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Workshop on Sphere Packing and Amorphous Materials

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Random Hard Sphere Packings and Constraint Satisfaction Problems

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Random hard sphere packings and constraint satisfaction problems

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Trieste, July 27, 2011

Presentation of the talk

Overview of the statistical mechanics (mean field) approach to the random packing problem

- The packing problem is a constraint satisfaction problem
- Discrete random constraint satisfaction problems (R-CSP) have been studied in detail by the statistical mechanics community
  Franz, Kirkpatrick, Krzakala, Kurchan, Marsili, Mézard, Monasson, Montanari, Parisi, Ricci-Tersenghi, Semerjian, Zdeborová, Zecchina, and many others
  in a very fruitful exchange with the mathematicians
- Review of results for simple R-CSP: structure of solution and *local* algorithms
- Difficulties in extending these results to the packing problem
- Results from the replica method (briefly)
  Cardenas, Franz, Kirkpatrick, Mézard, Monasson, Parisi, Thirumalai, Wolynes, FZ

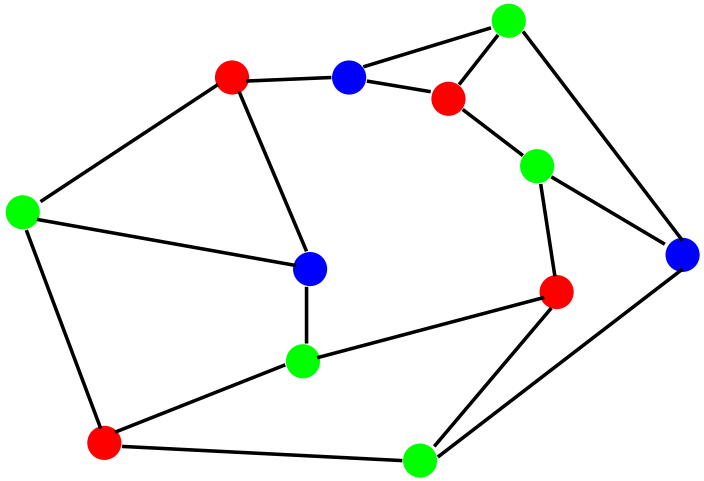
At this conference, see the talks by:
Brito, Chakraborty, Charbonneau, Ellenbroek, O'Hern, Kurchan, Miyazaki, Ramezanpour

Outline

1. Random Constraint Satisfaction Problems
   - The coloring problem
   - Statistical mechanics approach
   - Phase transitions in R-CSP
   - Consequences for *local* algorithms
   - A bridge between coloring and packing problemss
2. The sphere packing problem
   - Mean field phase diagram
   - Mean field and large d
   - Mean field and $3d$

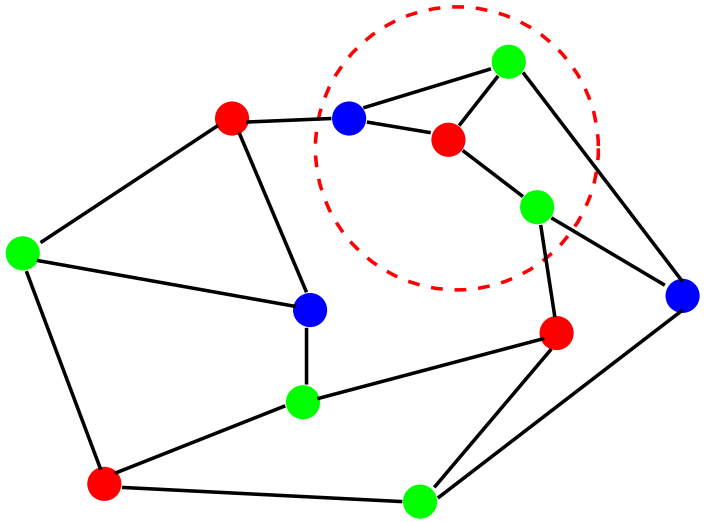
Outline

The coloring problem



Input: A graph of N nodes and M links, and q colors.
Problem: Assign a color to each node in such a way that no link connects two nodes of different colors
A constraint satisfaction problem

The coloring problem as a packing problem

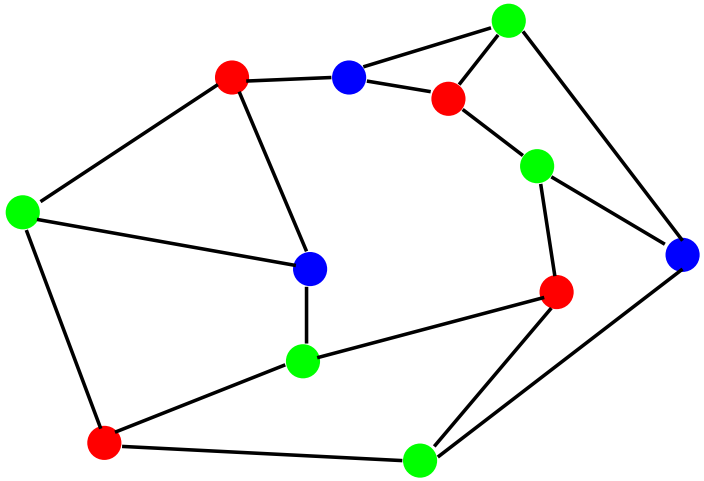


Input: A graph of N nodes and M links, and q types of particles.
Problem:

- On each site, put one particle (hard-core exclusion)
- If a site is occupied by a particle of color i, then adjacent sites cannot be occupied by particles of the same color (nearest-neighbor exclusion between particles of the same color)

