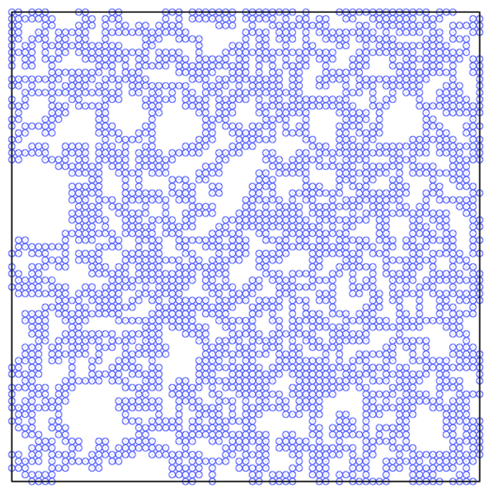
Glassy dynamics in kinetically constrained models

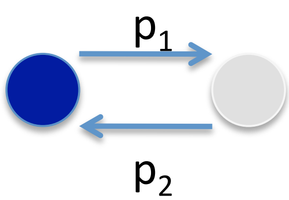
Hiroki Ohta
(LPTMS, Universite Paris Sud)
in collaboration with
Shin-ichi Sasa (Kyoto University)



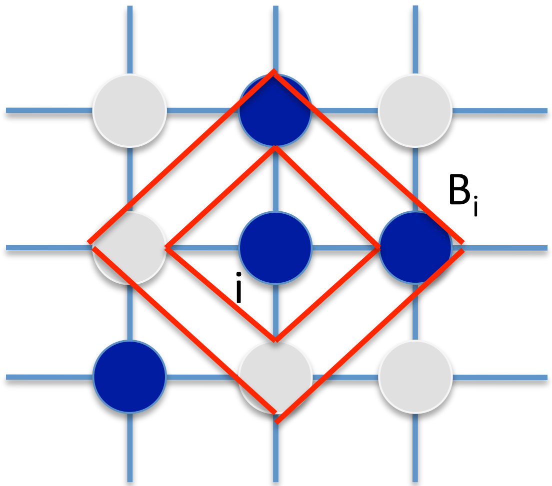
(arXiv:1112.0971)

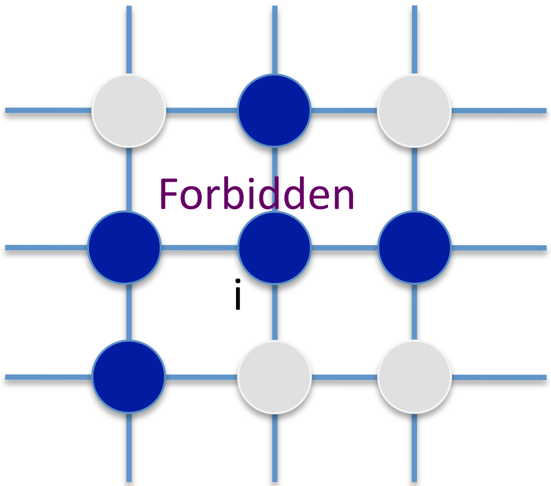
What are kinetically constrained models ?

[Fredrickson,Anderson,PRL,1984]



Square lattice





k =2

If the number of  at nearest neighbors of site i is more than k,
the change of states at site i is forbidden.

[Ritort,Sollich,AdvPhys,2001]

This might be a toy model for glassy dynamics such as cage effects
that the dynamics of a particle is suppressed by the neighbor particles.

