

**International Workshop on Statistical-Mechanical Informatics 2007
Kyoto, September 17**

Phase Transitions (and their meaning) in Random Constraint Satisfaction Problems

Florent Krzakala

In collaboration with:

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A. Montanari (Stanford)
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G. Semerjian (ENS Paris)
L. Zdeborová (LPTMS Paris)**

Find these slides on my webpage:
www.pct.espci.fr/~florent/

Random Constraint Satisfaction Problems

- **Random K-Satisfiability**

Consider N boolean variables x_i and M random clauses of K literals

The average number of constraints is $\alpha = \frac{M}{N}$.

Is it possible to find an assignment of the variables that satisfies all the constraints?

Ex: Random 3-SAT

$(x_1 \text{ OR } \sim x_2 \text{ OR } x_3) \text{ AND } (\sim x_2 \text{ OR } x_4 \text{ OR } x_5) \text{ AND } (\sim x_6 \text{ OR } x_7 \text{ OR } \sim x_3) \text{ AND } \dots$

- **Random q-Coloring**

Consider q colors, N points and a random set of M edges connecting them.

Is it possible to color the points so that none of them has the same color as one of its neighbors ?

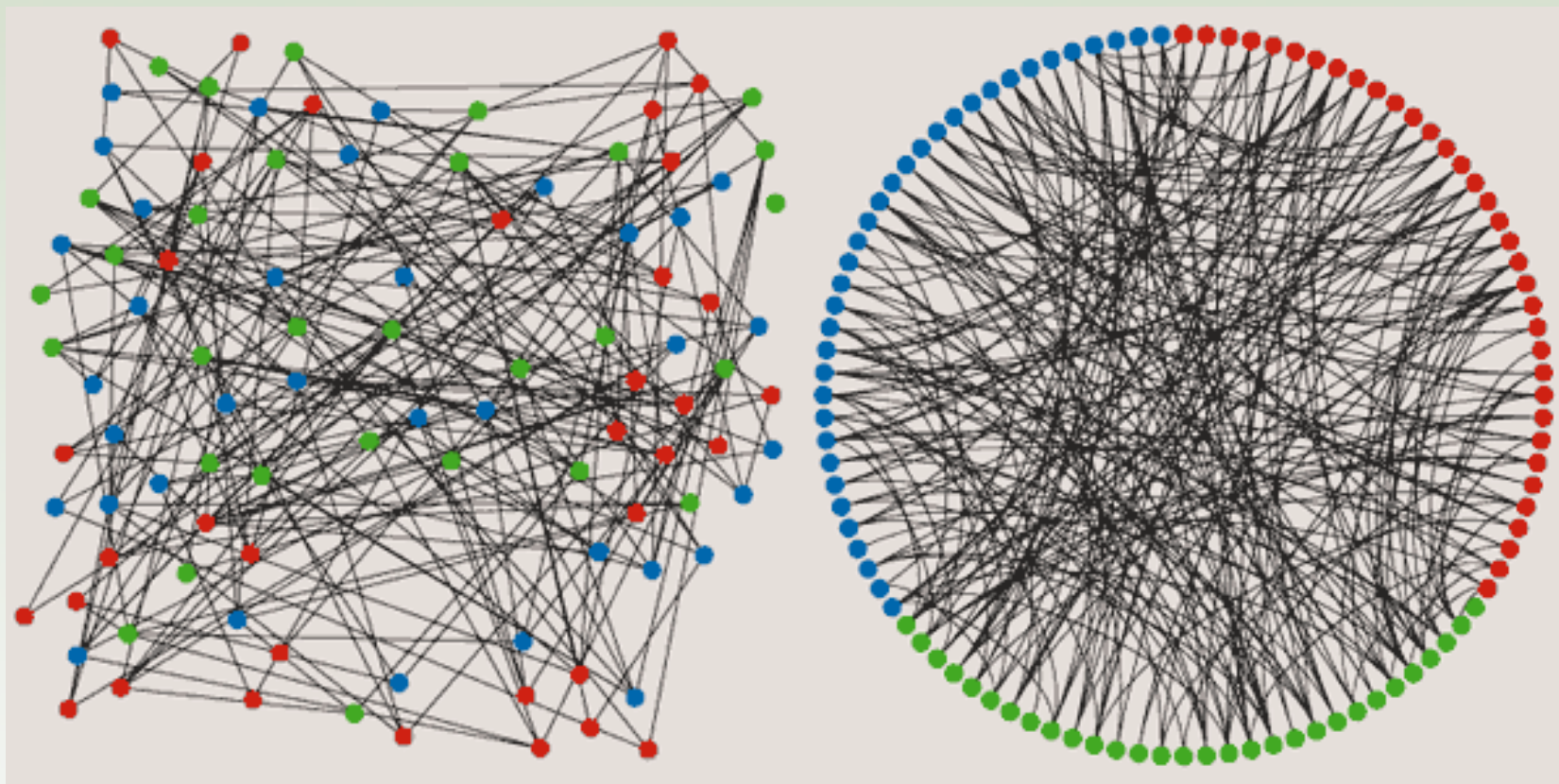
The average number of constraints is $\alpha = \frac{M}{N} = \frac{c}{2}$, where c is the average connectivity

Ex: Random 3-COL

COL and SAT are both NP-complete

Example of CSP: the Coloring of a random graph

N=100 vertices, M=218 edges, average degree $c=2M/N=4.36$



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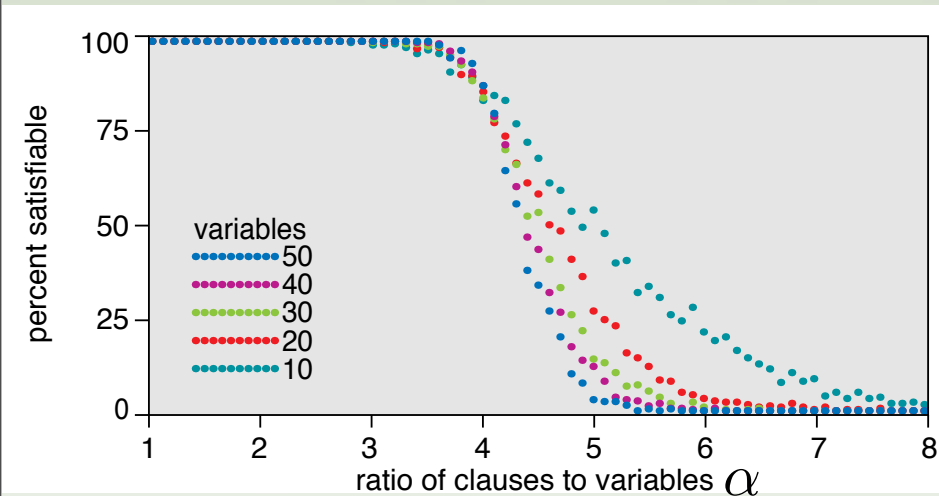
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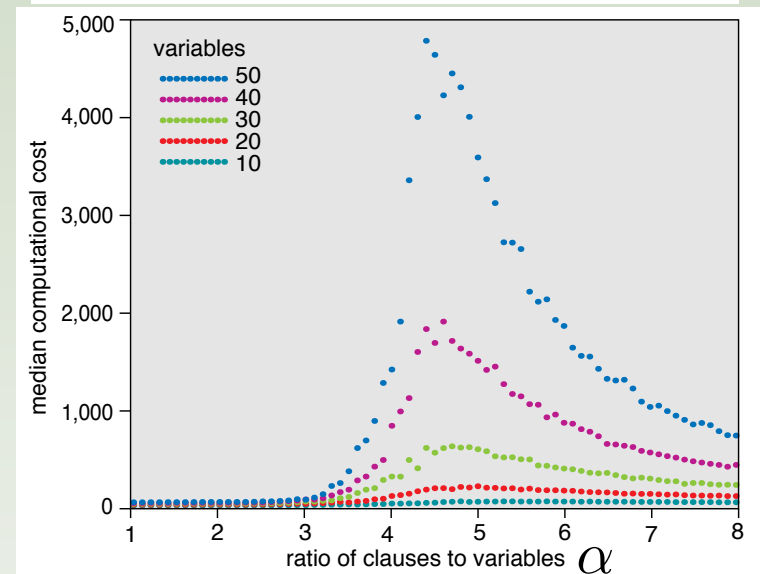
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Why is random constraint satisfaction interesting?

Existence of a sharp
SAT/UNSAT (or COL/UNCOL)
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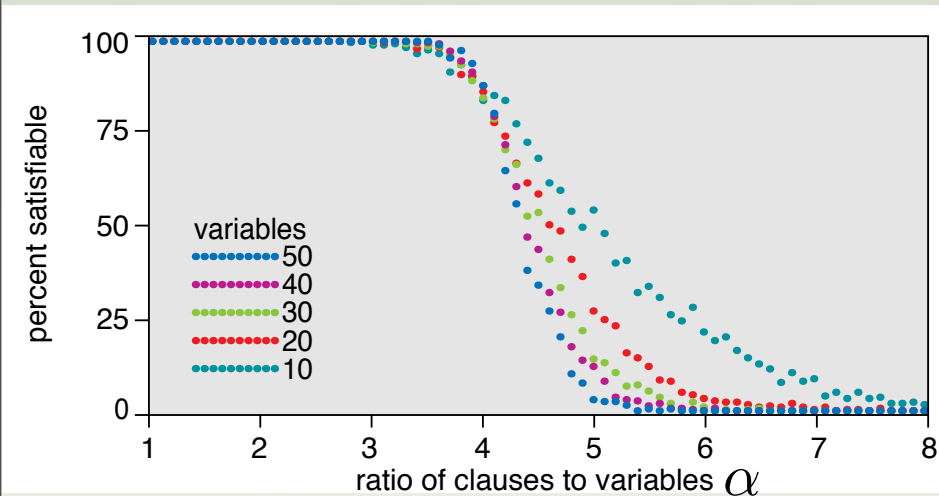
Computationally “hard” region
near to the threshold



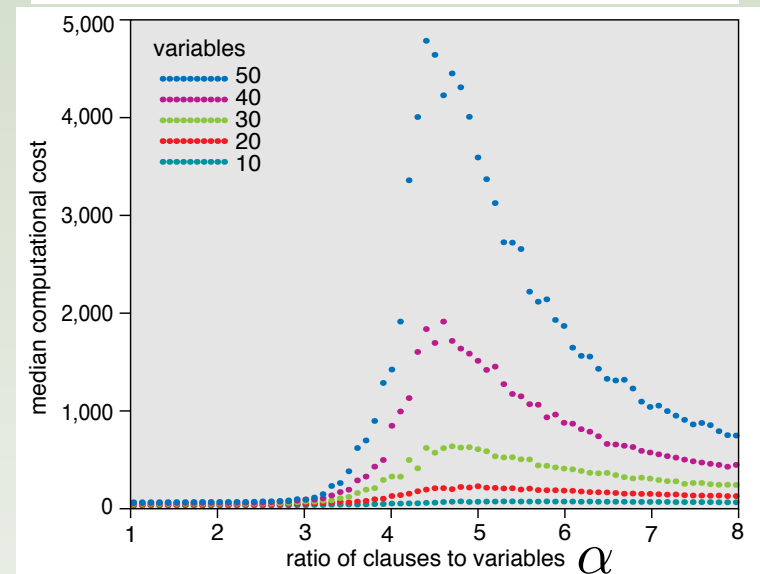
- **SAT/UNSAT threshold at average degree α_s**
 - w.h.p. colorable for $\alpha < \alpha_s$ and w.h.p. uncolorable for $\alpha > \alpha_s$
 - (A part of) **Proof of existence** (Friedgut 1997, Achlioptas, Friedgut, 1999)

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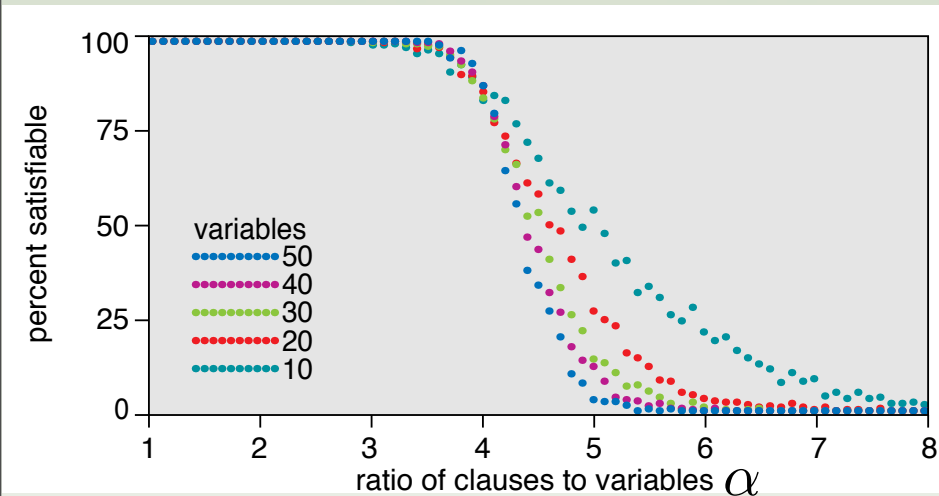
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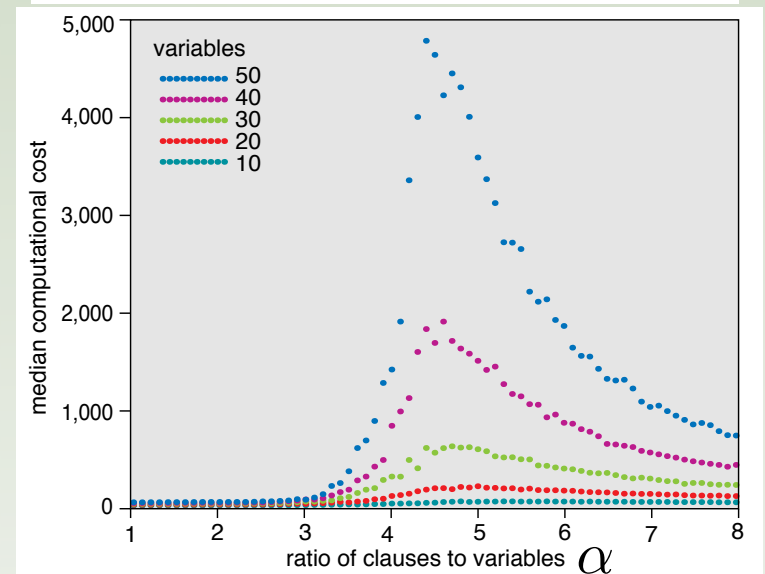
- The time needed to decide satisfiability increases a lot close to α_s
Computationally hard region near to the colorable threshold

Why is random constraint satisfaction interesting?

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Computationally “hard” region
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Can we compute the location of the COL/UNCOL threshold?

Are there other sharp transitions in the problem?

Why are some instances so hard? Is there a way to make them easy?

Coloring random graphs for physicist

• Consider the following Potts anti-ferromagnet Hamiltonian:

$$\mathcal{H} = \sum_{\langle ij \rangle} \delta(s_i, s_j)$$

• A configuration with zero energy is a proper coloring.

• To see if a graph is colorable just compute the ground-state energy and see if it is zero.

$$s_i = 1, 2, \dots, q$$

• A random graph is locally tree-like with large loops (of typical size $\log(N)$): mean field methods are exact!