A packing problem for a non-additive mixture of q types of particles

Coloring problem as a statistical mechanics problem

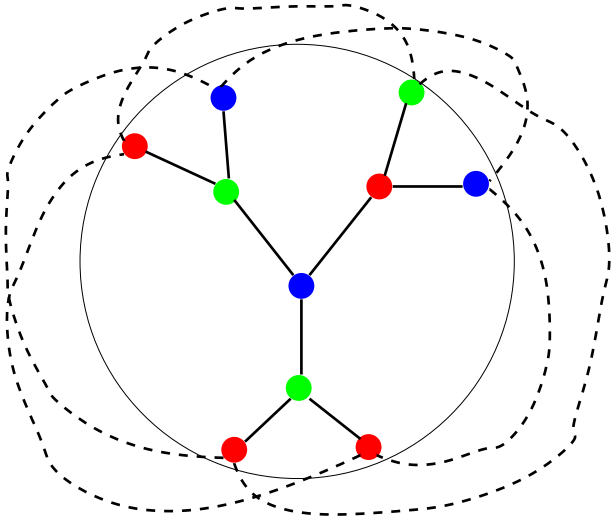


Input: A graph of N nodes and M links, and "Potts spins" $\sigma_i \in \{1, 2, \cdots, q\}$.
Problem:

- Define the Hamiltonian $H = \sum_{\langle i,j \rangle} \delta_{\sigma_i,\sigma_j}$
- Compute the partition function: $Z(\beta) = \sum_{\sigma_1,\cdots,\sigma_N} e^{-\beta H}$
- The ground state energy is $E_{GS} = \lim_{\beta\to\infty} \left[-\beta^{-1} \log Z(\beta) \right]$

A coloring exists $\Leftrightarrow E_{GS} = 0$, and $Z(\beta = \infty)$ =number of solutions
No coloring exist $\Leftrightarrow E_{GS} > 0$, and E_{GS} =minimal number of monochromatic links

Coloring of random graph as "spin glass" problem

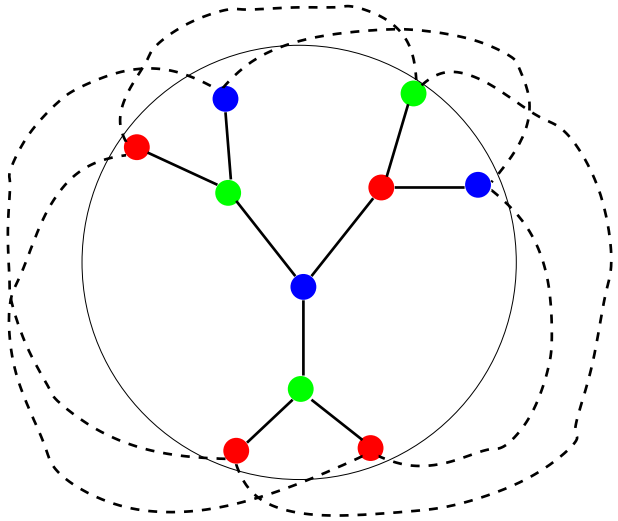


Solving the problem for each given graph is too hard
Introduce an ensemble of random graphs: e.g. Erdös-Rényi ensemble
Random Constraint Satisfaction Problem (R-CSP)

Key property of random graphs: locally tree-like for $N \to \infty$ and $M = cN/2$
Typical loops are long $\sim \log(N)$

The neighbors of a given spin are "far away" from each other
Hence, *they are decorrelated* (in absence of the central spin)
In physics, this is called a "mean field" model

Coloring of random graph as "spin glass" problem



Mean field statistical mechanics methods (replica and cavity methods) allow to compute exactly the partition function

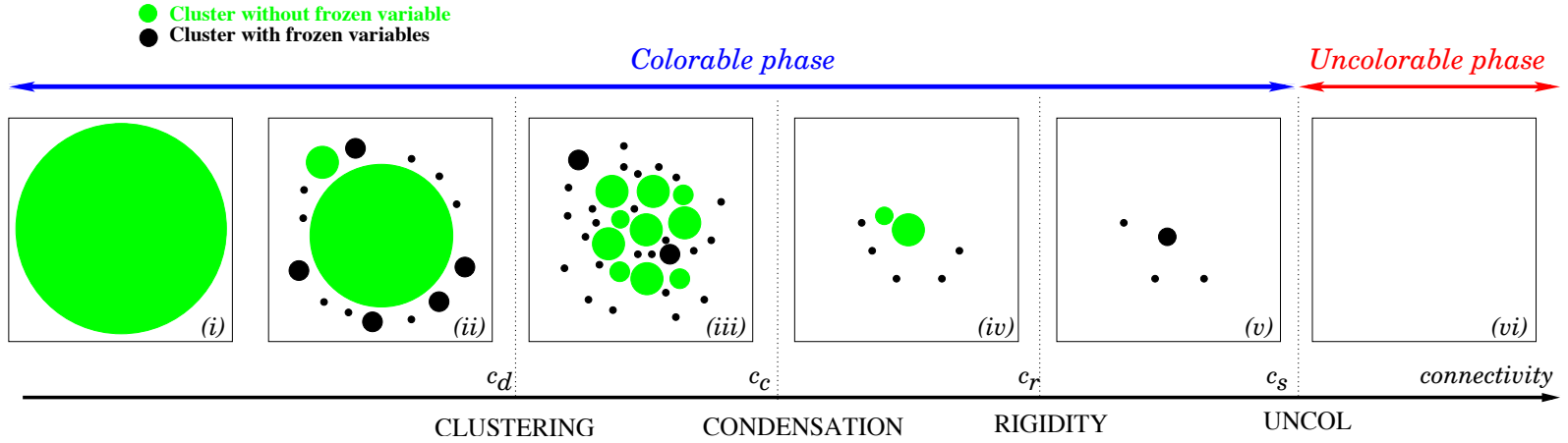
More precisely, the free energy averaged over the random graph:

$$f(\beta, c) = \lim_{N\to\infty\,,\, M=cN/2} \mathbb{E}\left[-\frac{1}{\beta N}\log Z(\beta)\right]$$

From this, all the information on the problem can be reconstructed: ground state energy, number of solutions, etc.