The same thing by more formal expressions

=1 =0 $\sigma_i \in \{0,1\}$ On the square lattice

Master equation

$$\partial_t P(\boldsymbol{\sigma},t) = \sum_{\boldsymbol{\sigma}'\neq\boldsymbol{\sigma}} [R(\boldsymbol{\sigma}'\to\boldsymbol{\sigma})P(\boldsymbol{\sigma}',t) - R(\boldsymbol{\sigma}\to\boldsymbol{\sigma}')P(\boldsymbol{\sigma},t)]$$

Transition rate

$$R(\boldsymbol{\sigma}\to\boldsymbol{\sigma}') = \sum_i \delta(\boldsymbol{\sigma}', F_i\boldsymbol{\sigma}) r(\boldsymbol{\sigma}\to\boldsymbol{\sigma}') \mathcal{C}_i(\boldsymbol{\sigma})$$

Spin flipping operator

$$(F_i\boldsymbol{\sigma})_j = (1-\sigma_i)\delta_{ij} + \sigma_j(1-\delta_{ij}).$$

$$\boxed{\mathcal{C}_i(\boldsymbol{\sigma}) = 0 \quad \text{If} \quad \sum_{j\in \mathrm{B}_i} \sigma_j \geq 3}$$

If we change this function,
Other behaviors can happen.

For example, we can choose

$$H(\boldsymbol{\sigma}) = \sum_{i\in\Lambda} \sigma_i \qquad r(\boldsymbol{\sigma}\to\boldsymbol{\sigma}') = \min\left[1, \exp\left(\frac{H(\boldsymbol{\sigma}) - H(\boldsymbol{\sigma}')}{T}\right)\right]$$

In this case, there is no equilibrium phase transitions in the model.

$T \to 0$ $p_1=1$

$$1 \underset{p_2=0}{\overset{p_1=1}{\rightleftarrows}} 0$$

$p_2=0$

Status of KCMs in the studies of glass?

Some experimental studies have attempted to understand the relationship between KCMs and realistic glass-forming materials.

[Candelier, Dauchot, Biroli, EPL, 2010]

-> Negative evidence

[Keys et al,PRX, 2011]

-> Positive evidence

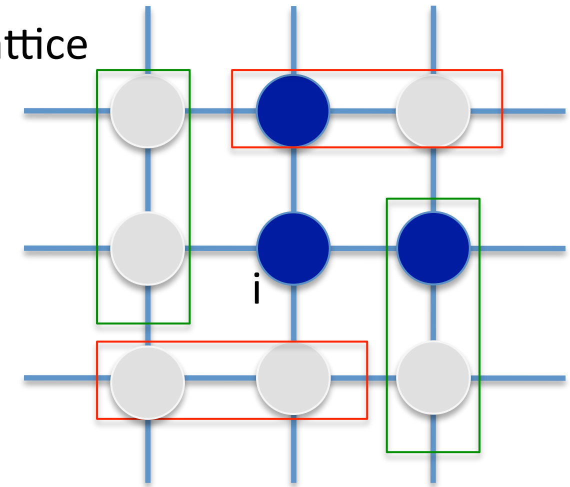
Anyway, the properties of KCMs themselves have not been understood sufficiently,
In particular, we need to understand phase transitions on finite dimensions.

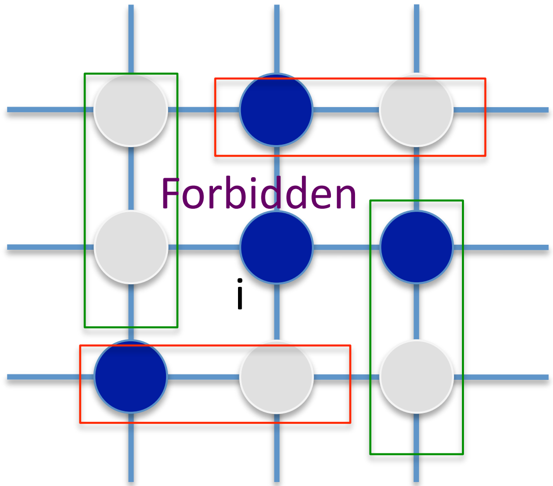
An oriented KCM

[Toninelli, Biroli, Fisher, PRL 2006]
[Toninelli, Biroli, EPJB 2008]