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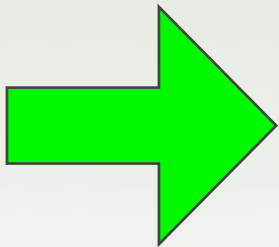
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Random Constraint Satisfaction Problems such as q -COL or K -SAT can be studied within mean field spin glass theory using the “cavity method”

Mézard, Parisi, Zecchina, Science (2002)

Overview

- **Brief presentation of the cavity method**
- **Computation of the phase diagram**
- **Algorithmic consequences**

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Statistical Physics of random CSP

Cavity approach: A mean field method for statistical physics models on tree-like graphs.
Equivalent to the replica method of disordered systems

Parisi, Mézard, Virasoro '87 , Parisi, Mézard '00,

Accomplishments

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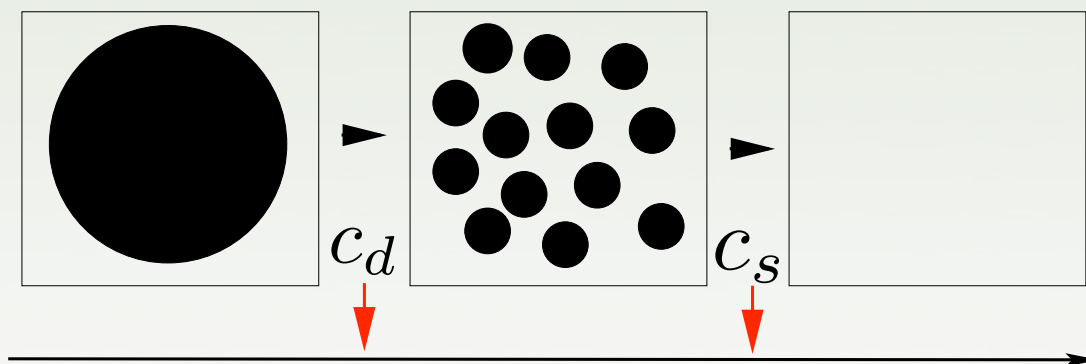


Prediction of a **glassy (clustered) phase** in the colorable region

Mézard, Zecchina, Parisi, '02, Biroli, Monasson, Weigt, '99

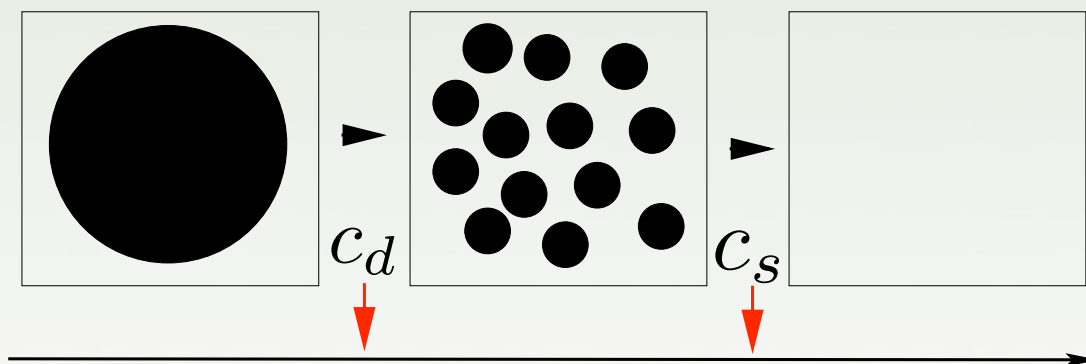
The exact **SAT/UNSAT** threshold computed. Survey Propagation algorithm designed.

*K-SAT: Mézard, Zecchina, Parisi, '02,
q-COL: Mulet, Pagnani, Weigt, Zecchina, '03*



What are clusters?

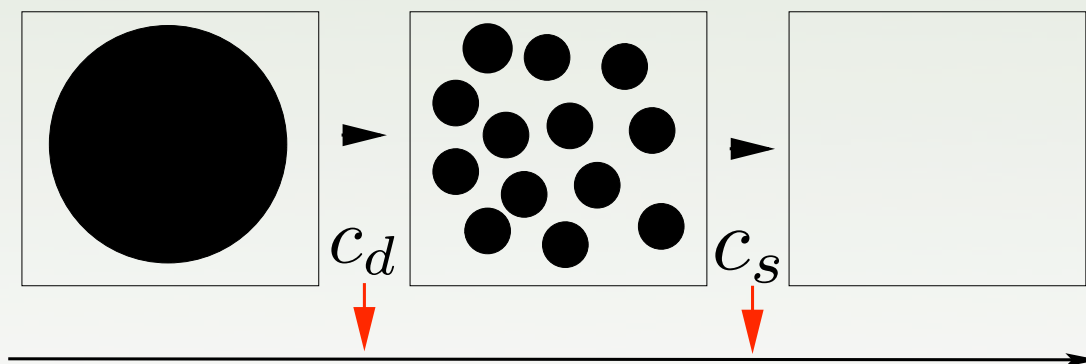
- **Roughly said:** Lumps (groups) of nearby solutions which are in some sense disconnected from each other.
- **For mathematical physicist:** “Extremal Gibbs measures = pure states”.
- **For computer scientist:** Fixed points of belief propagation.
- **For spin glass physicist:** Solutions of TAP equations.



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What is the distribution of the sizes of the clusters ?



A refined analysis of clusters

- ▶ **Entropy (size) of a cluster s :**

logarithm of the number of solutions belonging to the cluster (divided by the number of variables).

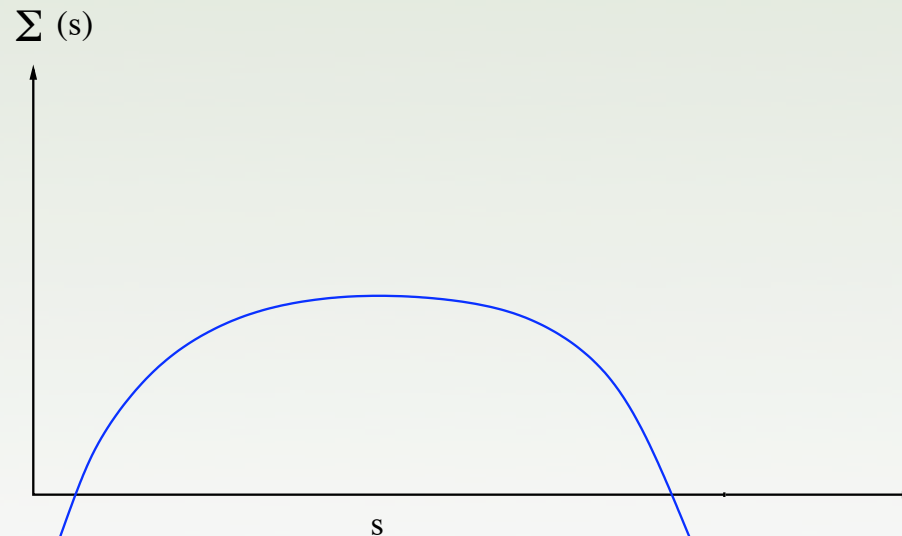
- ▶ **Complexity function $\Sigma(s)$:**

logarithm of the number of clusters of size s

$$\mathcal{N}(s) = e^{N\Sigma(s)}$$

If $\Sigma(s) > 0$, there are exponentially many states of size s .

If $\Sigma(s) < 0$, then states of size s become exponentially rare as N grows.



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- ▶ **We compute the complexity function using the zero temperature cavity method via a Legendre transform $\Phi(m)$ of $\Sigma(s)$.**

- ▶ **Main idea** (Mézard, Palassini, Rivoire, '05): **weight each cluster by its size to the power m :**

$$e^{N\Phi(m)} = \sum_{\alpha} (e^{Ns_{\alpha}})^m = \int e^{N[ms + \Sigma(s)]} ds \quad \Phi(m) = ms + \Sigma(s), \quad \frac{\partial \Sigma(s)}{\partial s} = -m$$

Note: the approach of Mézard, Zecchina, Parisi '02; Mulet, Pagnani, Weigt, Zecchina '02 was at $m=0$.

Solve (mostly numerically) the 1RSB cavity equations

+ Work out the several special cases when the equations simplify ($m=1$, $m=0$, frozen variables, regular graphs ...)

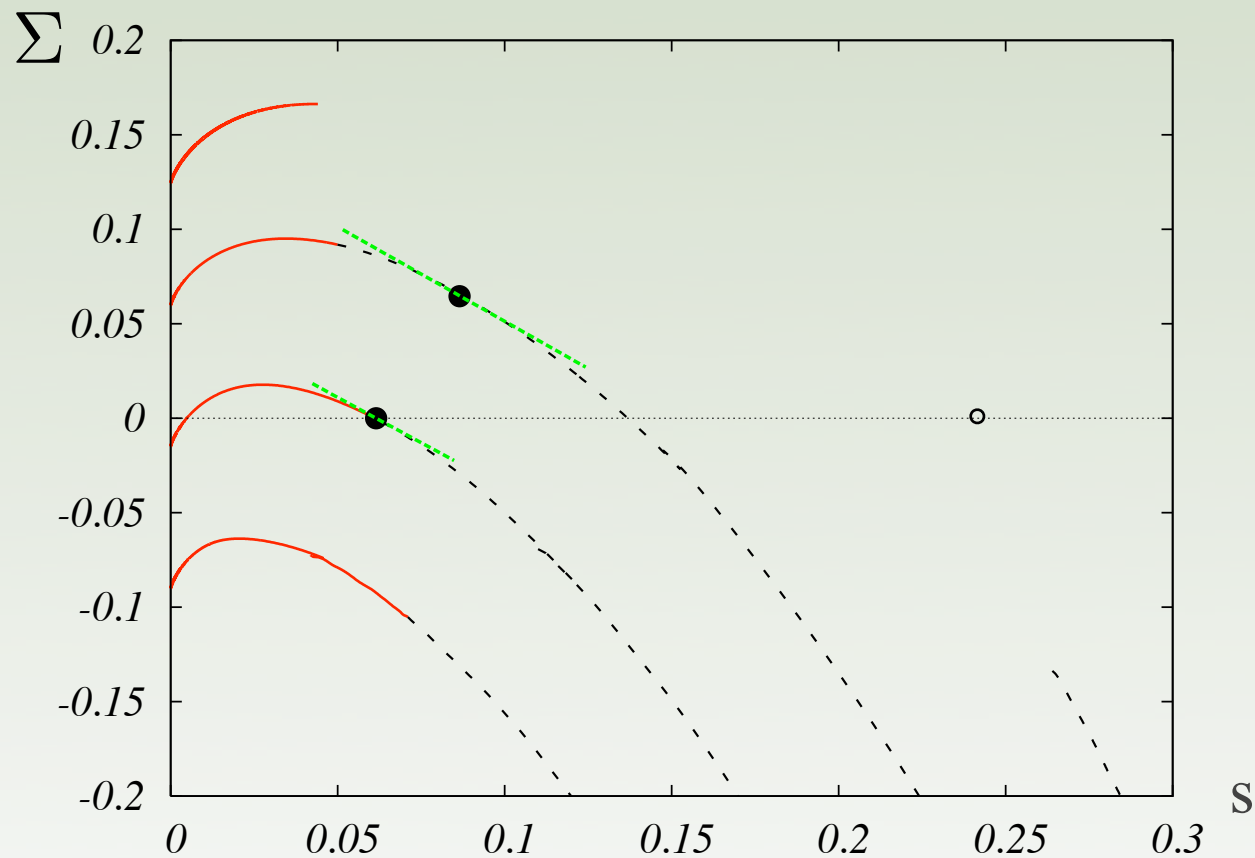


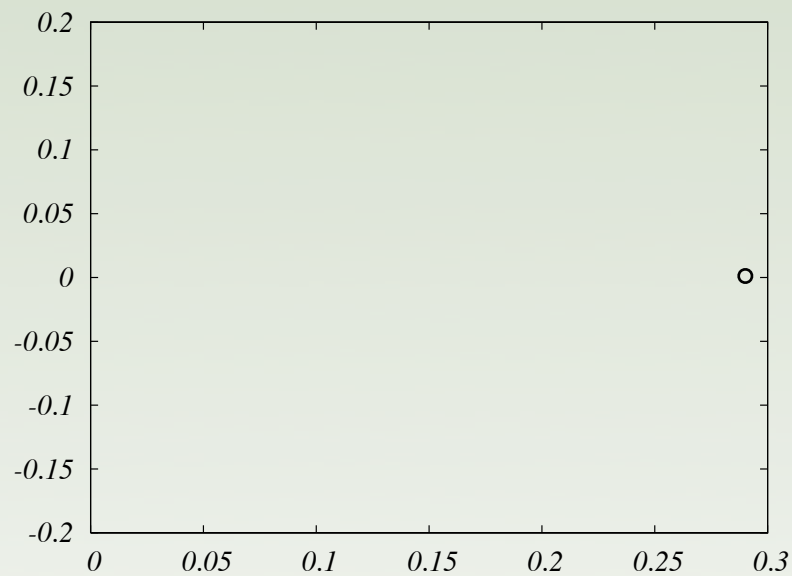
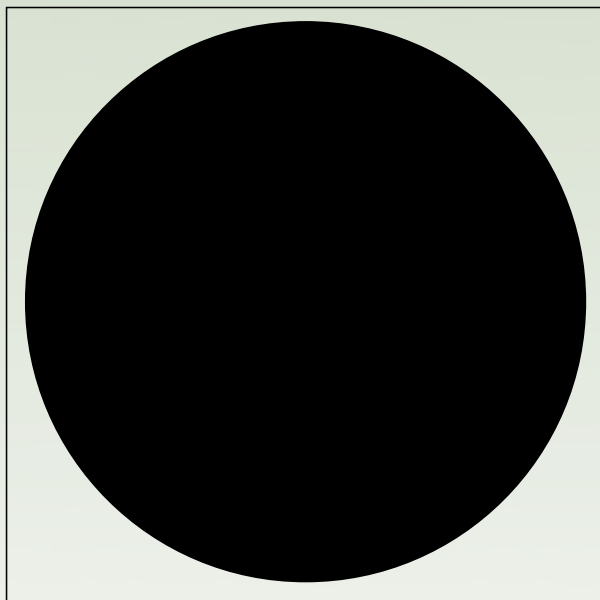
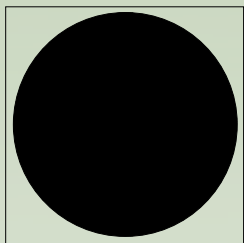
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Learning from $\Sigma(s)$

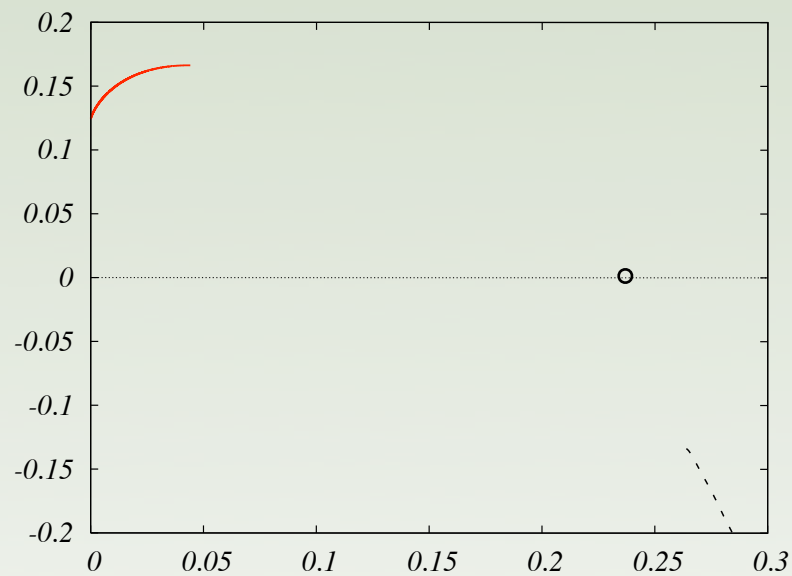
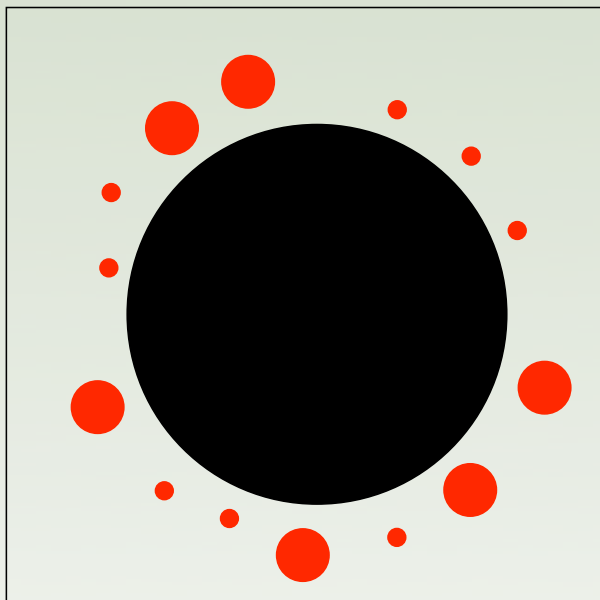
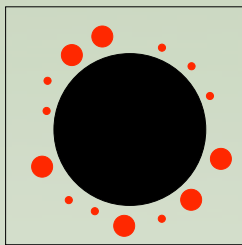
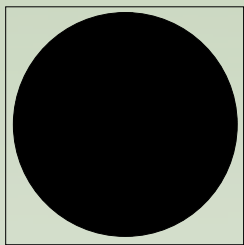
Example of 6-coloring, connectivities 17, 18, 19, 20 (from top).