Phase transitions in R-CSP, at zero temperature

Structure of the set of the solutions: [Krzakala et al. PNAS 104, 10318 (2007)]

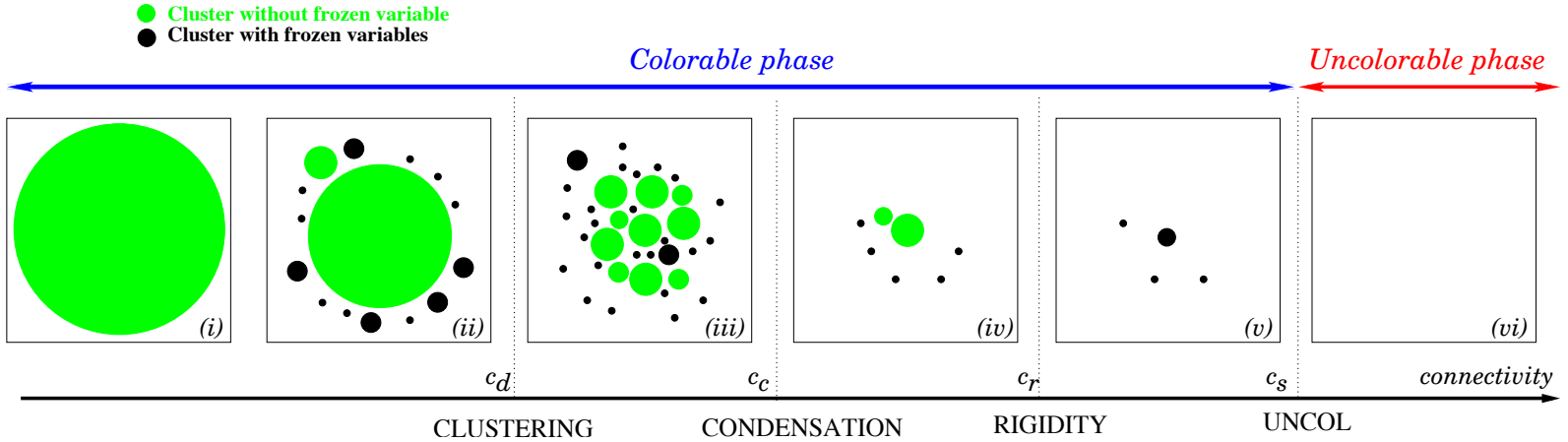


Phase transitions in Random CSP:

- $c < c_d$: Most of the solutions form a unique cluster
- $c_d < c < c_c$: The solutions form many ($\sim e^{N\Sigma}$) clusters
- $c_c < c < c_s$: A small number of clusters dominate
- $c_r < c < c_s$: Frozen variables in a cluster
- $c > c_s$: No colorings, $E_{GS} > 0$ (UNSAT)

Phase transitions in R-CSP, at zero temperature

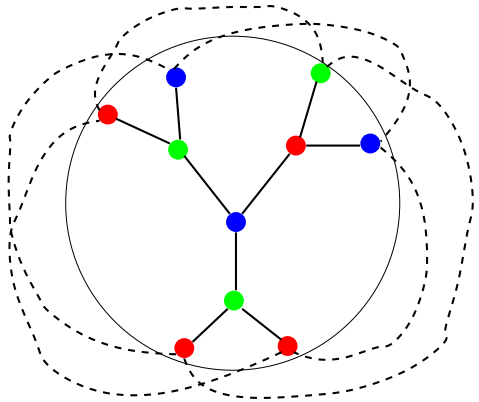
Structure of the set of the solutions: [Krzakala et al. PNAS 104, 10318 (2007)]



Condition for the clustering transition: $\forall c \leq c_d$ one has

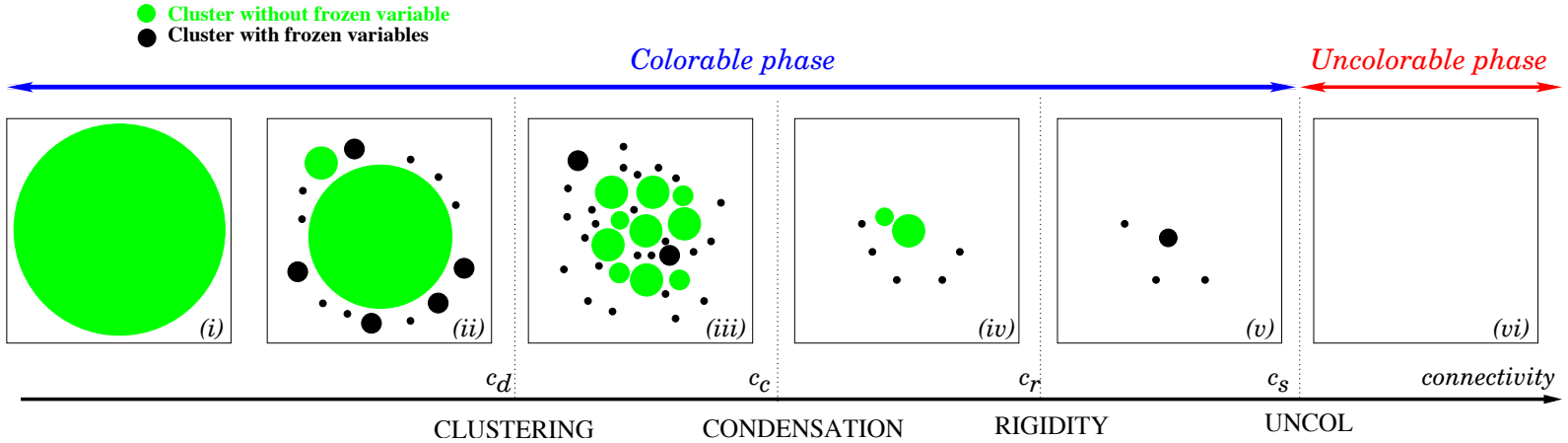
$\mu(\cdot)$: uniform measure over solutions
σ_i: a randomly drawn spin
$\underline{\sigma}_\ell$: set of spins at distance ℓ from i

$$\lim_{\ell\to\infty}\lim_{N\to\infty}\mathbb{E}\sum_{\underline{\sigma}_\ell}\mu(\underline{\sigma}_\ell)\sum_{\sigma_i}|\mu(\sigma_i|\underline{\sigma}_\ell)-\mu(\sigma_i)|=0$$