Spiral model

Square lattice



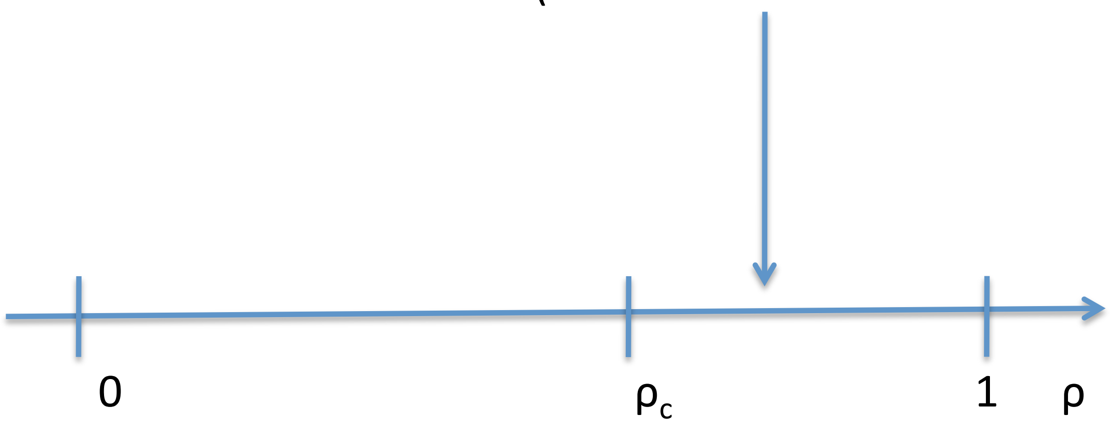


$\mathcal{C}_i(\boldsymbol{\sigma}) = 0$ If there is at least one in both boxes
or in both boxes
The change of the state at site i is forbidden.

we consider the initial condition where blue particles are put at each site with probability ρ.

Freezing transition

There is a set of constrained particles
by only constrained particles,
which we call "frozen" particles.
(The state at frozen sites never change.)



= the transition point
of the directed site percolation
in a cellular automton (Domany-Kinzel model)

Other models (Knight model by Toninelli, Biroli, Fisher PRL 2006,
Force-balance model by Jeng,Schwarz PRE 2010) also belong to the same universality class.
(We call it "TBF class".)

The purpose of our study

??) From a theoretical point of view,
one might ask how robust is the results in the oriented models?
Specifically, it is reasonable to think
“is the orientation a necessary condition for the freezing transition?”

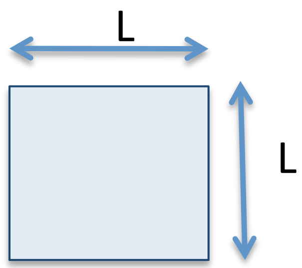
??) From the experimental point of view,
One might argue that this mechanism cannot occur in realistic glassy systems
because the model is already oriented, which is not true in realistic systems.
(It is not reasonable to argue that KCMs is not relevant only because of
the nature of lattice models. Remember critical phenomena in Ising models)

Our work can answer to these questions in the way that
The orientation is not necessary, therefore, we cannot still exclude possible relations
between the realistic glassy systems and KCMs only because of the above reason.

Unoriented Model

$$\sigma_i \in \{0, 1\}$$

On the square lattice



(Filled boundary condition)

Master equation

$$\partial_t P(\boldsymbol{\sigma}, t) = \sum_{\boldsymbol{\sigma}' \neq \boldsymbol{\sigma}} [R(\boldsymbol{\sigma}' \to \boldsymbol{\sigma}) P(\boldsymbol{\sigma}', t) - R(\boldsymbol{\sigma} \to \boldsymbol{\sigma}') P(\boldsymbol{\sigma}, t)]$$

Transition rate

$$R(\boldsymbol{\sigma} \to \boldsymbol{\sigma}') = \sum_i \delta(\boldsymbol{\sigma}', F_i \boldsymbol{\sigma}) r(\boldsymbol{\sigma} \to \boldsymbol{\sigma}') \mathcal{C}_i(\boldsymbol{\sigma})$$