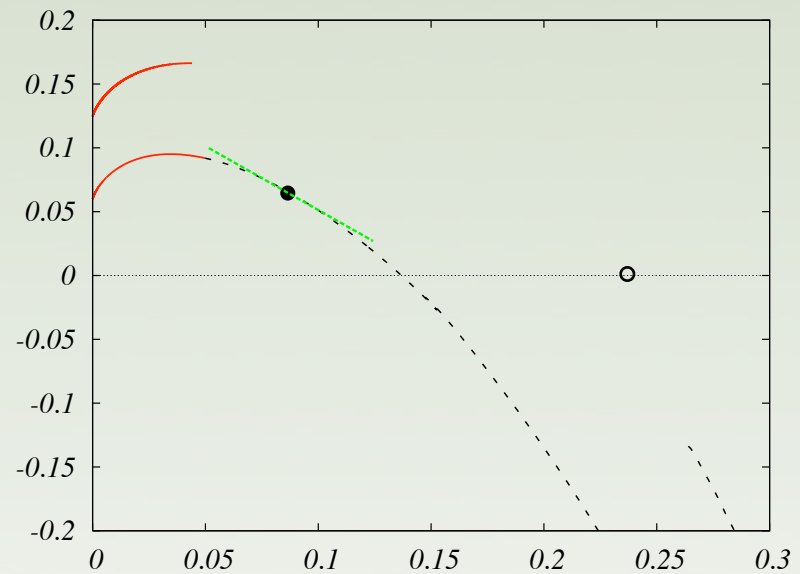
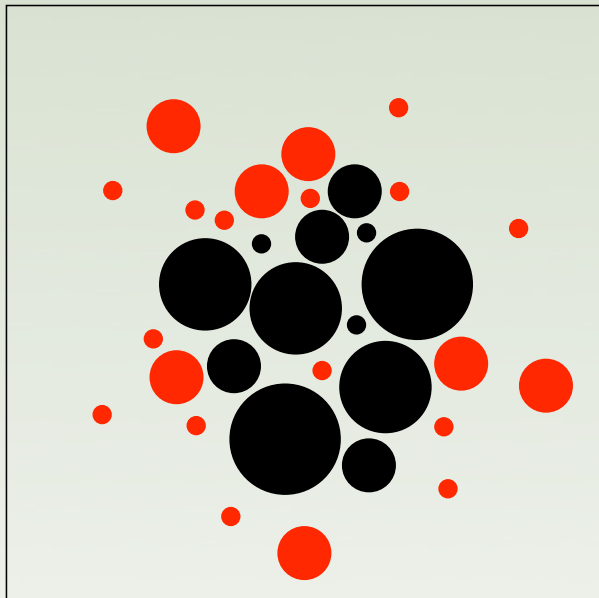
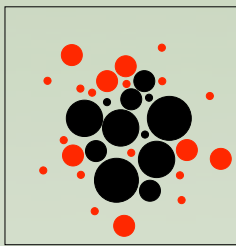
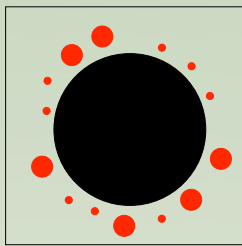
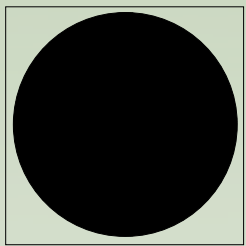
6 coloring of regular random graph

very low connectivity



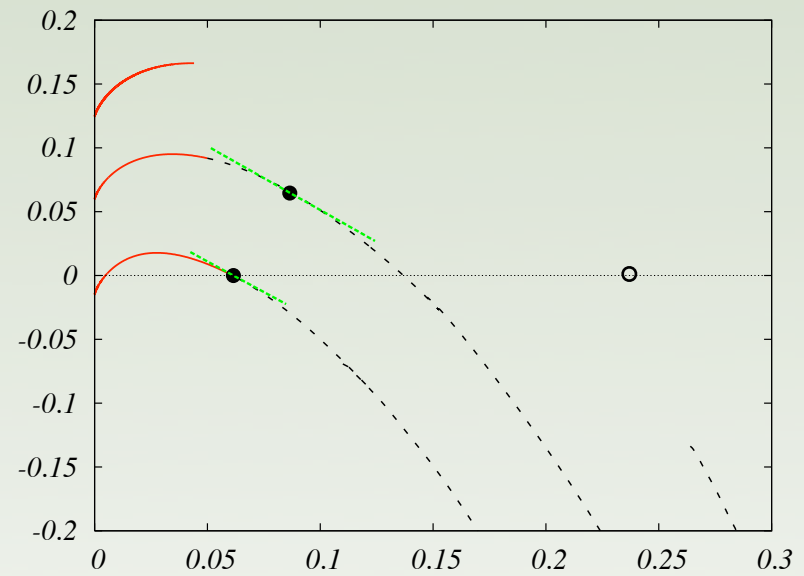
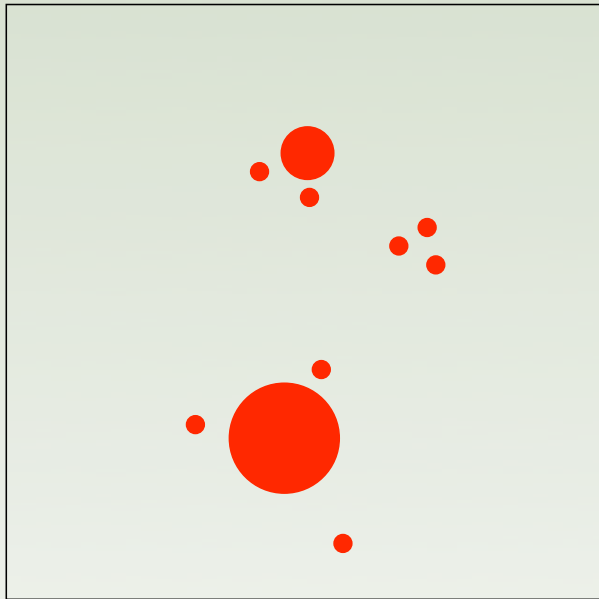
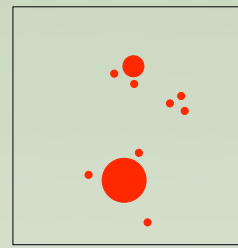
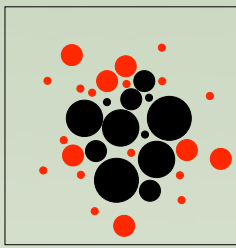
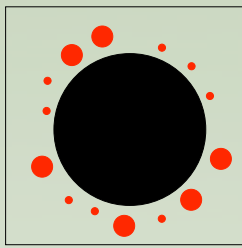
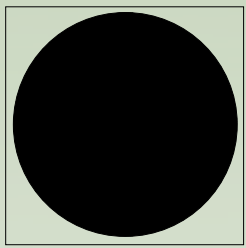
6 coloring of regular random graph

connectivity $c=17$



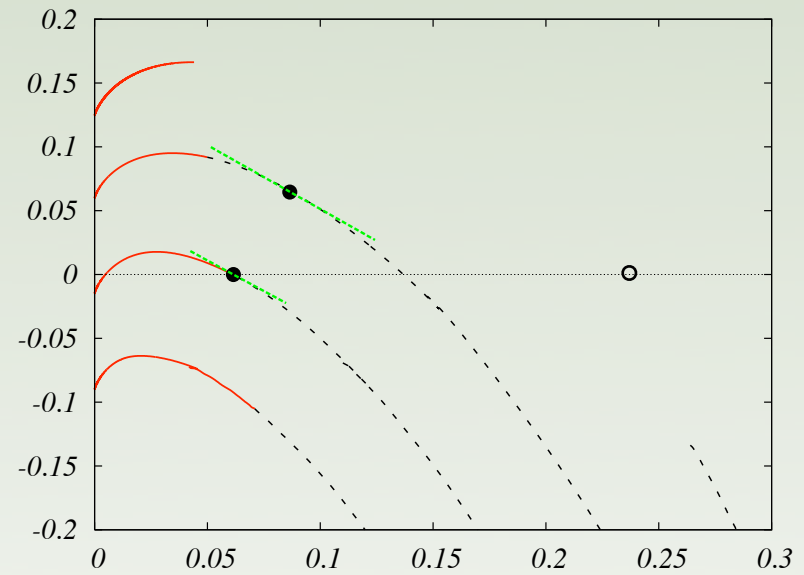
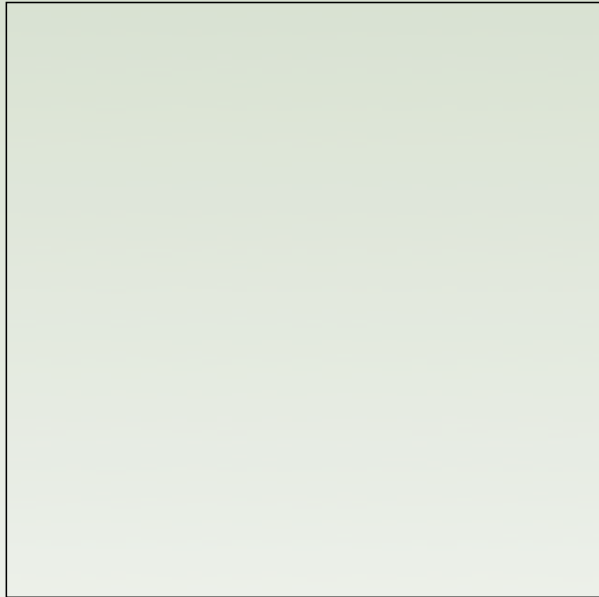
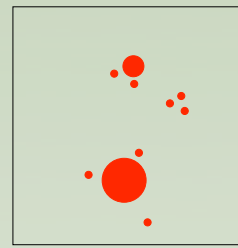
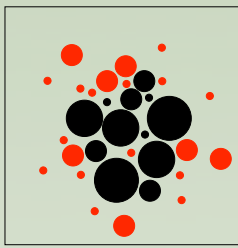
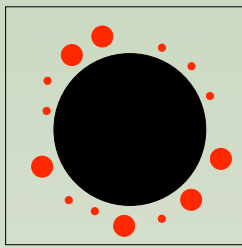
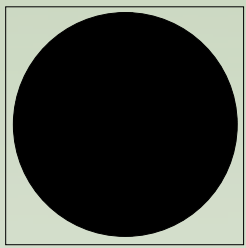
6 coloring of regular random graph

connectivity $c=18$



6 coloring of regular random graph

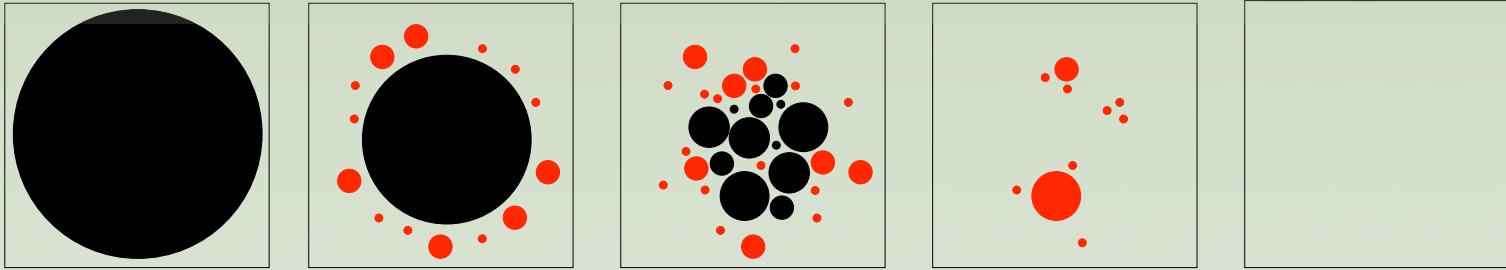
connectivity $c=19$



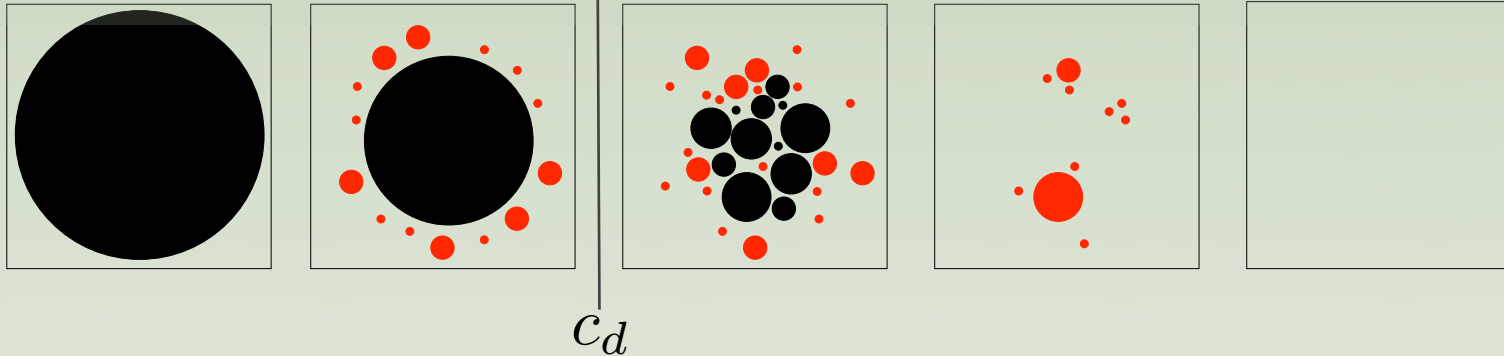
6 coloring of regular random graph

connectivity $c=20$

Many phase transitions



Many phase transitions

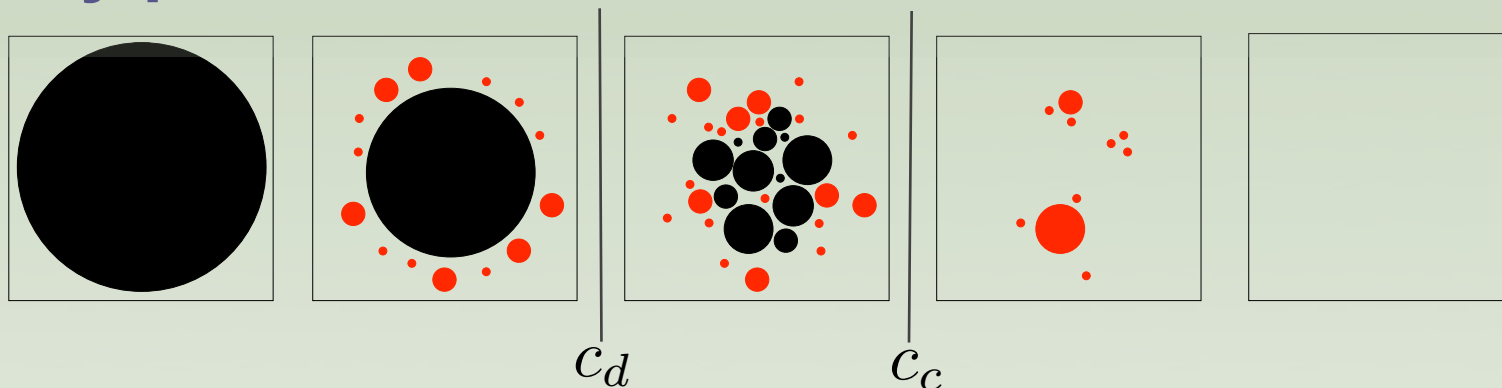


★ Clustering transition

🗣 The phase space splits into exponentially many states

$$c_d(3) = 4, c_d(4) = 8.35, c_d(5) = 12.84$$

Many phase transitions



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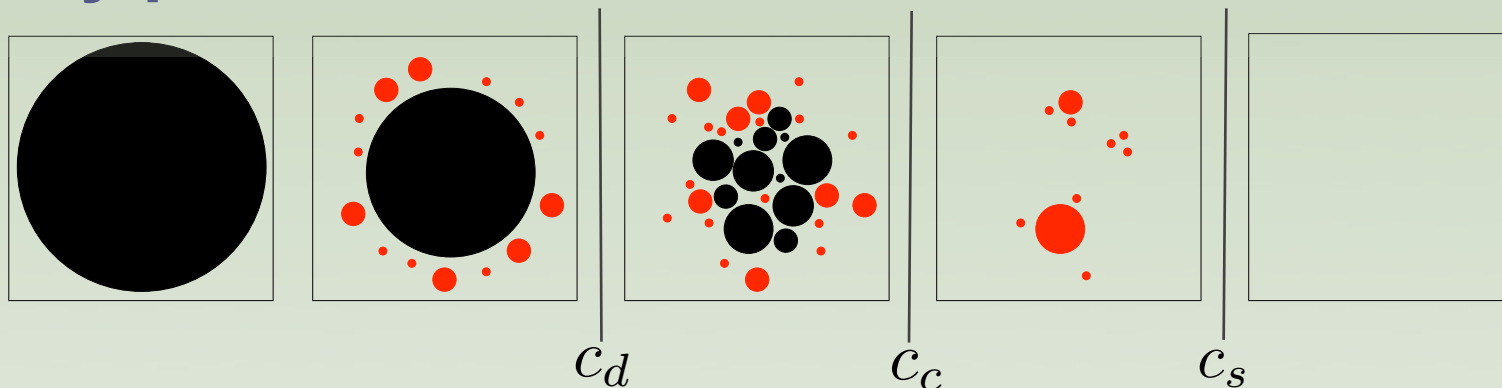
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★ Condensation transition