Phase transitions in R-CSP, at zero temperature

Structure of the set of the solutions: [Krzakala et al. PNAS 104, 10318 (2007)]



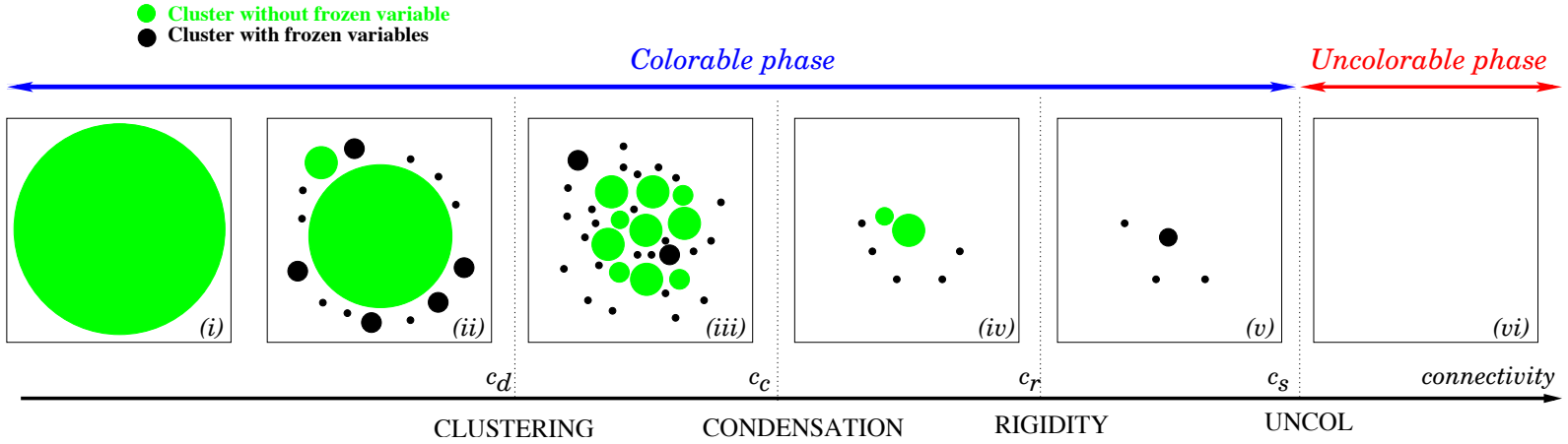
Condition for the condensation transition: draw n random spins $i_1, \cdots, i_n$, then one has, $\forall n$ and $\forall c \leq c_c$,

$$\lim_{N\to\infty} \mathbb{E} \sum_{\sigma_{i_1},\cdots,\sigma_{i_n}} |\mu(\sigma_{i_1},\cdots,\sigma_{i_n}) - \mu(\sigma_{i_1})\cdots\mu(\sigma_{i_n})| = 0$$

Hence c_c is really a "phase transition"!

Phase transitions in R-CSP, at zero temperature

Structure of the set of the solutions: [Krzakala et al. PNAS 104, 10318 (2007)]

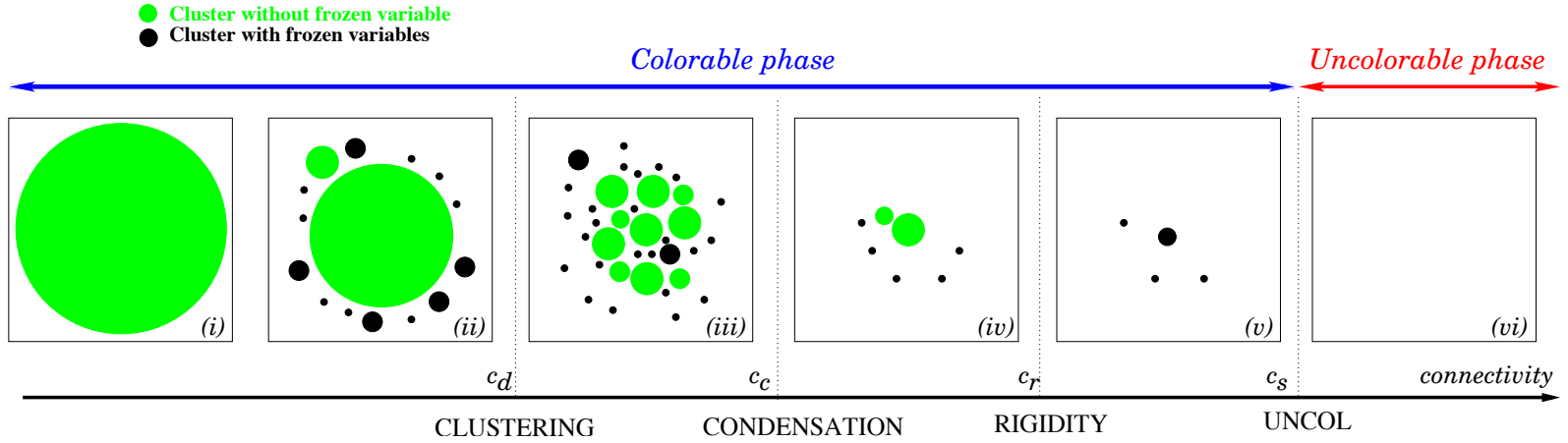


Condition for the satisfiability transition: $\forall c > c_s$, one has

$$\lim_{N\to\infty} P(Z > 0) = 0$$

Phase transitions in R-CSP, at zero temperature

Structure of the set of the solutions: [Krzakala et al. PNAS 104, 10318 (2007)]



In the limit of large q, one has

$c_d \sim q(\log q + \log\log q + O(1))$

[Theorem: Sly CMP 288, 943 (2009)
Gerschenfeld, Montanari, IEEE FOCS'07, 194 (2007)]