Spin flipping operator

$$(F_i \boldsymbol{\sigma})_j = (1 - \sigma_i)\delta_{ij} + \sigma_j (1 - \delta_{ij}).$$

$$\mathcal{C}_i(\boldsymbol{\sigma}) = 0$$

If $\sum_{j \in \mathrm{B}_i} \sigma_j \geq 3$

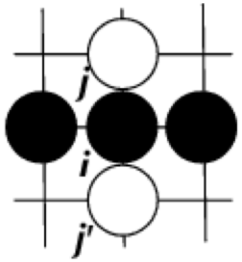
Or

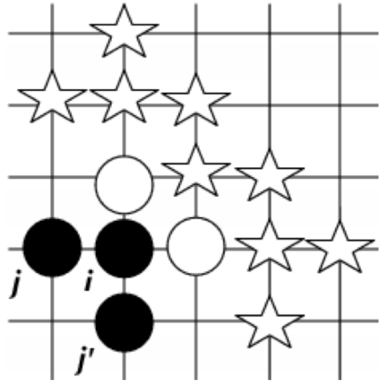
$\sum_{j \in \mathrm{B}_i} \sigma_j = 2$ and $\sum_{j \in \mathrm{B}_i} \delta(f_j, 2) \leq 1$

where $f_i \equiv \sum_{j \in \mathrm{B}_i} \delta(\sigma_j, 0) \left[\prod_{\ell \in \mathrm{B}_j} \delta(\sigma_\ell, 0) \right]$

Examples of some configurations

Forbidden





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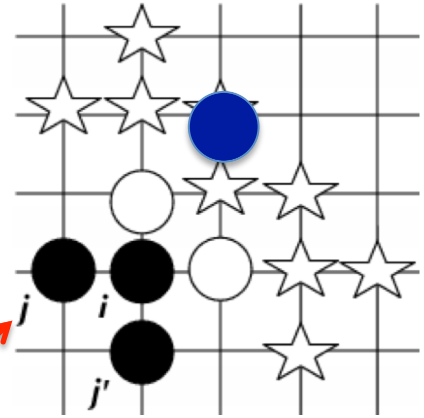
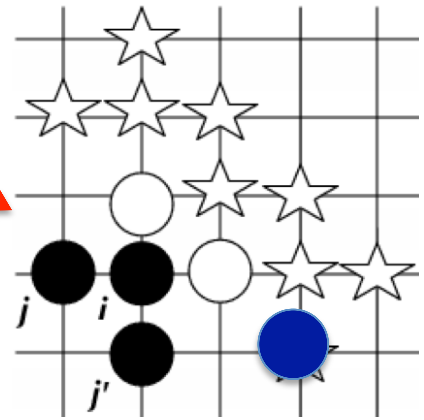


The change of
the state at site i is forbidden.

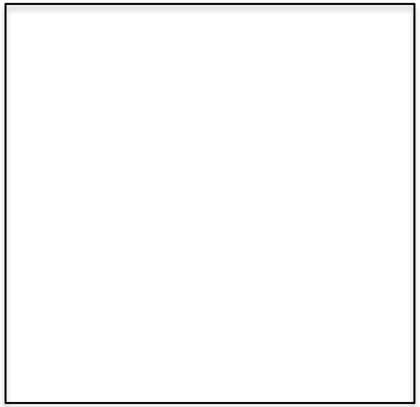
If there is at least one particle
at the sites marked with
the star symbol, the change of
the state at site i is forbidden.