🔊 Entropy dominated by finite number of the largest states.

$$c_c(3) = 4, c_c(4) = 8.46, c_c(5) = 13.23$$

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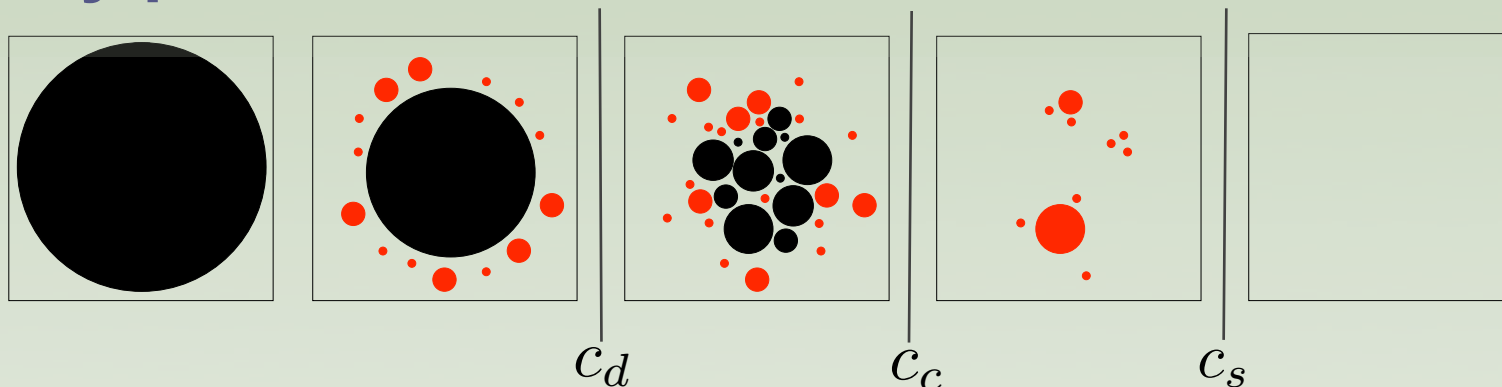
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★ COL/UNCOL transition

🔊 No more clusters, uncolorable phase

$$c_s(3) = 4.69, c_s(4) = 8.90, c_s(5) = 13.67$$

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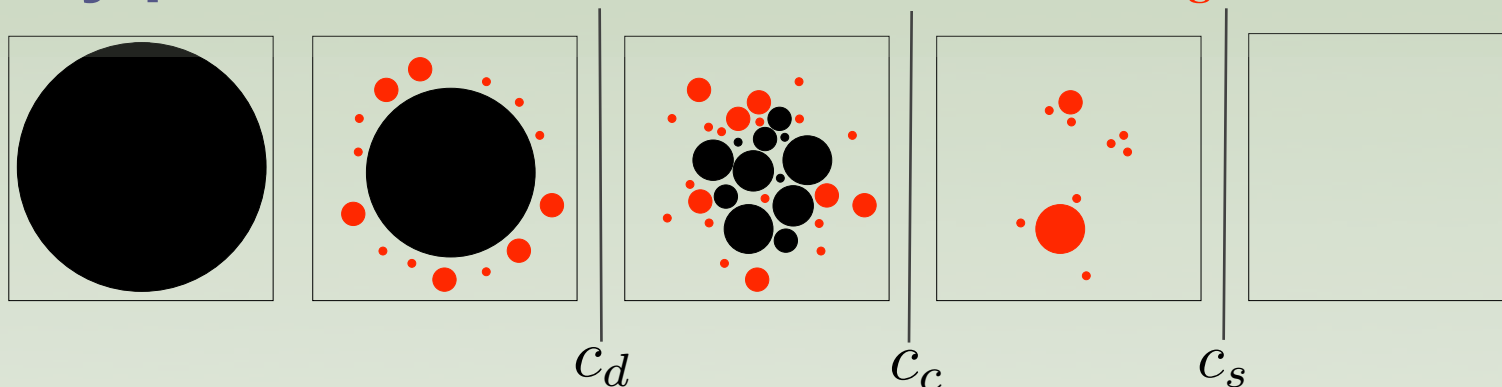
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Moreover: The entropically dominating clusters are 1RSB stable in the colorable phase
(at least for $q > 3$)

Many phase transitions

Same phenomenology as in the ideal glass transition (ex: p-spin)



★ Clustering transition

- The phase space splits into exponentially many states
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*Dynamic
(Ergodicity Breaking) transition*

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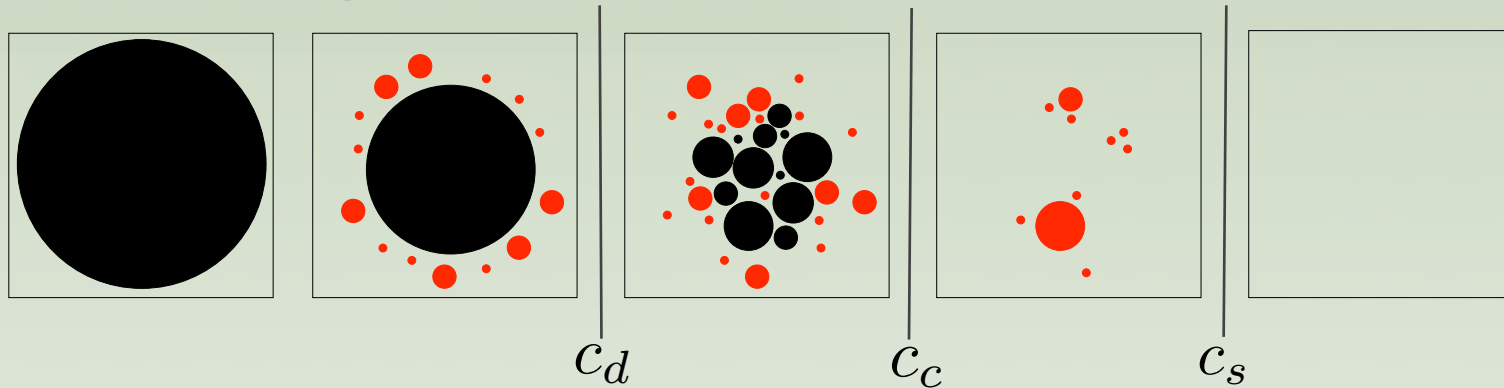
Static (Kauzmann) transition

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The freezing of clusters



Two types of clusters are found

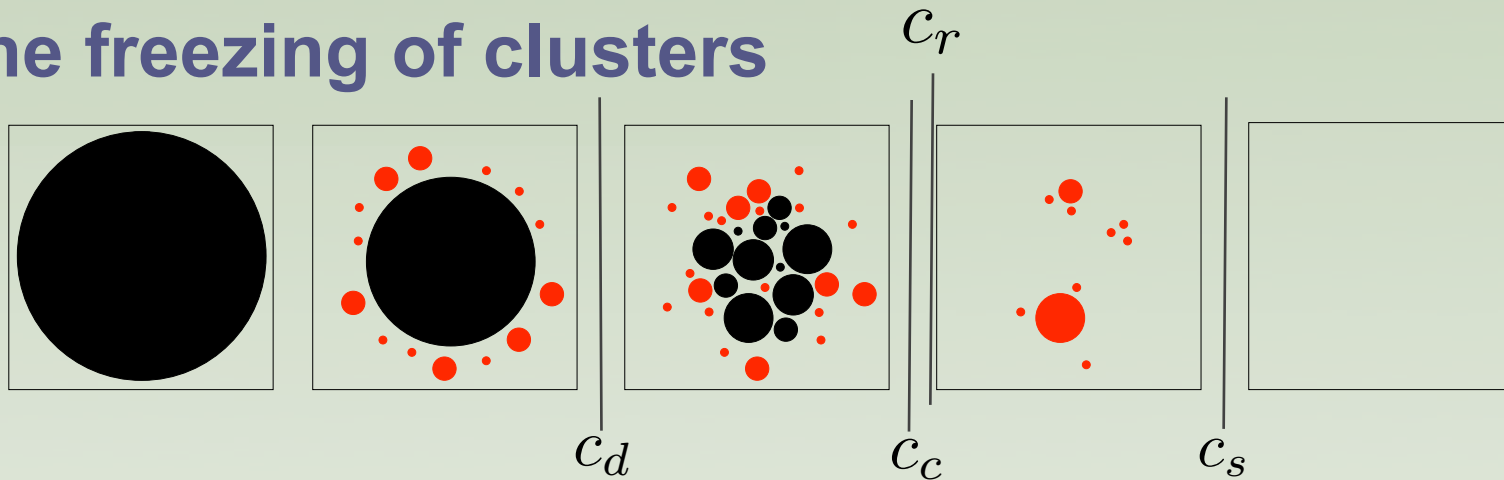
Soft or “unfrozen” clusters

All variables are allowed at least two different colors in the cluster

Hard or “frozen” clusters

A finite fraction of variables are allowed only one color in all solutions belonging to the cluster: we say that these variables “freeze”

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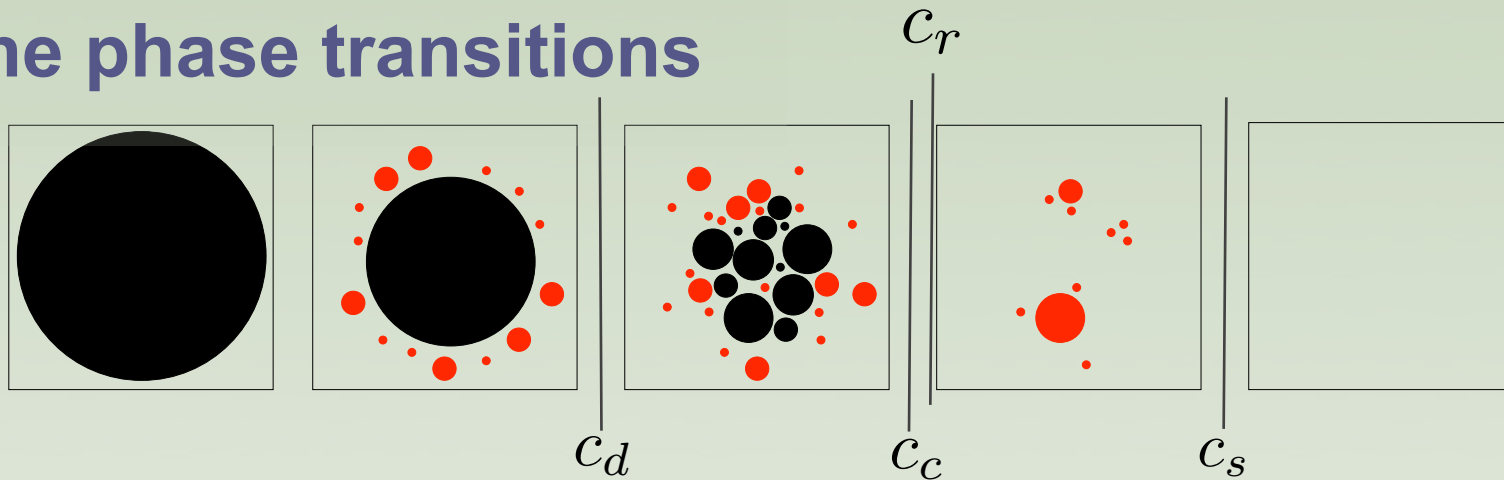
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★ Rigidity transition

📌 Frozen variables appears in the dominating states.

$$c_r(3) = 4.66, c_r(4) = 8.83, c_r(5) = 13.55$$

The phase transitions



★ Clustering/Dynamic transition

★ Condensation/Static transition

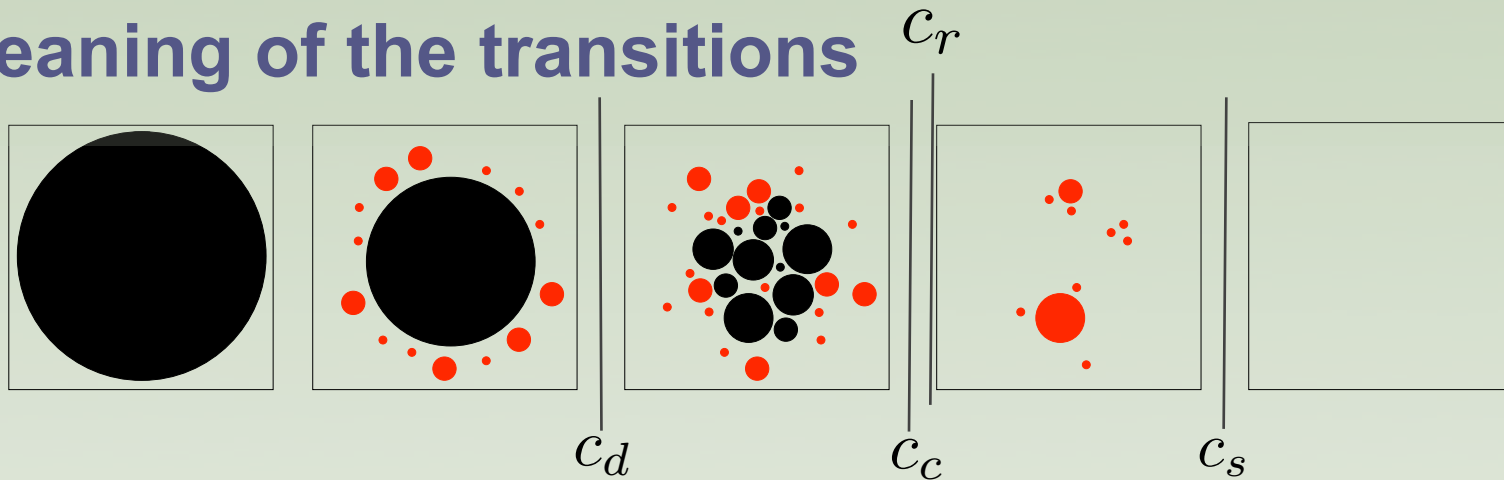
★ COL/UNCOL transition

★ Freezing of clusters and the rigidity transition

Overview

- **Brief presentation of the cavity method**
- **Computation of the phase diagram**
- **Algorithmic consequences**

Meaning of the transitions



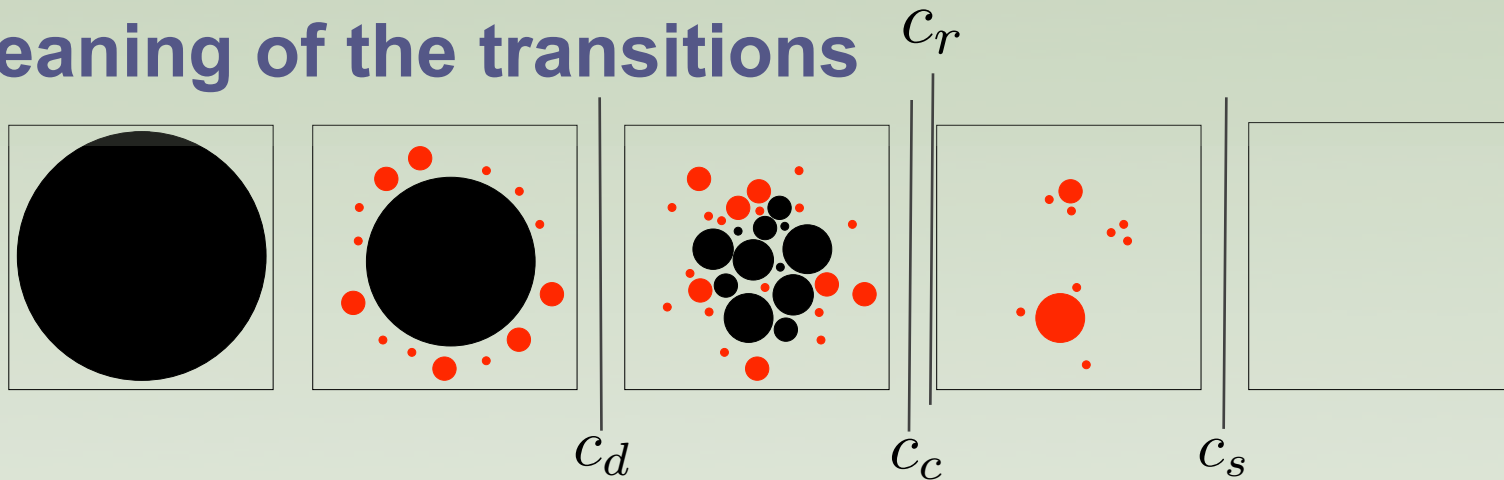
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★ Clustering/Dynamic transition

