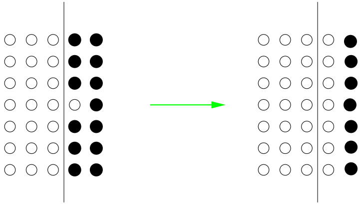
Example 2-neighbour model







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

$\Rightarrow$ $\tau(q) \leq e^{1/q\log(1/q)^2}$ = mean distance from 0 to nearest empty droplet

$\Rightarrow$ $\tau(q) \sim e^{\frac{\pi^2}{18q}(1+o(1))}$ via a (much) more refined argument

Critical universality class

The general critical case:

- *Difficulty* of a stable direction :
  $d(\vec{u})$ = minimal number of empty sites to unstabilize $\vec{u}$, i.e. to empty an infinite number of sites in direction $\vec{u}$

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

$\Rightarrow$ size of the droplet (= empty region from which we can expand) is $\sim 1/q^{\alpha}$

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

$\Rightarrow$ $q_c = 0$

Subcritical universality class

Two equivalent definitions

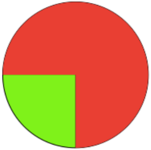
$\mathcal{U}$ is subcritical iff it is neather supercritical nor critical

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



Kinetically Constrained Models, a.k.a. KCM

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

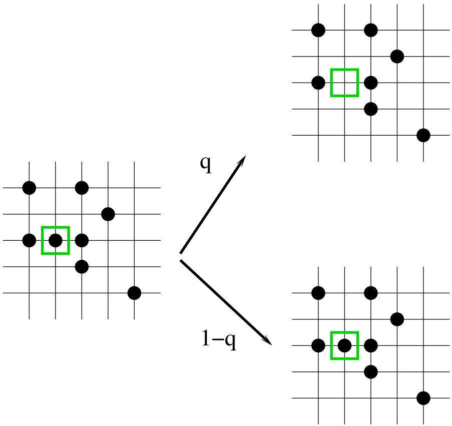
Dynamics: continuous time Markov process of Glauber type, i.e. birth / death of particles

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 $1-q$.

- $\Rightarrow$ 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 in the '80's to model the liquid/glass transition

- If a liquid is cooled sufficiently rapidly it avoids crystallisation and freezes in an amorphous solid, the glass;
- understanding the liquid/glass transition is a major open problem in condensed matter physics;
- sharp divergence of timescales;
- no significant structural changes.

Origins of KCM

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

- If a liquid is cooled sufficiently rapidly it avoids crystallisation and freezes in an amorphous solid, the glass;
- understanding the liquid/glass 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

Supercritical KCM: a new classification

We introduce a refined classification. A supercritical model is

- rooted if there are two non opposite stable directions
- unrooted otherwise.

Examples.

- 1-neighbour model: unrooted
- East model: rooted

Supercritical KCM : results

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

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

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

$\Rightarrow$ Rooted models: $\tau^{\mathrm{KCM}}(q) \gg \tau^{\mathrm{BP}}(q)$

Critical KCM: first example

Theorem 2. [Martinelli, C.T. '16]

For the 2-neighbour KCM

$$\exp\left(\frac{\pi^2}{18q}\right) \leq \tau(q) \leq \exp\left(\frac{\log(1/q)^2}{q}\right)$$

- Heuristic / ideas of proof in a moment ...
- new flexible toolbox: we can analyse all critical models

Critical KCM : a new classification

We introduce a refined classification.

A critical KCM with difficulty α is

- rooted if $\exists$ two non opposite directions of difficulty $> \alpha$
- unrooted otherwise.

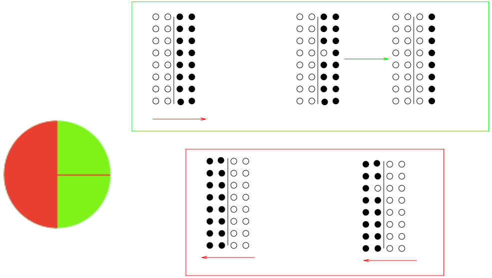
Examples

- **2-neighbour model**:
  $\pm\vec{e}_1, \pm\vec{e}_2$ have difficulty $= 1$
  $\rightarrow \alpha = 1$ and **unrooted**

- **Duarte model** (*at least 2 empty among S , W, and N*):
  $\alpha = 1$ and **rooted. Why?**

Duarte model is critical rooted

Duarte model (*at least 2 empty among S , W, and N*):



- $\vec{e}_1$ has difficulty 1;
- $-\vec{e}_1$ and all the directions in the red semicircle have ∞ difficulty
- $\alpha = 1$ and **rooted** (there are a lot of non opposite stable directions with difficulty > 1!)

Critical KCM : results

Theorem 2. [Martinelli, C.T. '16 + Martinelli,Morris,C.T. '17]

- for unrooted critical KCM with difficulty α

$$\tau^{\mathrm{KCM}} = \exp\left(\frac{c|\log(1/q)|^{\Theta(1)}}{q^{\alpha}}\right)$$

- for rooted critical KCM with difficulty α

$$\exp\left(\frac{c|\log(1/q)|^{\Theta(1)}}{q^{\alpha}}\right) \leq \tau^{\mathrm{KCM}} \leq \exp\left(\frac{c|\log(1/q)|^{\Theta(1)}}{q^{\gamma}}\right)$$

$$\gamma > \alpha$$

$$\gamma = \min(2\alpha, \beta) \quad \text{with} \quad \beta = \min_{\mathcal{C}} \max(d(\mathcal{C}), d(-\mathcal{C})) \geq \alpha + 1$$

$$d(\mathcal{C}) = \max_{\vec{u} \in \mathcal{C}} d(\vec{u})$$

Conjecture for rooted KCM

For rooted KCM we conjecture that the upper bound is correct:

$$\tau^{\text{KCM}} \gg \tau^{\text{BP}}$$

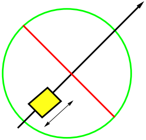
With L.Marêché and F.Martinelli we proved the conjecture for Duarte model ($\alpha = 1, \gamma = 2$)

$$\tau^{\text{KCM Duarte}} \sim \exp(1/q^2) \gg \tau^{\text{BP Duarte}} \sim \exp(1/q)$$

Work in progress for general case ...