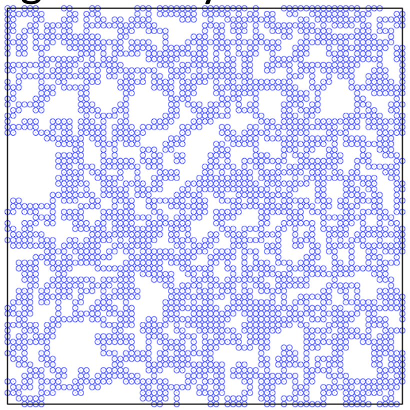
Results

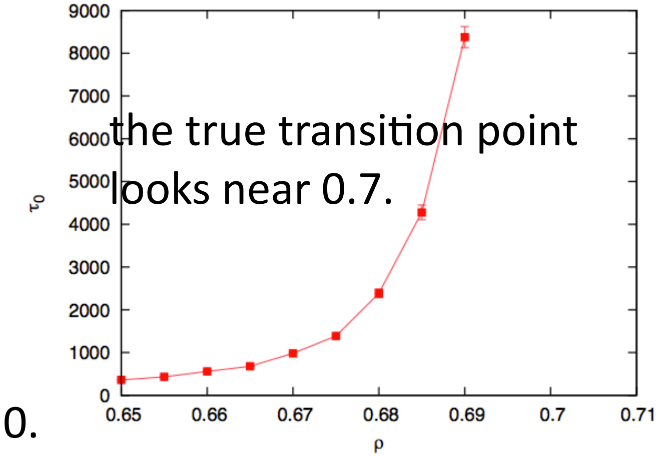
Initially, particles are located with probability ρ.

Low density



High density





the true transition point looks near 0.7.

Result) we can prove that there is a freezing transition at ρ_c where $0<\rho_l \leqq \rho_c \leqq \rho_u<1$.

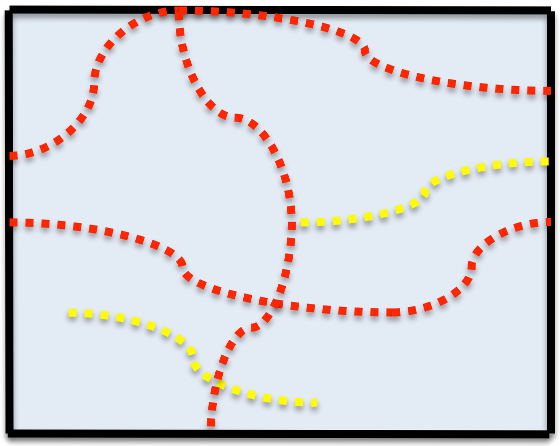
ρ_u=0.984…
(ρ_l=1/24)

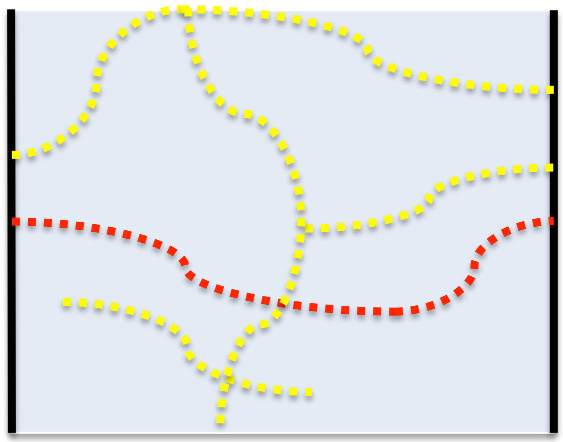
Relaxation time τ_0 when $\Sigma_i\sigma_i$ becomes 0.

numerical experiments near the transition point

Red: The sequence of frozen sites
Yellow: unfrozen particles

: filled boundary





Numerical experiments are quite hard
In a sense that we might need the time of exp(L).

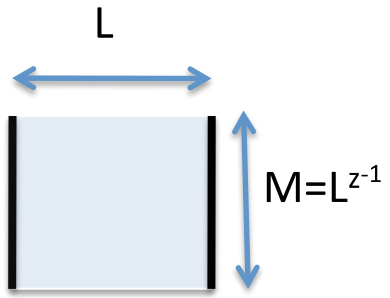
Numerical experiments are not so hard
In a sense that the difficulty is the same as the ones in usual percolation problems.