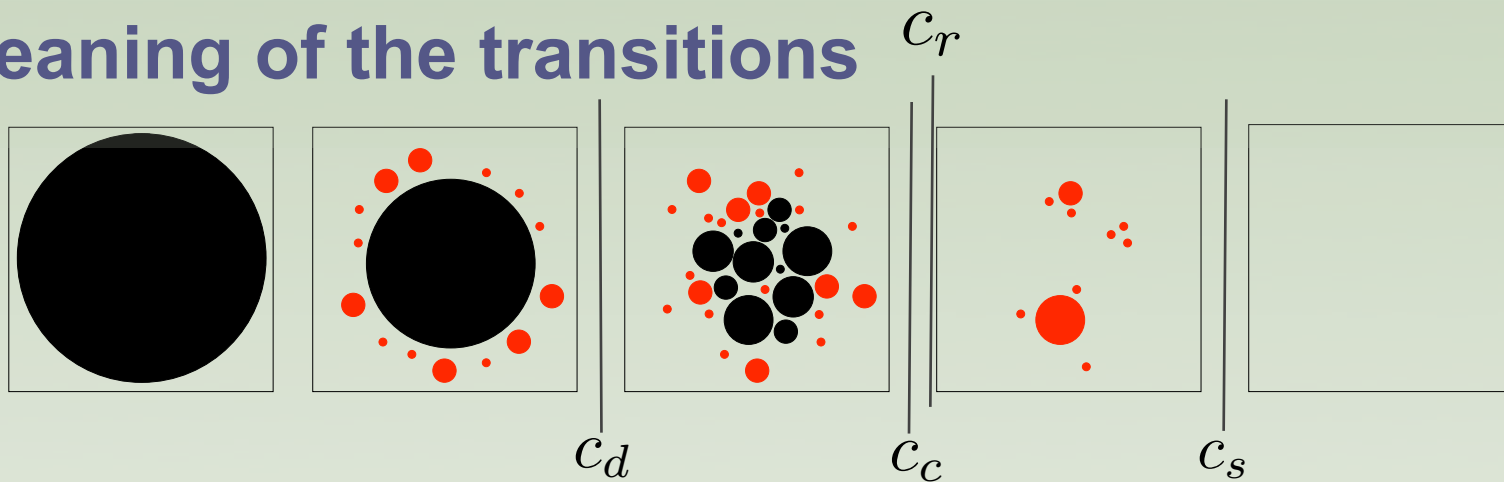
- ▶ “Ergodicity breaking transition”, equilibration time diverges
- ▶ Metropolis Monte-Carlo inefficient for sampling

★ Condensation/Static transition

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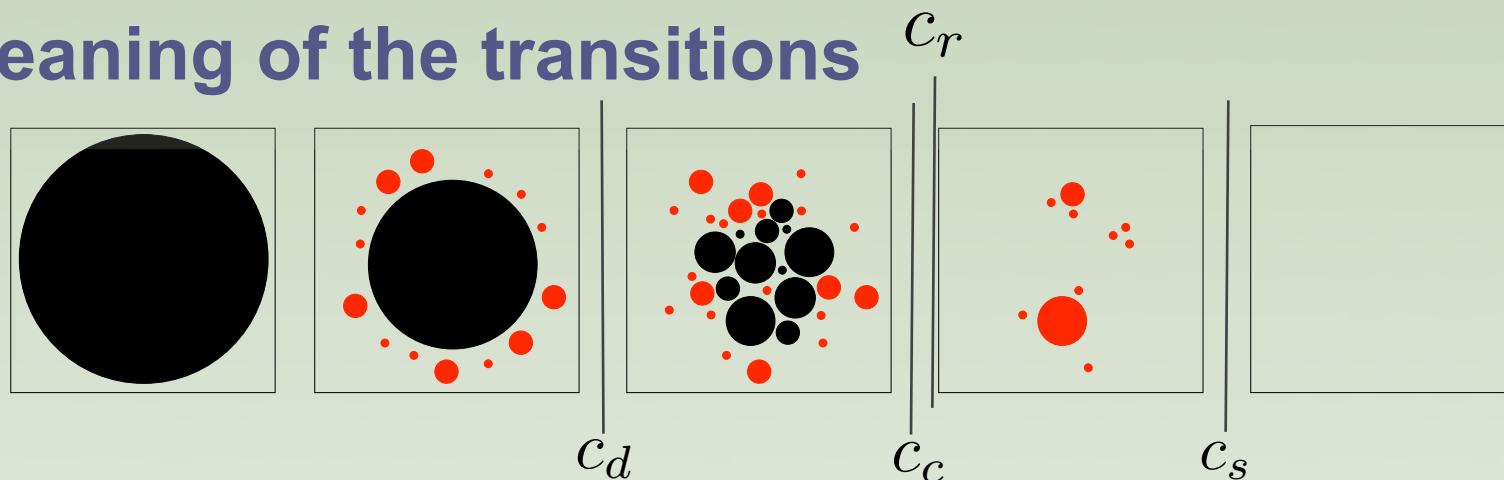
**Easy/Hard transition for
the “MC sampling” problem
(but not for the “solving” problem)**

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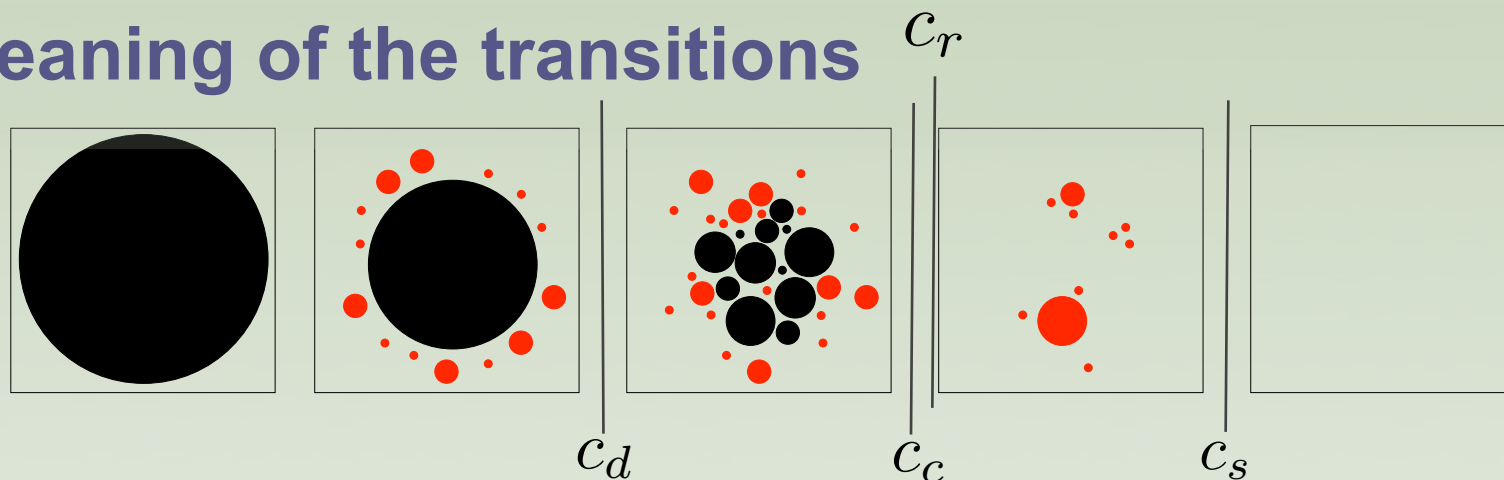
★ Condensation/Static transition

- ▶ “Static replica symmetry breaking transition”
- ▶ Many clusters exist, but a finite number of them covers almost all solutions
- ▶ The overlap function $P(q)$ becomes non-trivial

★ COL/UNCOL transition

★ Freezing of clusters and the rigidity transition

Meaning of the transitions



★ Clustering/Dynamic transition

- ▶ “Ergodicity breaking transition”, equilibration time diverges
- ▶ Metropolis Monte-Carlo inefficient for sampling

Easy/Hard transition for the “MC sampling” problem (but not for the “solving” problem)

★ Condensation/Static transition

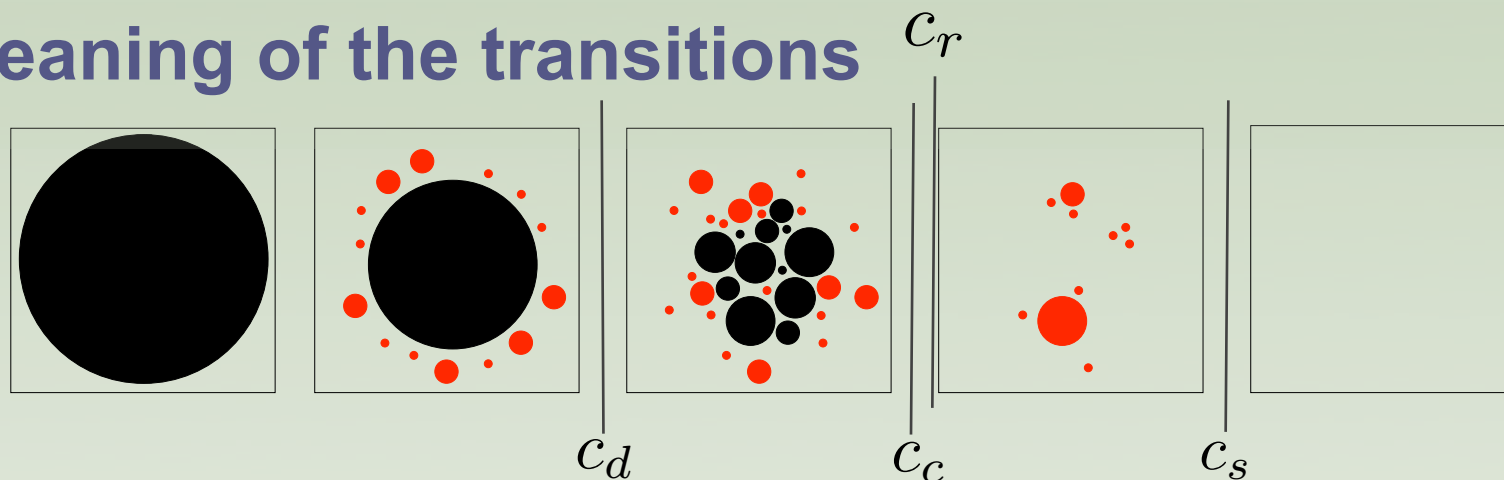
- ▶ “Static replica symmetry breaking transition”
- ▶ Many clusters exist, but a finite number of them covers almost all solutions
- ▶ The overlap function $P(q)$ becomes non-trivial

★ COL/UNCOL transition

- ▶ No solutions exist anymore

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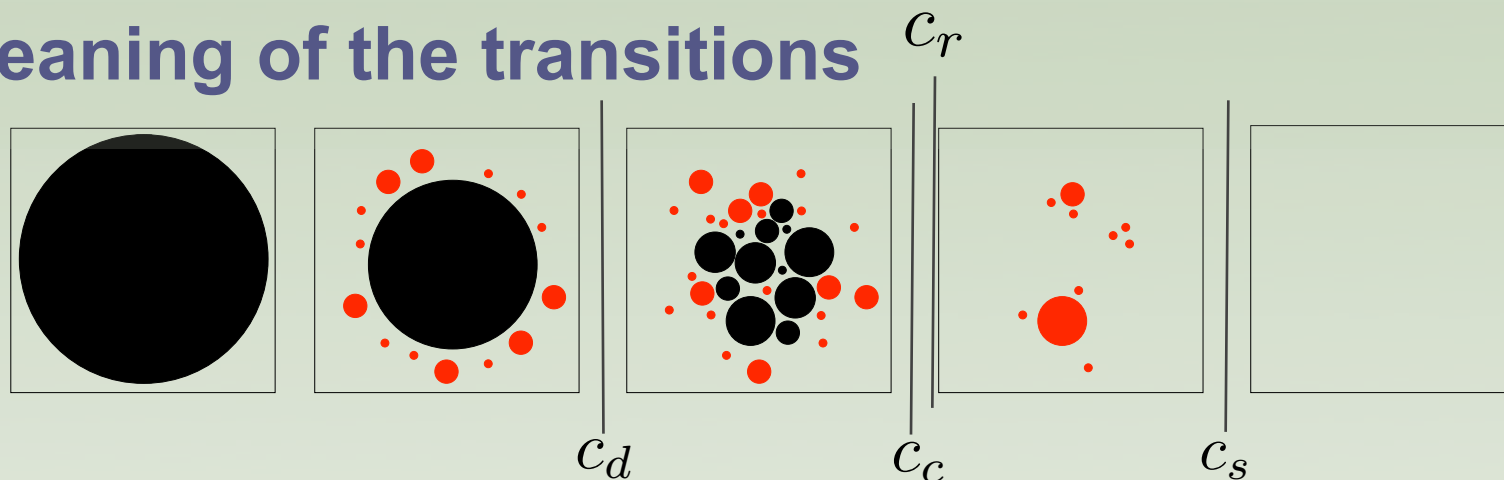
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- ▶ Solutions are hardly constraint within the cluster
- ▶ For $c > c_r$, most solutions belong to frozen clusters

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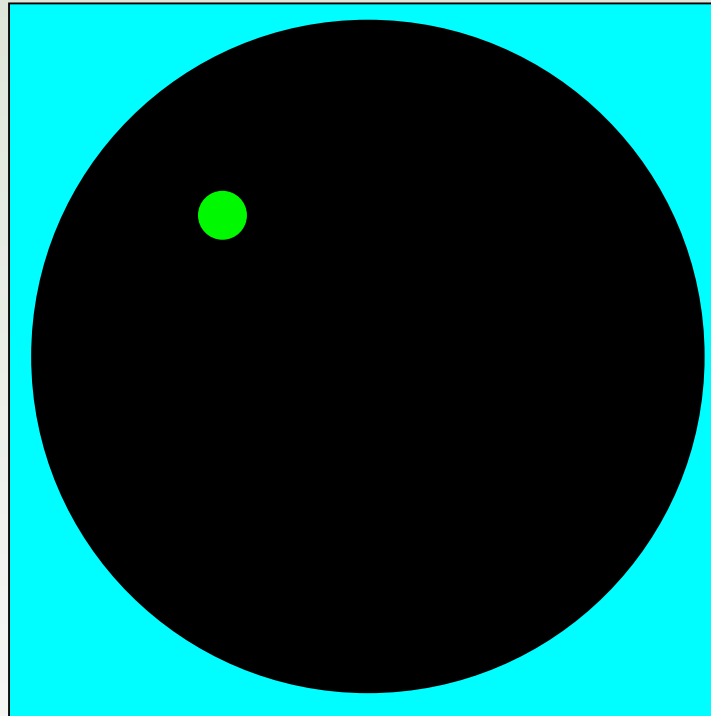
- ▶ Solutions are hardly constraint within the cluster
- ▶ For $c > c_r$, most solutions belong to frozen clusters

The frozen clusters are responsible for the difficulty of finding solutions (not the clustering in itself)