$c_c \sim 2q\log q - \log q - 2\log 2 + o(1)$

Existence of this transition proven in a similar model

[Coja-Oghlan, Zdeborova, arXiv:1107.2341]

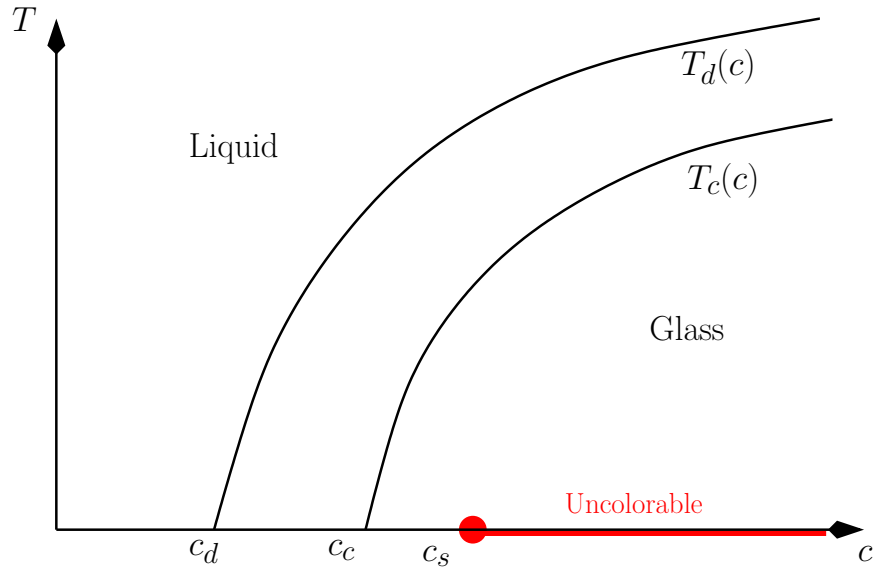
$c_s \sim 2q\log q - \log q - 1 + o(1)$

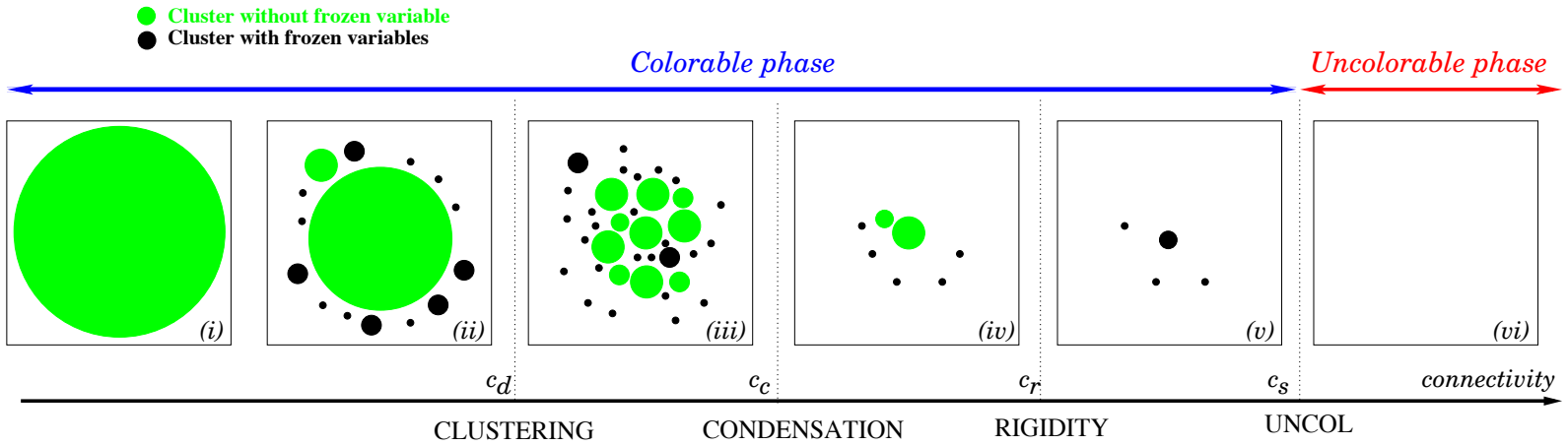
[Theorem ($2q\log q$): Achlioptas, Naor, Ann. Math. 162, 1335 (2005)]

Phase transitions in R-CSP, at non-zero temperature

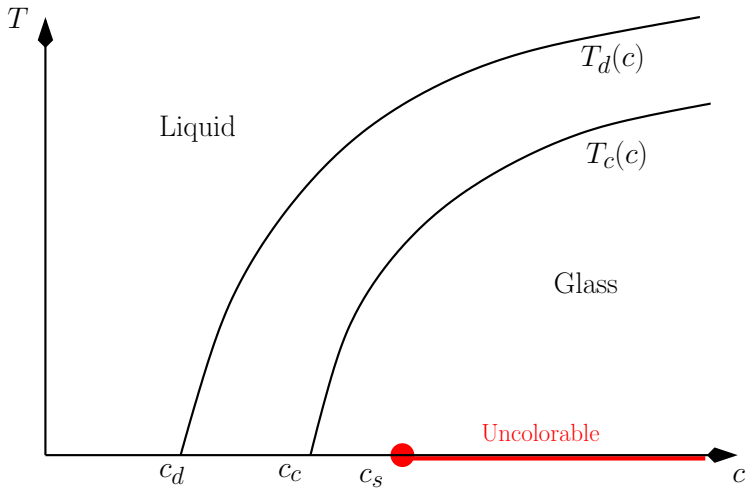
The temperature-connectivity phase diagram:

[Krzakala, Zdeborová, EPL 81, 57005 (2008)]