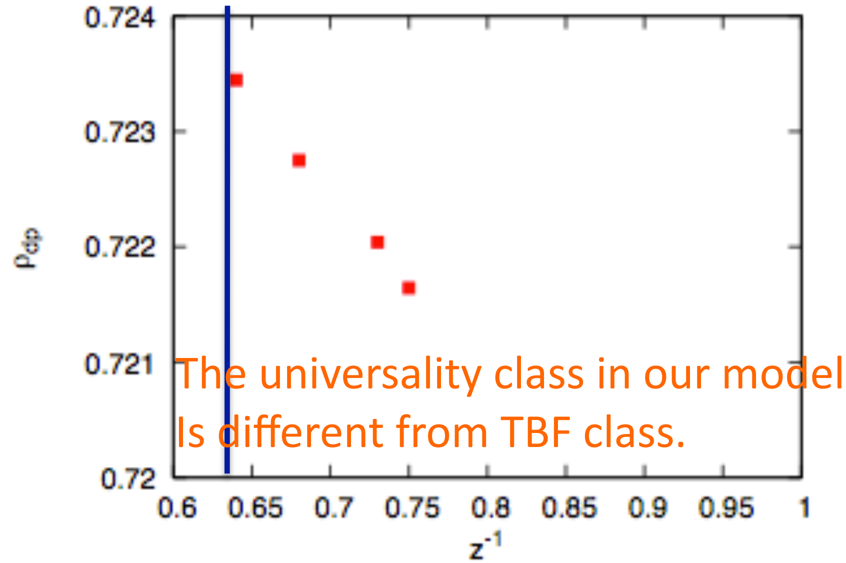
$$\rho_c \leqq \rho_{dp}$$

If there are frozen particles in the modified system,
We can find frozen particles in the original system.

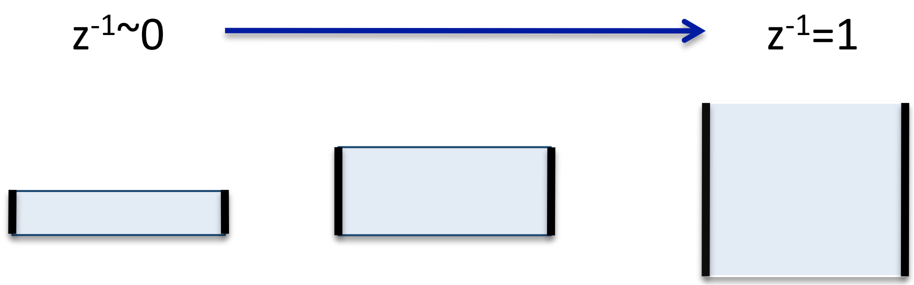
Conjecture

The modified system

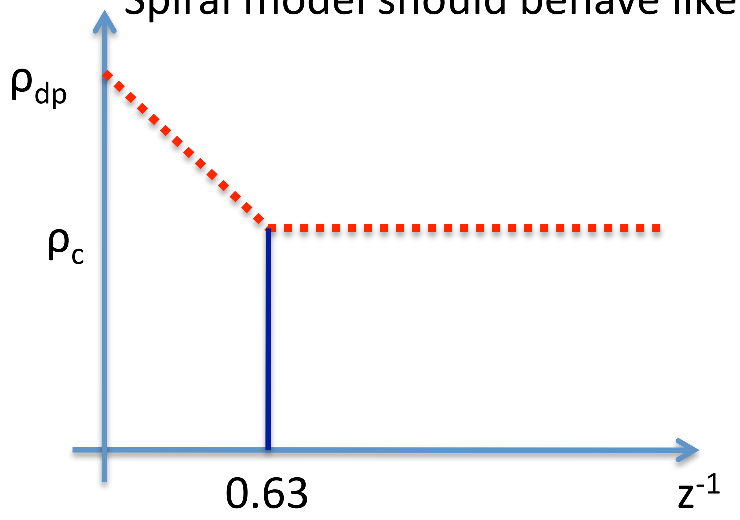




We expect that $\rho_c \leftarrow \rho_{dp}$ (M->L,L->infinite)