“Wet toes” algorithm

Arkless strategy for flood victims

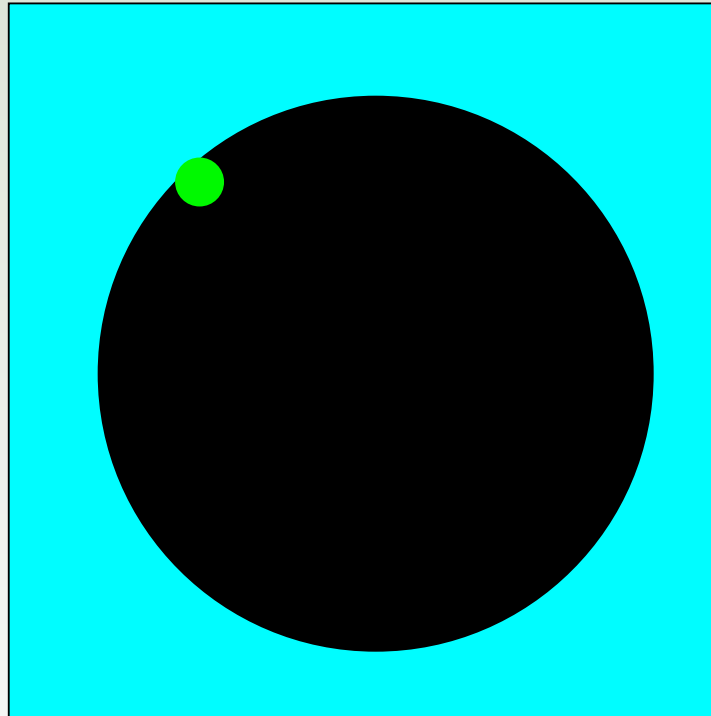
You are on a rugged landscape that is being flooded



“Wet toes” algorithm

Arkless strategy for flood victims

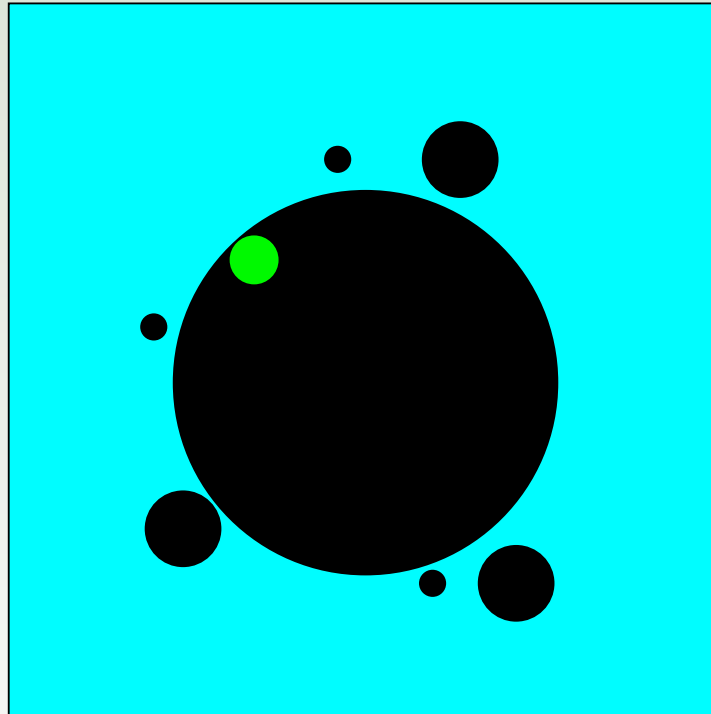
Water goes up. When your toes are wet
step back on the land!



“Wet toes” algorithm

Arkless strategy for flood victims

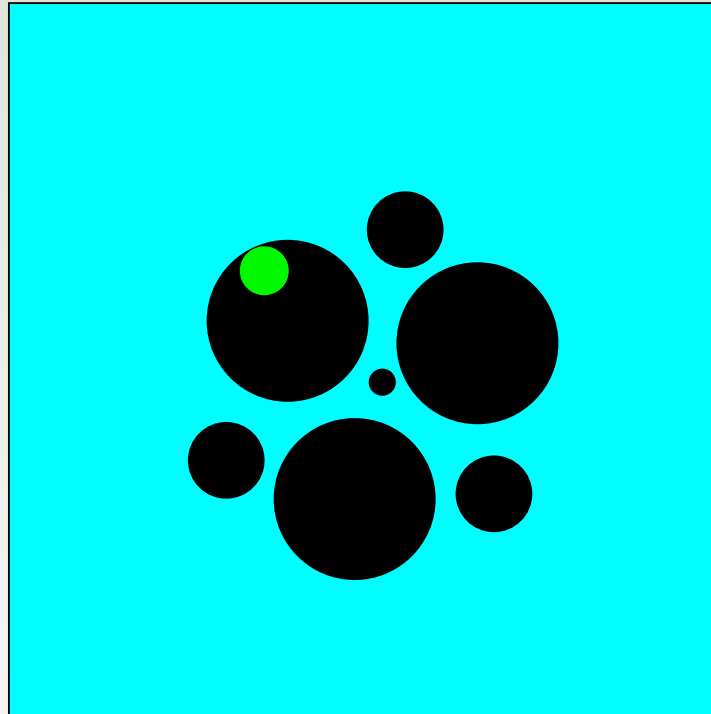
And wait until your toes get wet again...



“Wet toes” algorithm

Arkless strategy for flood victims

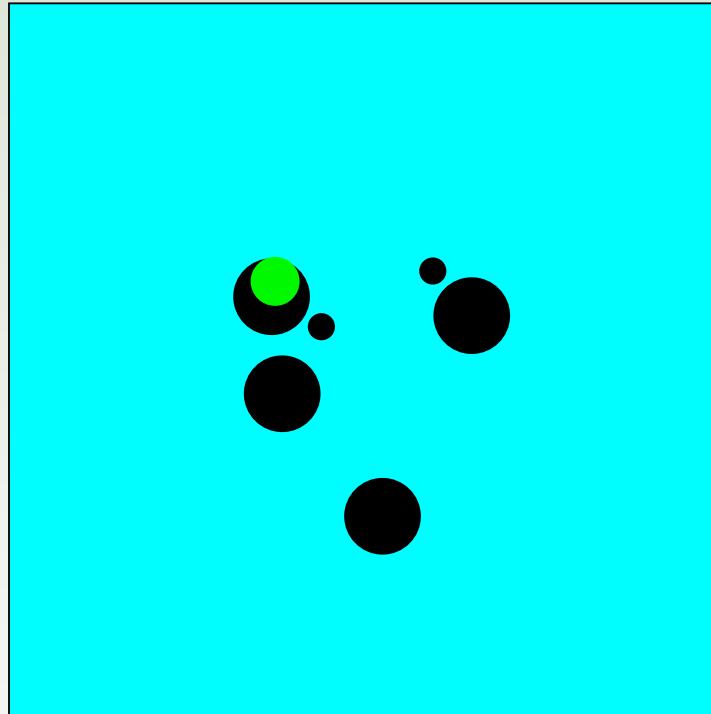
Sooner or later you’ll find yourself on a smaller island...



“Wet toes” algorithm

Arkless strategy for flood victims

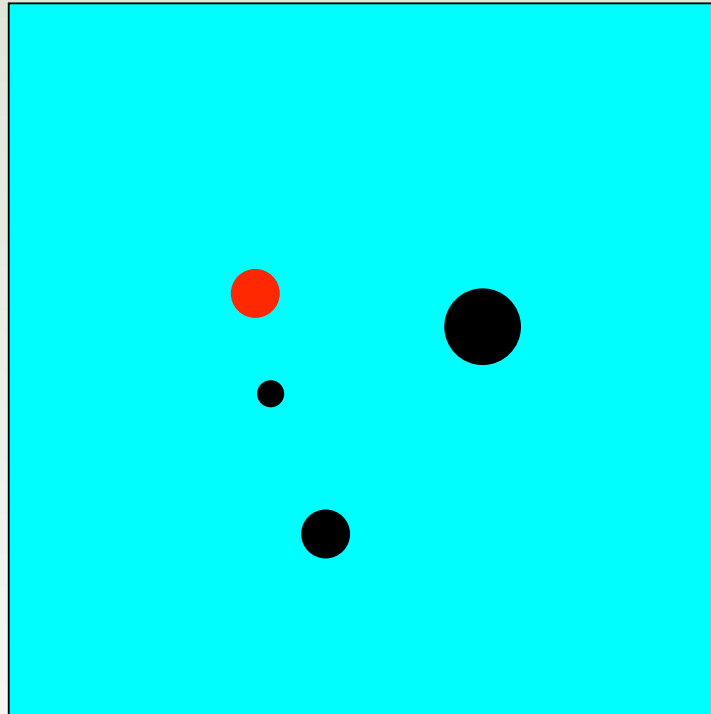
Then even a smaller one...



“Wet toes” algorithm

Arkless strategy for flood victims

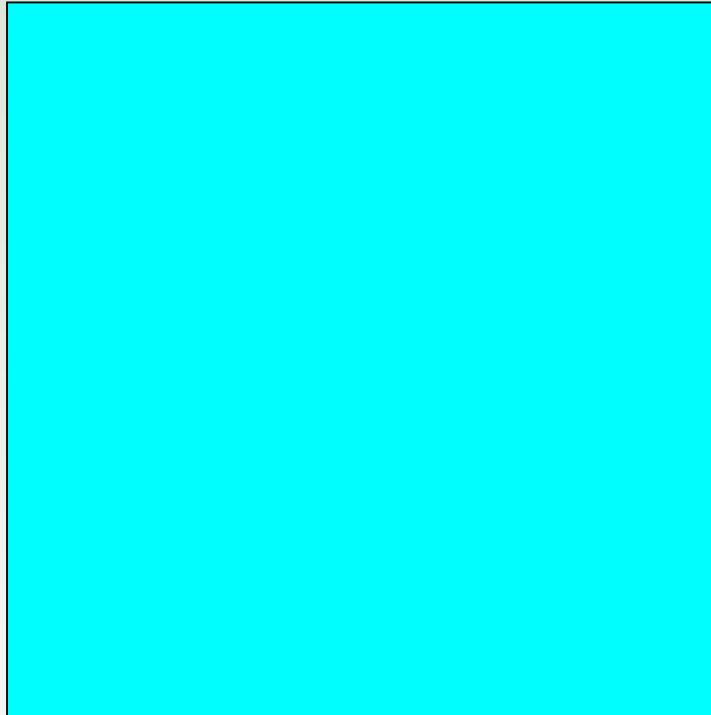
Until eventually you'll drown (if you can't swim!)



“Wet toes” algorithm

Arkless strategy for flood victims

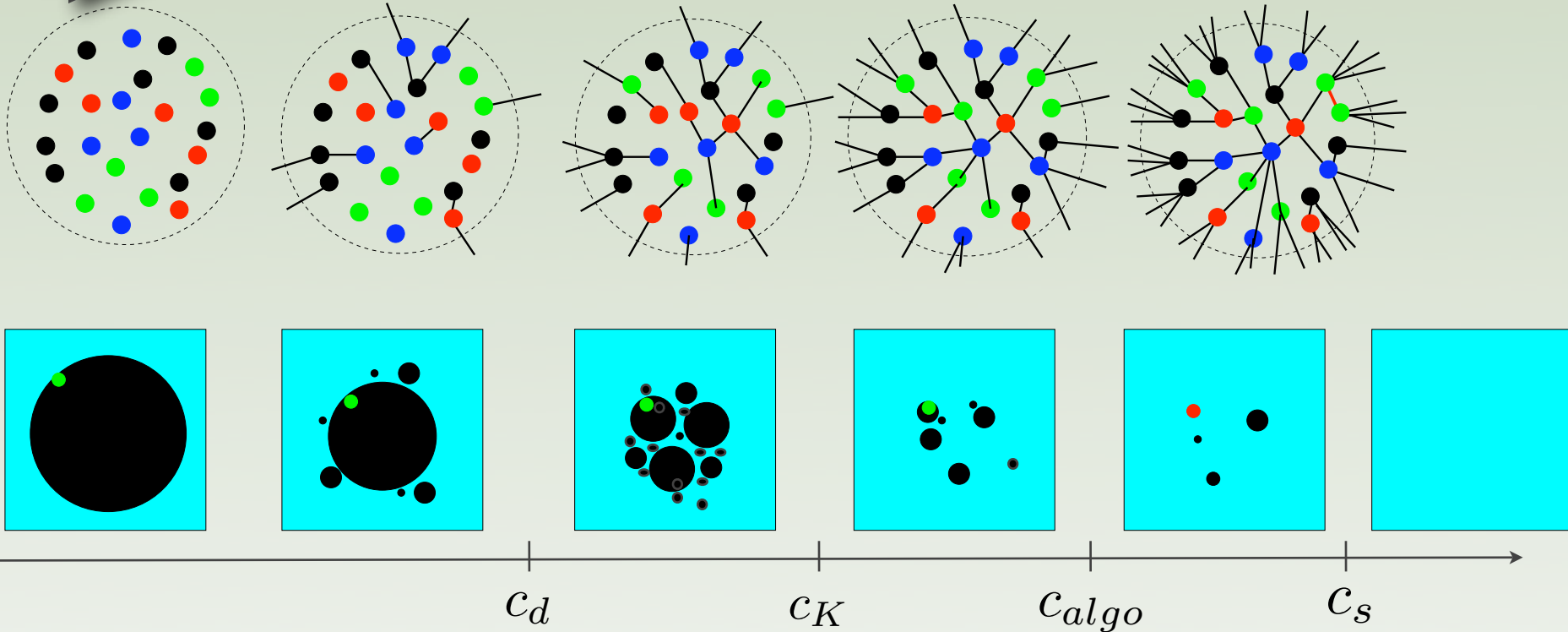
Finally, all land will be flooded!



“Wet toes” algorithm



Add links one by one and use a local algorithm to solve contradictions

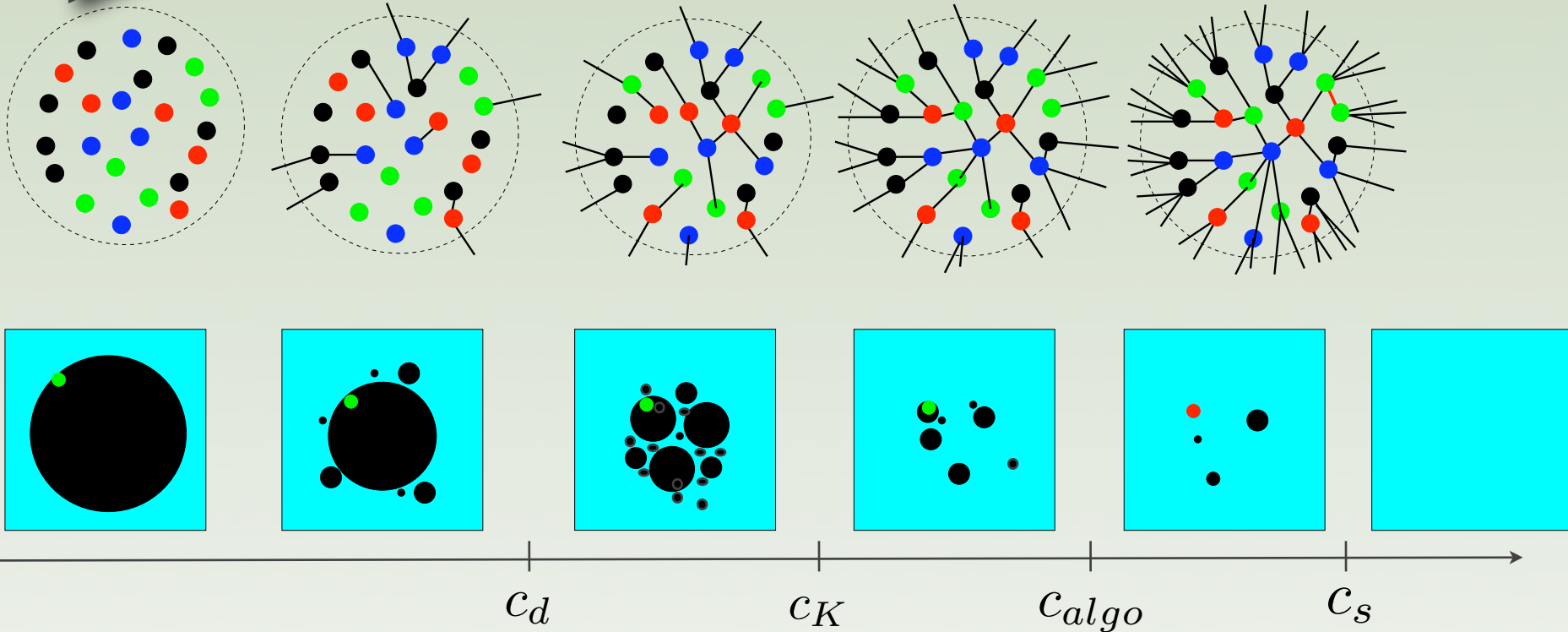


The algorithm works until the cluster disappears

Frozen clusters make it hard!