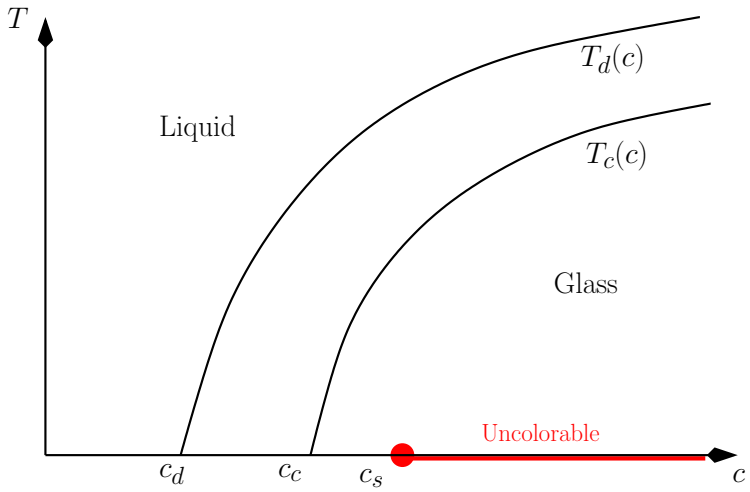


Consequences for *local* algorithms



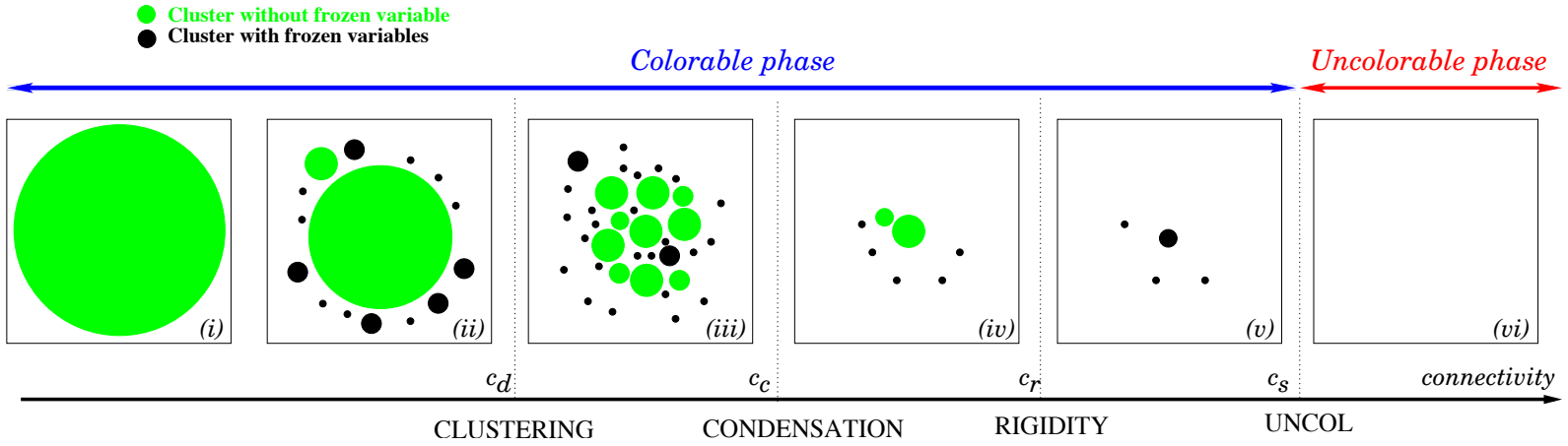
- Theorem: [Montanari, Semerjian, J. Stat. Phys. 125, 23 (2006)]
  Local Monte-Carlo algorithms do not equilibrate for $T < T_d(c)$
- This means that sampling is hard in this region - it takes a time $\sim \exp(N)$
- This means that dynamics becomes very algorithm-dependent in this region
- This *does not* mean that finding a solution is hard in this region

Consequences for *local* algorithms



- Sometimes, even thermal annealing is able to find a solution for $c > c_d$
- Several algorithms (WalkSAT, Belief Propagation, etc.) are able to find solutions quite close to c_s
- The point c_j where the algorithm fails is algorithm-dependent

Consequences for *local* algorithms



- Main message: whatever *local* algorithm will get stuck in one cluster
- There is a wide distribution of clusters and it is hard to predict in which cluster a given algorithm will get stuck
- In some cases, a more precise analysis can be done

[Krzakala, Zdeborová PRB 81, 224205 (2010)]

[Ricci-Tersenghi, Semerjian, J. Stat. Mech. P09001 (2009)]

A bridge between coloring and packing problems

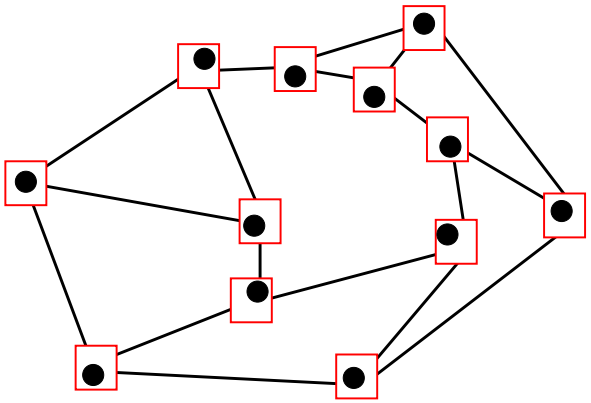
On each site, a variable $r_i \in [0,1]^d$
"*a continuous color*"