Heuristic for supercritical unrooted/rooted result

Unrooted KCM:

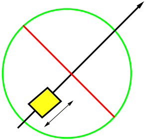


- empty droplet D moves back and forth
- D behaves roughly as a random walk of rate $q^{|D|}$
- distance of origin to first empty droplet $\sim 1/q^{|D|}$

$\Longrightarrow \tau^{\mathrm{KCM}} \sim 1/q^{\Theta(1)}$

Heuristic for supercritical unrooted/rooted result

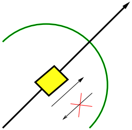
Unrooted KCM:



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

$\Longrightarrow \tau^{\mathrm{KCM}} \sim 1/q^{\Theta(1)}$

Rooted KCM:



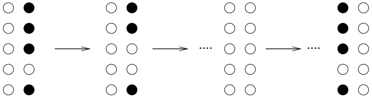
- empty droplet moves only in one direction
- $\to$ logarithmic energy barriers [L.Marêché '17]: to create new droplet at distance $n \sim 1/q^{\Theta(1)}$ we have to go through a configuration with $\log n$ empty sites

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

2-neighbour KCM: ideas of the proof

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

- a box is good if it contains at least one empty site on each column and on each line
- a droplet is an empty column or row of length ℓ
- $\mu_q(\text{good}) \sim 1 \to$ good boxes percolate
- droplets can freely move on the good cluster without creating more then one extra droplet



2-neighbour KCM: ideas of the proof

Heuristics:

- at $t = 0$ w.h.p. the origin belongs to a cluster of good boxes containing a droplet at distance $L \sim \exp(c/q \log(1/q)^2)$
- in time poly(L) the droplet moves near origin and we can empty the origin $\to \tau \leq \exp(c/q \log(1/q)^2)$

Main difficulties when turning heuristics into a proof:

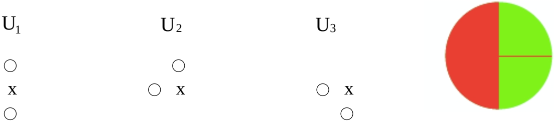
- the good cluster evolves
- the droplet can be destroyed
- no monotonicity, no coupling arguments

Critical KCM: the general case

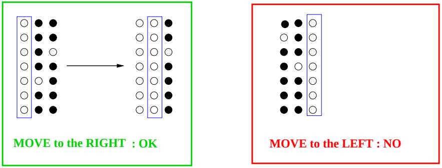
- Very flexible strategy: changing the notion of droplet, good box, and the length scales we cover all critical models
- Why do we get $\tau^{\mathrm{KCM}} \gg \tau^{\mathrm{BP}}$ for critical rooted models?

An example of critical rooted KCM: Duarte model

Duarte model: ≥ 2 empty among N, W and S neighbours



- $d(\vec{e}_1) = 1, \quad d(\vec{u}) = \infty$ for all $u \in$ red semicercle
- an empty column of height $\ell = 1/q \log 1/q$ can (typically) empty next column to its right, but never to its left!



Duarte model

- an empty column of height $\ell = 1/q \log(1/q)$ is a droplet that moves only to its right
- logarithmic barriers: to move the droplet a distance L on the good cluster we have to go through a configuration with $\log(L)$ simultaneous droplets
- to bring the droplet near the origin we typically have to move it a distance $L = \exp(1/q \log(1/q))$

$$\tau^{\text{KCM Duarte}} \sim \frac{1}{q^{\ell}}^{\log L} = e^{1/q^2 \log(1/q)^{\Theta(1)}} \gg e^{1/q \log(1/q)^{\Theta(1)}} = \tau^{\text{BP Duarte}}$$

$\Rightarrow$ τ^{BP} = length of the optimal path to empty origin

$\Rightarrow$ τ^{KCM} = length of optimal path $\times$ time to go through it !

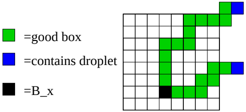
2-neighbour KCM: more on the proof

- First step: upper bound infection time with relaxation time

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

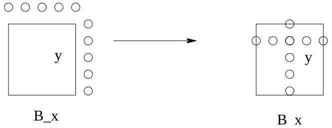
$c_x = 1_{x \text{ has at least 2 empty neighbours}}$

- 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 $\to$ we "reconstruct" the update of block B_x via allowed elementary moves



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

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 captures the universality classes of KCM;
- we construct a new (flexible) toolbox to analyse T_{rel} and τ

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)

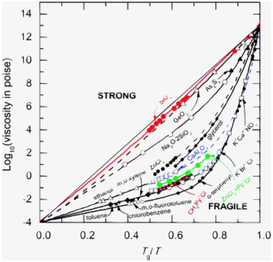
- *2-neighbour KCM:*

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

- *k-neighbour KCM:*

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

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 $c_x = 1_{A_x}$