Add links one by one and use a local algorithm to solve contradictions



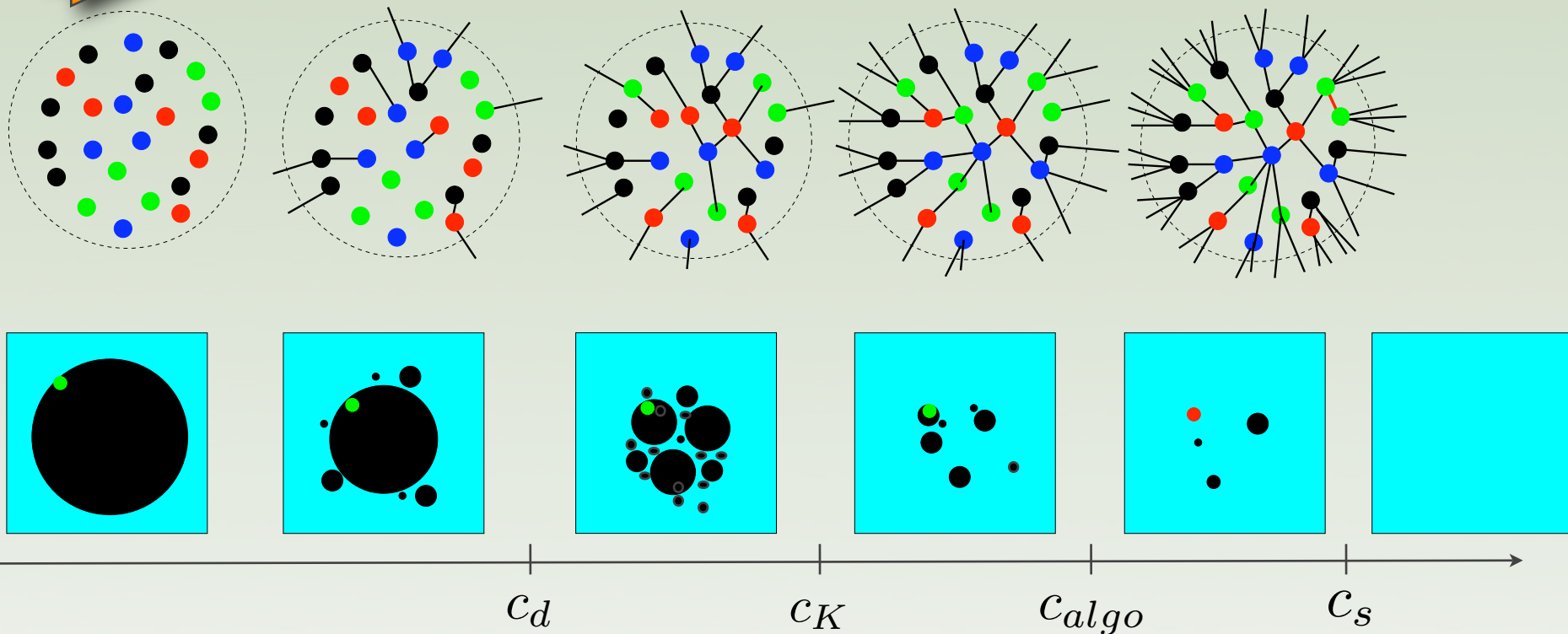
- A fundamental properties of frozen clusters:

- ➡ Frozen clusters are fragile and disappear after the addition of few links.
- ➡ The number of needed changes is finite in unfrozen clusters and infinite in frozen ones *Semerjian '07*

Frozen clusters make it hard!

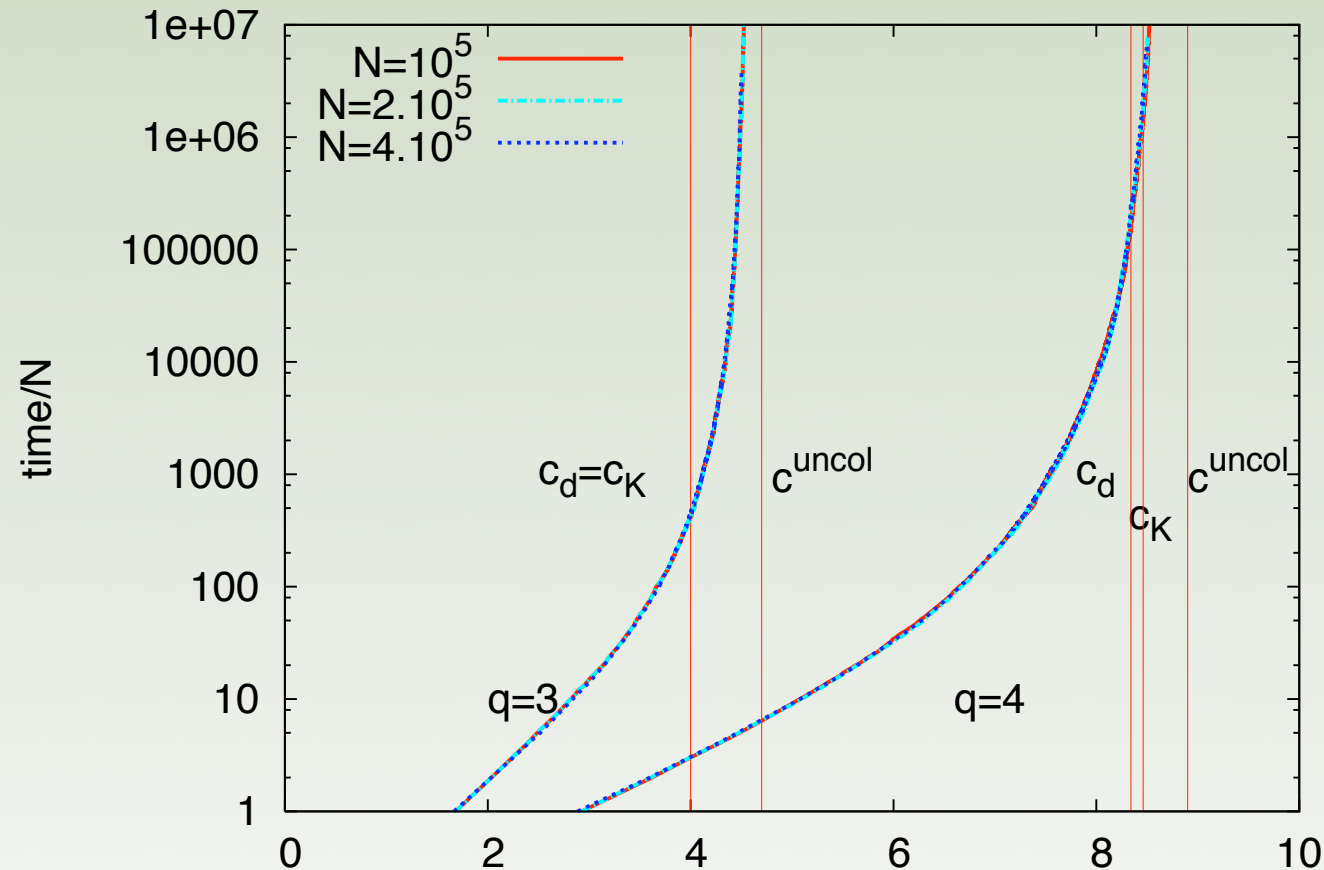


Add links one by one and use a local algorithm to solve contradictions



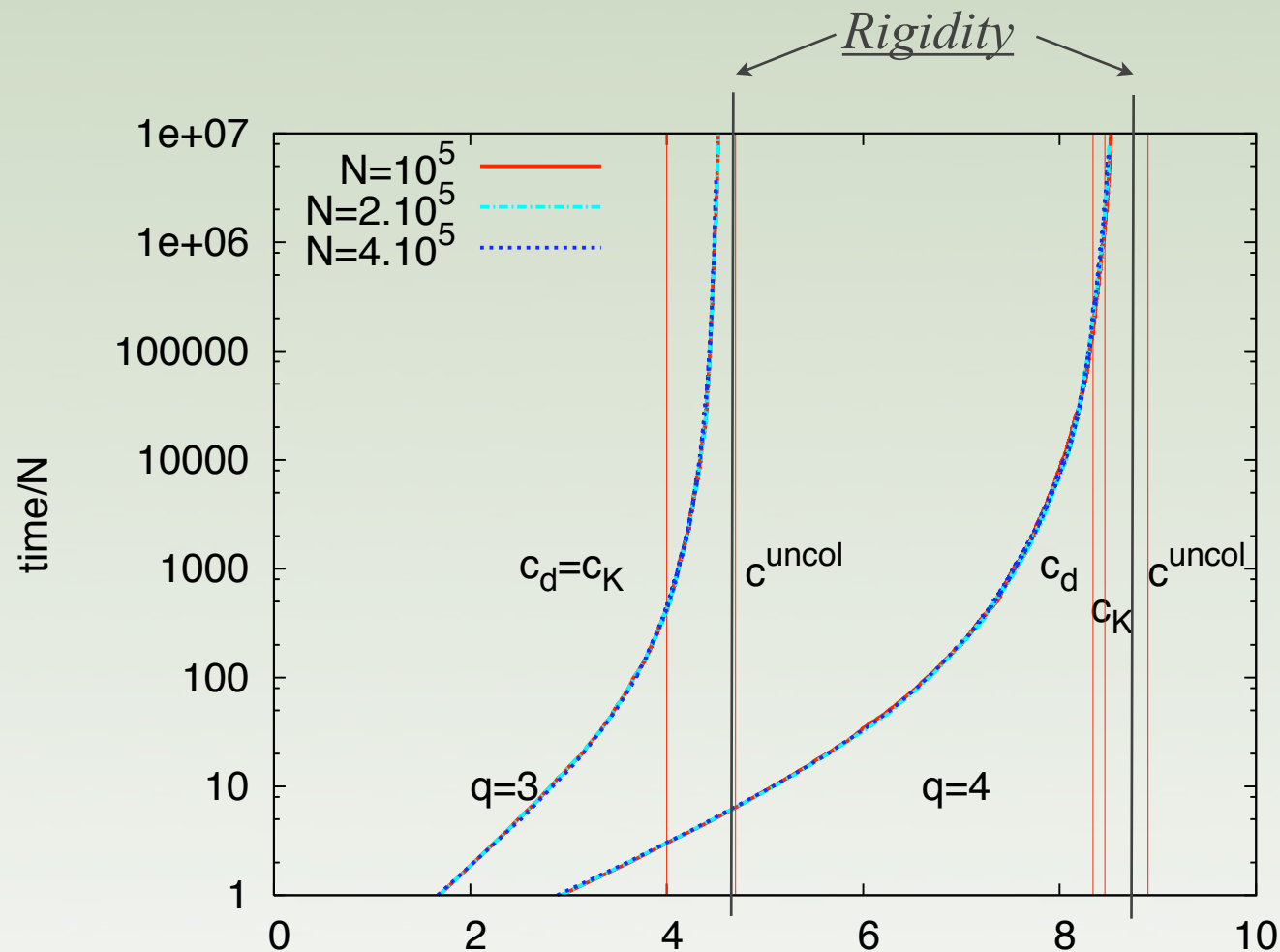
*The algorithm works until the cluster disappears
and this happens when frozen variables appear*

Performance of the “Wet toes” algorithm



Goes beyond the dynamical and the condensation transition for $q=3$ & 4

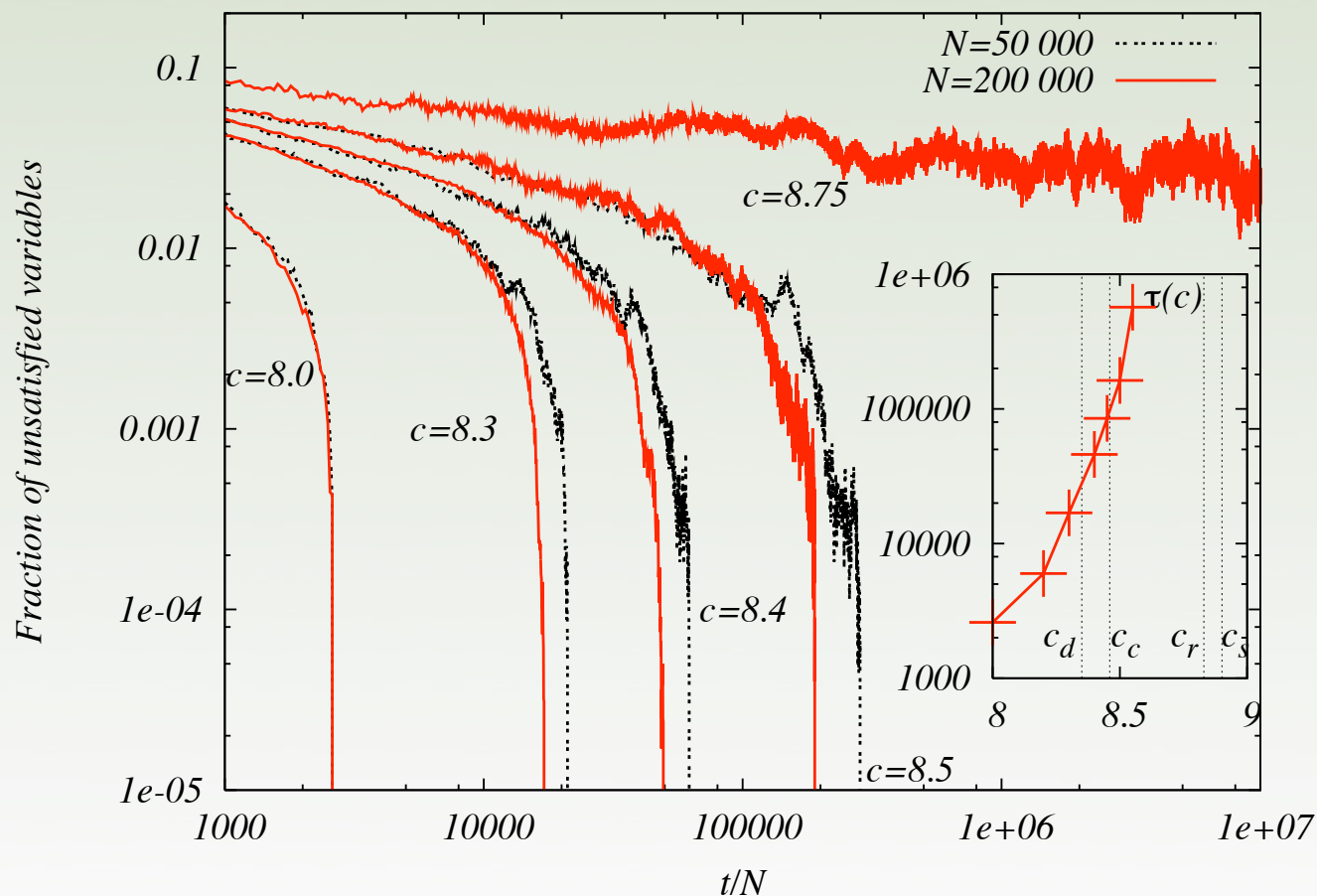
Performance of the “Wet toes” algorithm



Goes beyond the dynamical and the condensation transition for $q=3$ & 4
But stops before the rigidity transition !

Another example: Walk-COL algorithm

- (1) Randomly choose a spin that has the same color as at least one of its neighbors.
- (2) Change randomly its color. Accept this change with probability one if the number of unsatisfied spins has been lowered, otherwise accept it with probability p .
- (3) If there are unsatisfied vertices, go to step (i) unless the maximum running time is reached.