Spiral model should behave like



Possible next problems

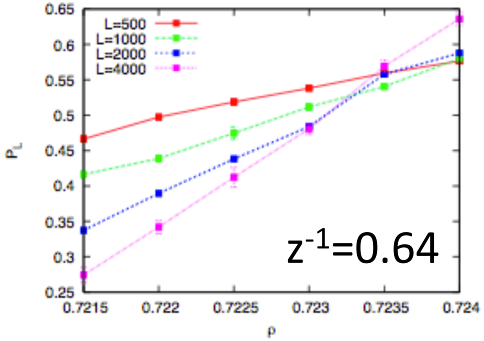
1) Theoretical determination of universality class (mathematics)

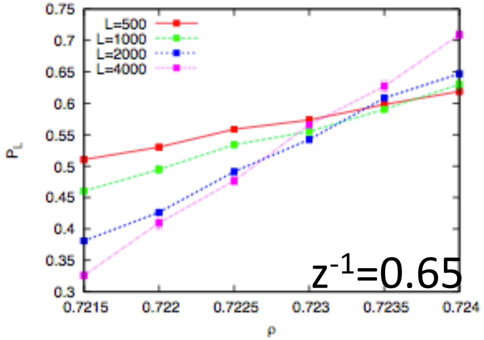
2) The dependence of the geometry of lattices (statistical physics)

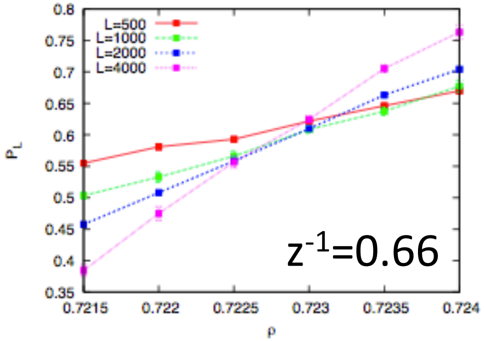
3) What happen if we do the “similar” experiments for realistic glassy systems?
although it is not trivial to set up the experimental conditions,
which are “similar” to that of KCMs. (experiments)

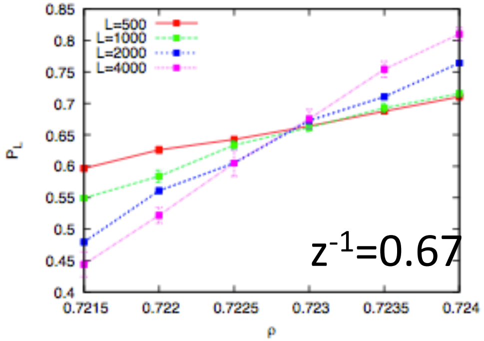
Thanks for your attentions!