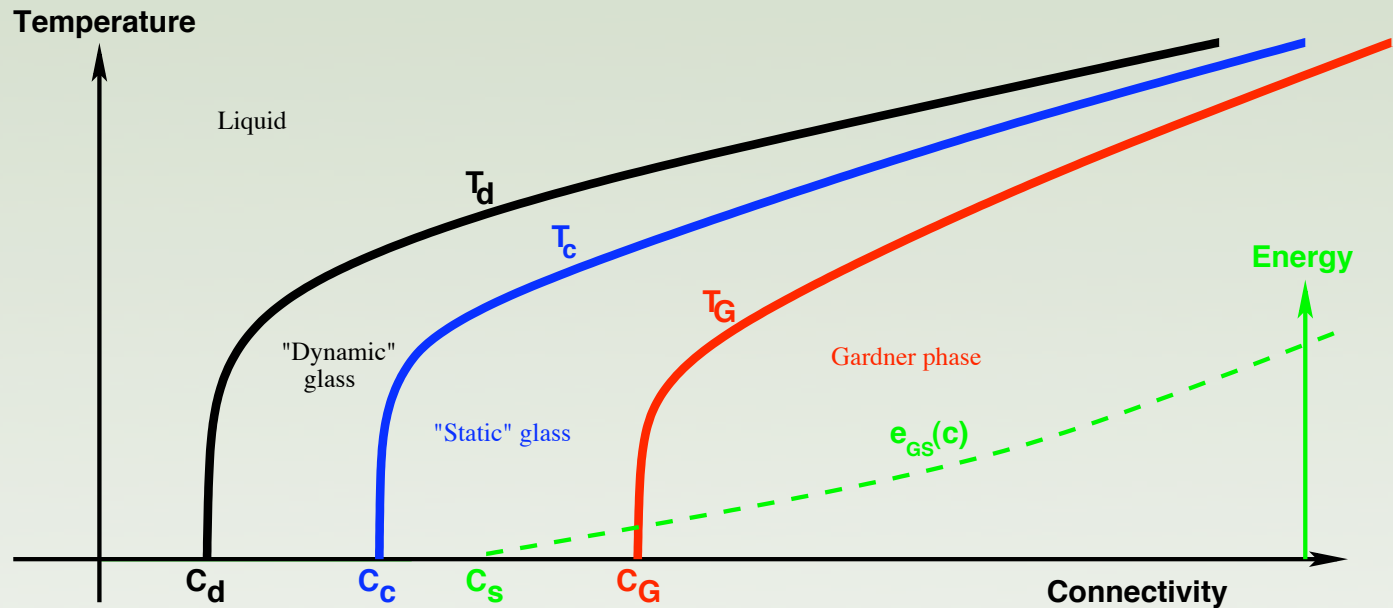
Conclusions & perspectives

- ~ Determination of the phase diagram of the random coloring problem. A rich “glassy”-like phenomenology is found :
 - ~ dynamical transition
 - ~ condensation/Kauzmann transition
 - ~ “rigidity/freezing” transition
 - ~ COL/UNCOL transition
- ~ Discussion of the algorithmic implications
- ~ Frozen variables are responsible for the computational hardness

- ~ Future directions :
 - ~ More (and possibly exact) results on the EASY/HARD transition and frozen clusters ?
See next talk by F. Zamponi
 - ~ Toward a rigorous formulation of the cavity results? Numerical check of static and dynamic predictions?
 - ▶ *Enumeration (c.f. Last talk by A. Hartmann)*
 - ▶ *Monte-Carlo simulations?*
 - ~ Better algorithms using message passing (BP and SP)?

Monte-Carlo simulations?

The typical phase diagram in a temperature/connectivity plane



Is it possible to confirm these predictions in a Monte-Carlo simulation and to find the dynamic, static and Gardner transition?

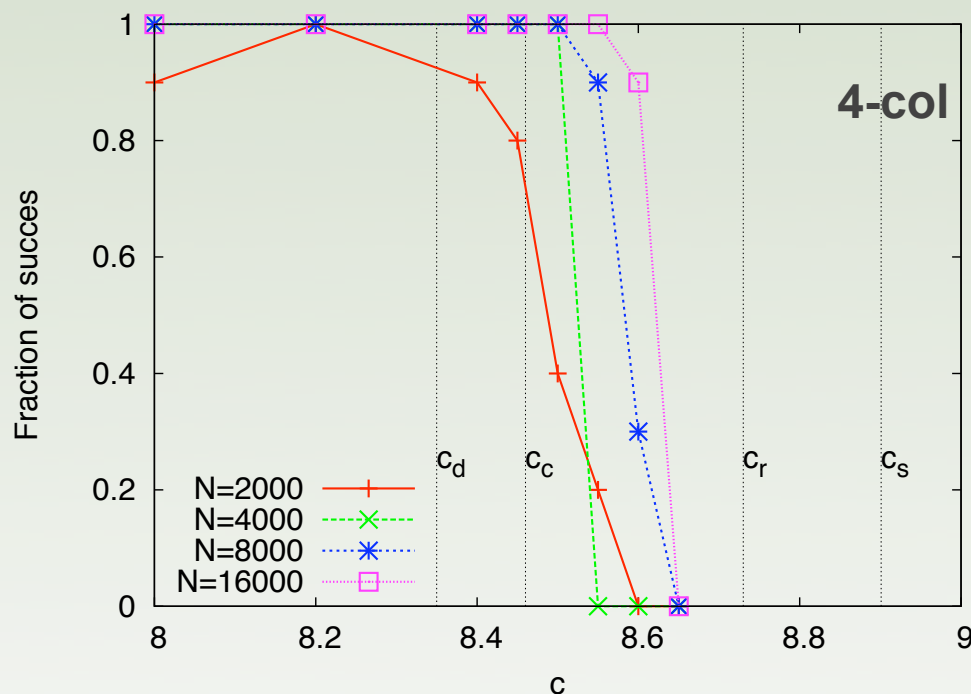
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Message Passing algorithms beyond SP ?

- Survey Propagation (cavity recursion on a single graph at $m=0$) is currently the best solver for random SAT
- Belief Propagation (replica symmetric cavity recursion on a single graph) can also be used with very good results (as it actually asymptotically gives exact marginals until the condensation)



- What is the limit of these algorithms?
- What is the best way to use message passing in order to find a solution?

➡ See the recent paper by Montanari et al. [arxiv:0709.1667](https://arxiv.org/abs/0709.1667)

References

- ~ **FK**, A. Montanari, F. Ricci-Tersenghi, G. Semerjian and L. Zdeborová : Gibbs States and the Set of Solutions or Random Constraint Satisfaction Problems, **PNAS 104, 10318 2007**
- ~ L. Zdeborová and **FK**: Phase Transitions in the Coloring of Random Graphs, **Accepted in PRE, arXiv:0704.1269**
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References

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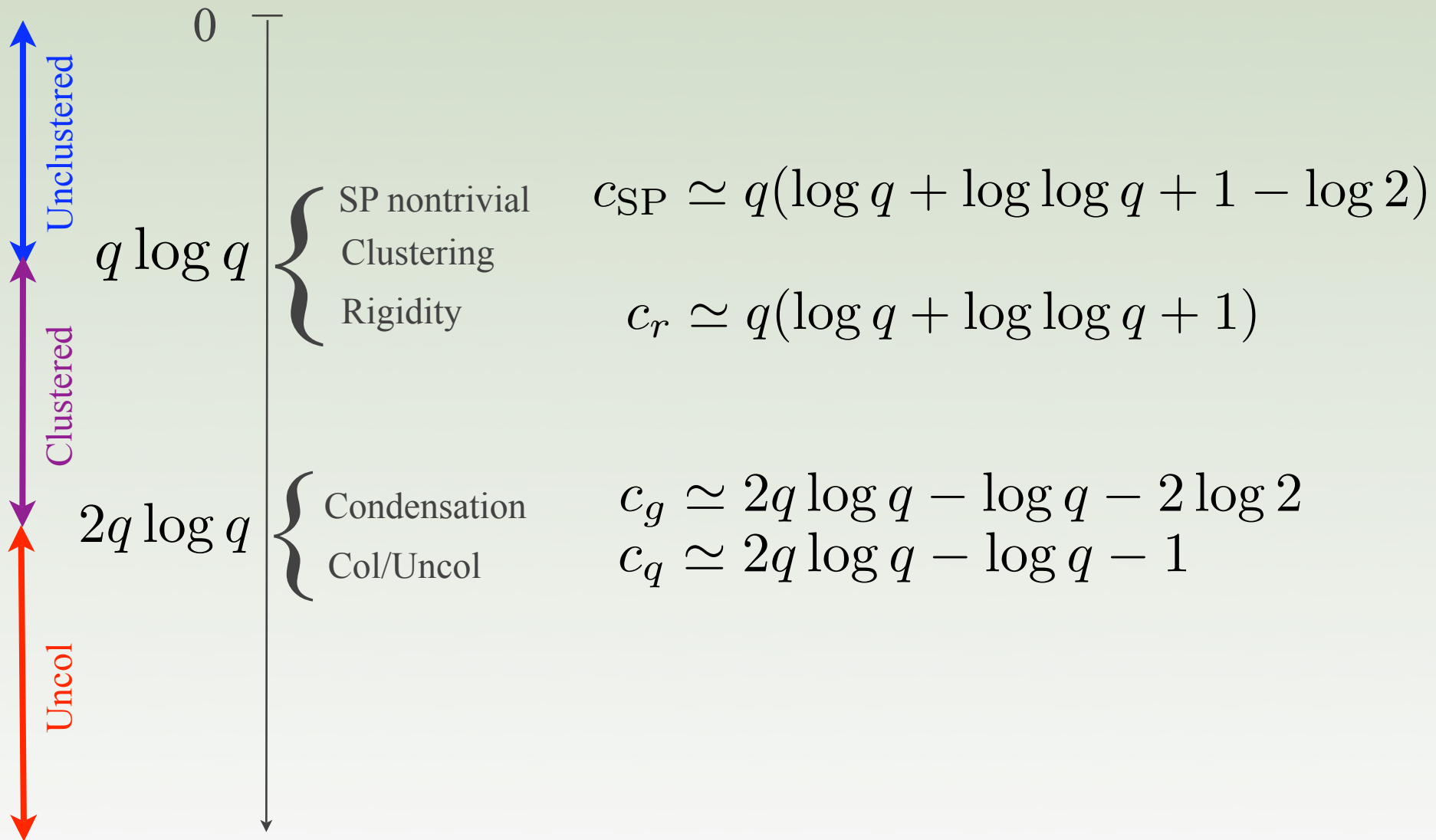
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... and to the audience for your attention.

Bonus Section

Large number of colors (analytical results)



The Cavity Method

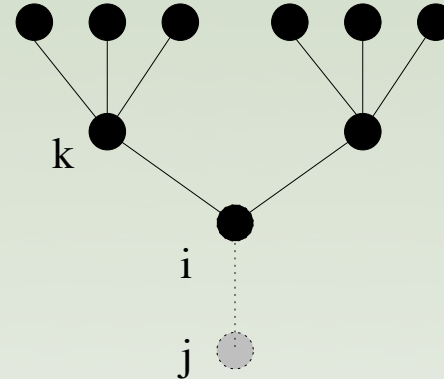
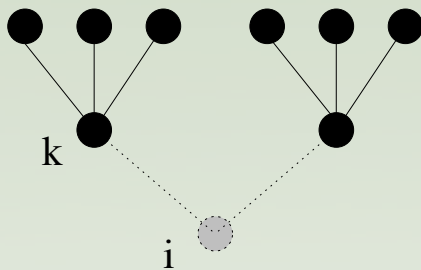
Parisi, Mézard, Virasoro '87

Parisi, Mézard '00

Parisi, Mézard, Zechinna '02

The iterative solution on a tree

Coloring = anti-ferromagnetic Potts model at zero temperature



Recursive equations on a tree (Belief propagation):

$$\begin{aligned}\psi_{s_i}^{i \rightarrow j} &= \frac{1}{Z^{i \rightarrow j}} \prod_{k \in V(i) - j} \sum_{s_k} (1 - \delta_{s_i s_k}) \psi_{s_k}^{k \rightarrow i} \\ &= \frac{1}{Z^{i \rightarrow j}} \prod_{k \in V(i) - j} (1 - \psi_{s_i}^{k \rightarrow i})\end{aligned}$$

$\psi_{s_i}^{i \rightarrow j}$ is the set of probabilities that the spin i takes the color q in absence of the spin j

The replica symmetric solution on a graph

A random graph being locally tree-like, assume a “fast” decay of correlations, then the RS solution should be correct.

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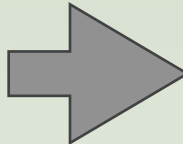
➔ Rigorously proven for regular random graphs for $c < q-1$

Bandyopadhyay, Gamarnik '05

... and believed to be correct even beyond (until $c \sim q \log q$).

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 Rigorously proven for regular random graphs for $c < q-1$

Bandyopadhyay, Gamarnik '05

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Solution of the self-consistent equation:

Only the “paramagnetic” $\psi = (1/q, 1/q, \dots)$ in the COL phase.

This leads to the following entropy:

$$s_{\text{RS}} = \log q + \frac{c}{2} \log \left(1 - \frac{1}{q} \right)$$

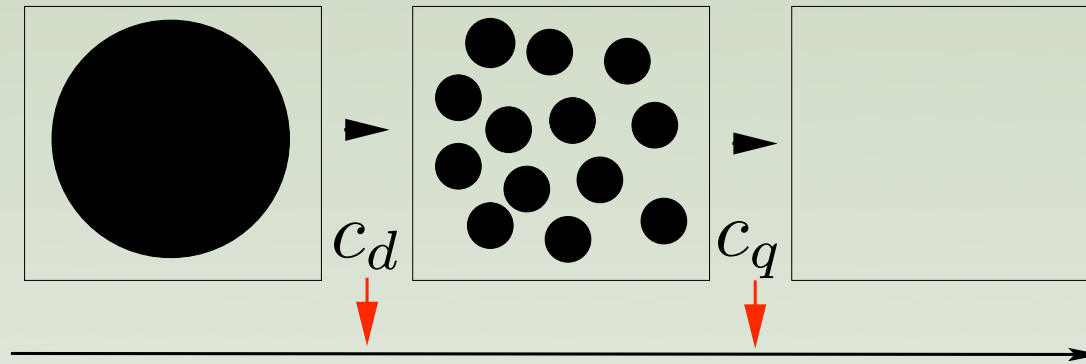
When is the tree solution expected to be correct ?

★ If we are in a “paramagnetic phase” .

★ From spin glass theory, we expect however a transition to a spin glass phase.

- 🕒 1) Continuous transition (divergence of the Spin glass susceptibility)
like in the Sherrington-Kirkpatrick model
- 🕒 2) Discontinuous transition (like in the p-spin or the Random Energy model model)

Replica symmetry breaking



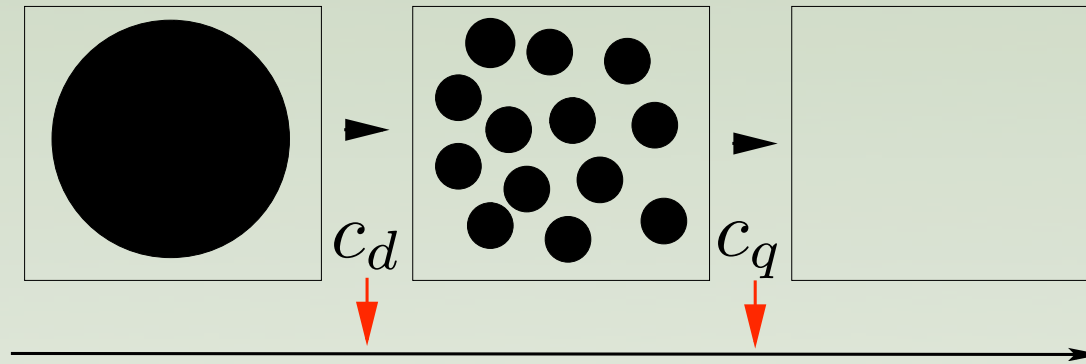
The phase space splits into an exponential number \mathcal{N} of components.

Define the complexity (or configurational entropy) Σ as $\mathcal{N} = e^{N\Sigma}$

The complexity can be computed using a “modified” partition sum:

$$\sum_{\alpha} Z_{\alpha}^m = \sum_{\alpha} \left(\sum_{s \in \alpha} e^{-\beta E(s)} \right)^m = \int f df e^{-N(\beta m f(\beta) - \Sigma(f))} = e^{-\beta m N \Phi(\beta, m)}$$

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The “Replicated” free energy is the Legendre transform of the complexity

$$-\beta m \Phi(m, \beta) = -\beta m F(\beta) + \Sigma(F)$$

The replica symmetry breaking recursion

Order Parameter:

Probability distribution $P^{i \rightarrow j}(\psi)$ **of fields for every edge.**

Self-consistent equation:

$$P^{i \rightarrow j}(\psi) = \frac{1}{Z^{i \rightarrow j}} \int \delta[\psi_{s_i}^{i \rightarrow j} - \mathcal{F}(\{\psi_{s_i}^{k \rightarrow i}\})] e^{m \Delta S^{i \rightarrow j}} \prod_{k \in V(i) - j} dP^{k \rightarrow i}(\psi)$$

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Numerical Solution - Population dynamics: very heavy!!!

Simplifications : m=0, m=1, regular graphs, hard fields...

Large q expansion