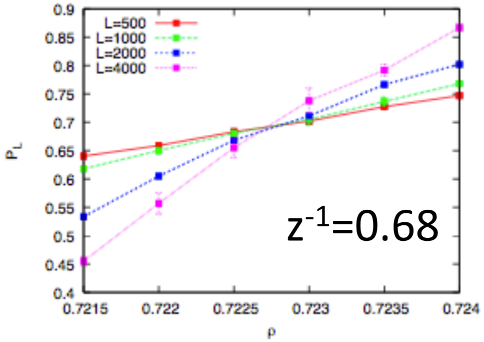
Appendix1

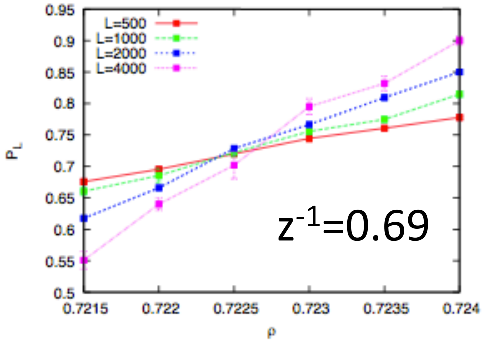








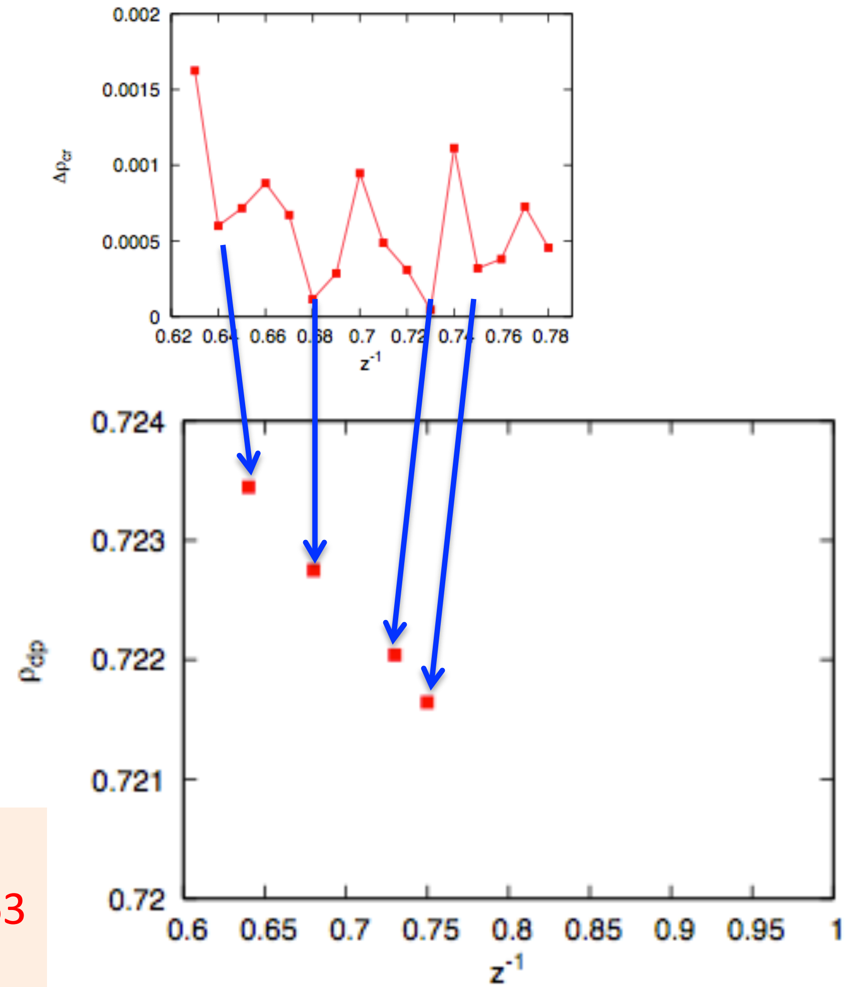




These suggest that there are several directed percolations with different dynamical exponents z.

$$\bar{\rho}_{\rm cr} \equiv \sum_{i=1}^{3} \rho_{\rm cr}^{L_i}(z^{-1})/3 \text{ with } L_i = 500 \times 2^i$$

$$\Delta\rho_{\rm cr} \equiv \sqrt{\sum_{i=1}^{3}(\rho_{\rm cr}^{L_i} - \bar{\rho}_{\rm cr})^2/3}$$



This also indicates that
the dynamical exponent is not the same as z=1/0.63 which is that of the standard directed percolation.

Appendix2

Rough sketch for the prrof

Existence of freezing transition

<lower bound>

P: probability that there are frozen particles at the initial condition.
Q: probability that a "specially" connected sequence of the particles from a boundary to a another faced boundary in the initial condition.

$P<Q$ $Q < (24\rho)^{M/3}$ $P \to 0$ (in the thermodynamic limit $M\to\infty$)

If $\rho<1/24$

<Upper bound>

We map the present problem to
a directed bond percolation problem by the auxiliary variable β_i^+,β_i^-
which locates at each site with probability ζ where $\rho = 1- (1-\zeta)^2$.

With using the transition point ρ_{dp}(=0.644…)of the directed bond percolation on the square lattice, We can get the relation $\rho_u= 1- (1-\zeta_c)^2$ where $\zeta_c^3=\rho_{dp}$