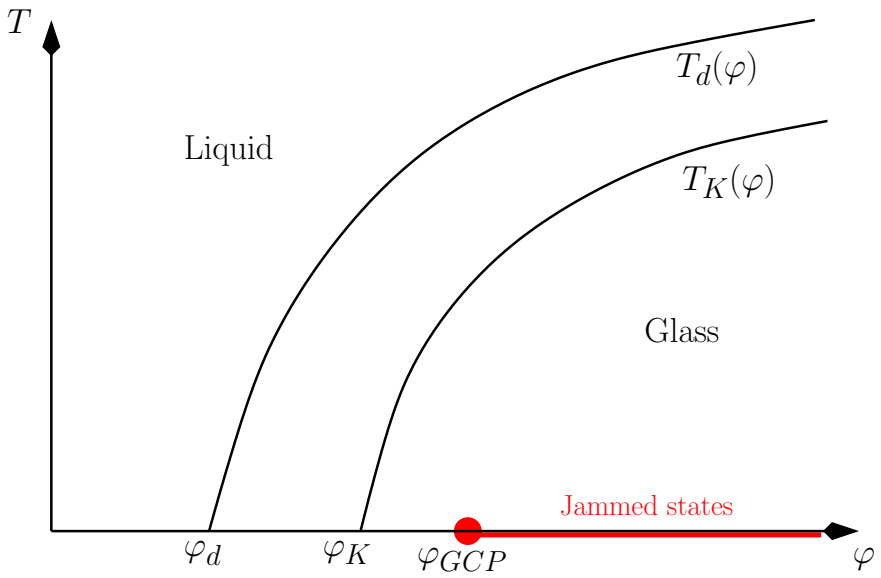
Hamiltonian $H = \sum_{\langle i,j \rangle} v(|r_i - r_j|)$
with $v(r) = (D-r)^2 \theta(D-r)$

Random graphs as for the COL problem

Same qualitative phase diagram:

[Mari, Krzakala, Kurchan, PRL 103, 025701 (2009)]





Outline

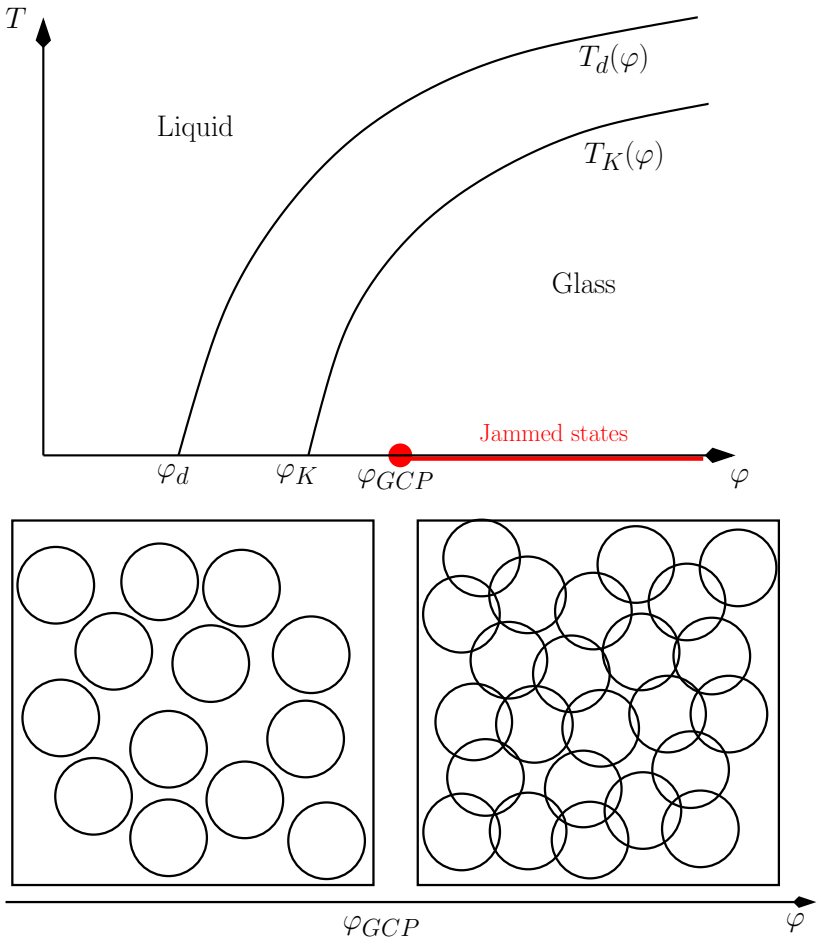
Mean field phase diagram for the sphere packing problem

The temperature-packing fraction phase diagram:

N particles in a volume V
d dimensions

$$H = \sum_{\langle i,j \rangle} v(|r_i - r_j|)$$
$$v(r) = (D - r)^2 \theta(D - r)$$

$$Z(\beta) = \int dr_1 \cdots dr_N \, e^{-\beta H}$$



Mean field phase diagram for the sphere packing problem

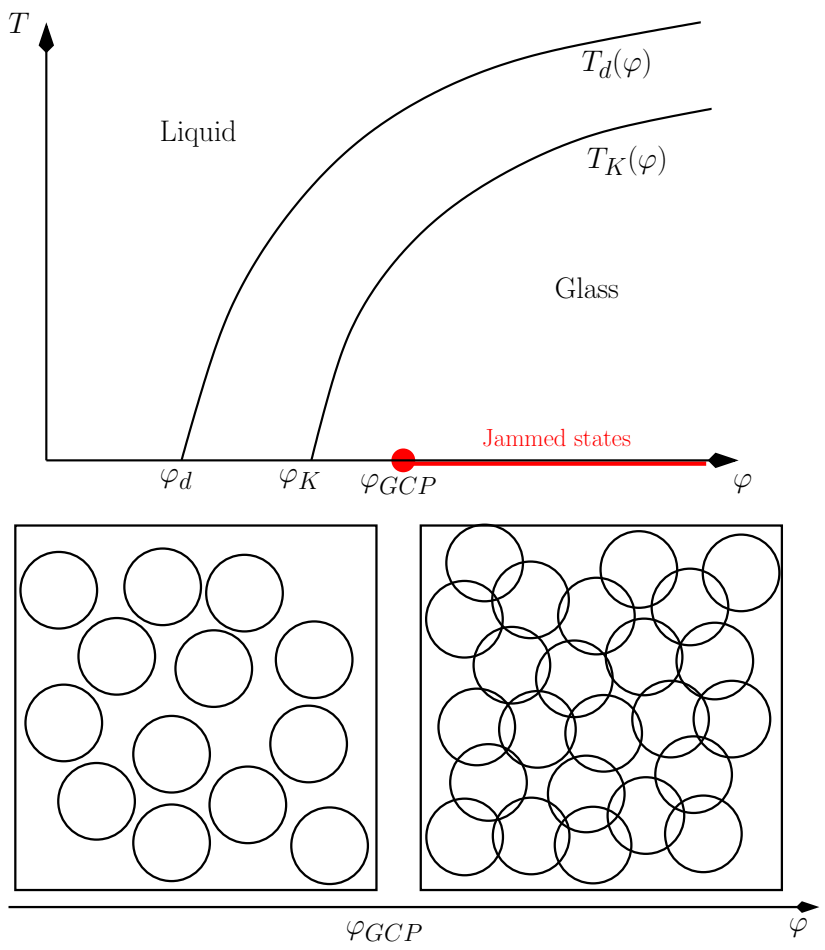
The temperature-packing fraction phase diagram:

New difficulties:

- Neighbors are correlated
- Geometry, crystallization

New interesting properties:
(C.Brito's talk)

- Mechanical properties
- Soft modes
- Scaling laws
- A large correlation



Mean field phase diagram for the sphere packing problem

The temperature-packing fraction phase diagram:

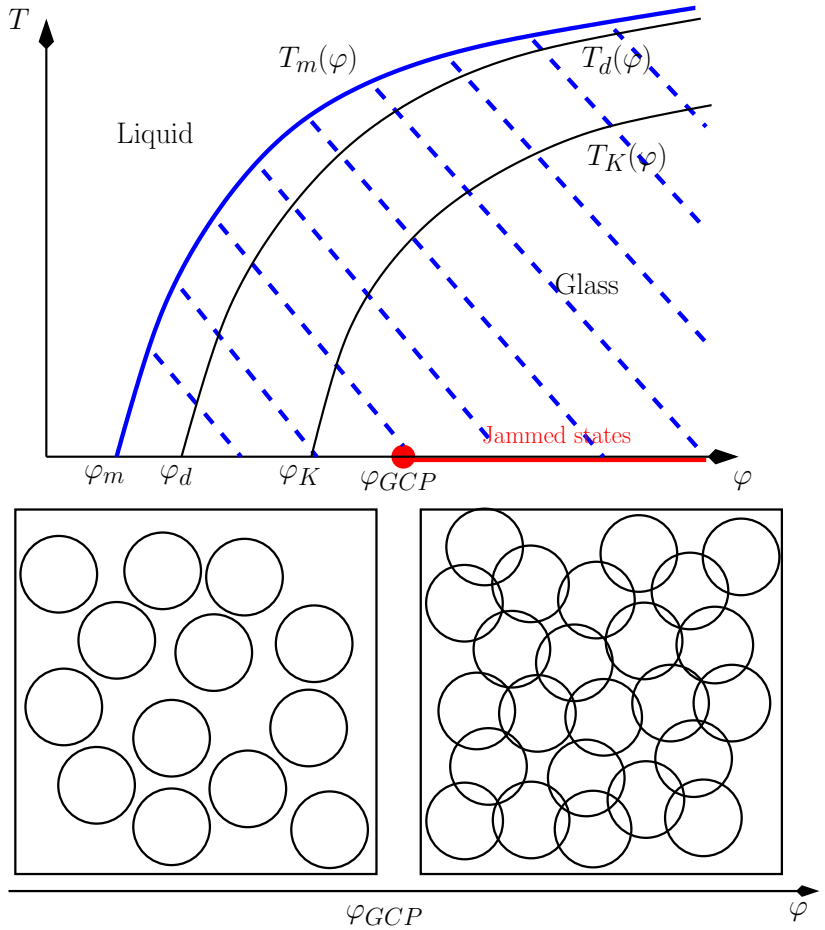
New difficulties:

- Geometry, crystallization

Because of crystallization, the amorphous region becomes metastable

Additional history dependence effects

In large dimensions, crystallization is suppressed (P.Charbonneau's talk)



Mean field phase diagram for the sphere packing problem

The temperature-packing fraction phase diagram:

New difficulties:

- Neighbors close to each others, hence correlated

Mean field theory cannot be used

In large dimensions:

$z = 2d$ (isostaticity)

$z \geq e^{d\,(-\log\sin(\pi/3))}$ (individual kissing number)

[Wyner, Bell System Tech. J. 46, 2111 (1967)]

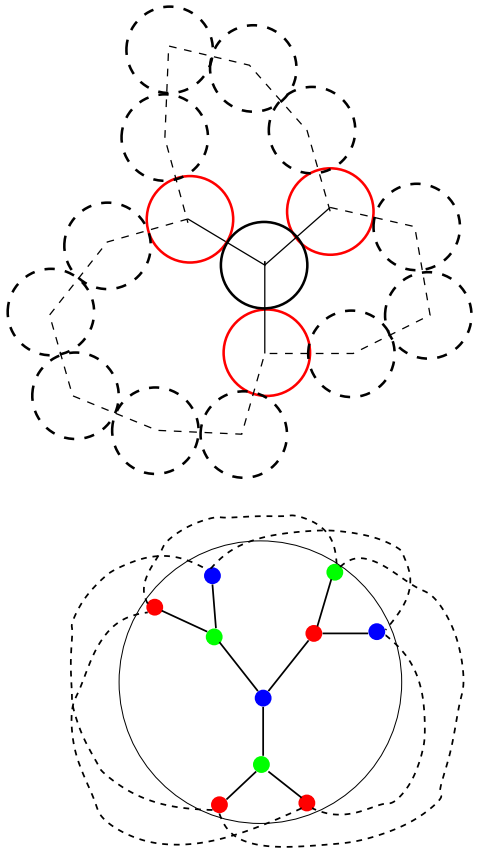
Neighbors are "far" from each others

The liquid lacks any short range structure

The Van der Waals equation is exact

Parisi, Slanina, PRE 62, 6554 (2000)

Skoge et al., PRE 74, 041127 (2006)



Mean field phase diagram for the sphere packing problem

Mean field theory of the glass transition in hard spheres has been formulated in many (almost) equivalent ways:

- Density functional theory

  `Singh, Stoessel, Wolynes, PRL 54, 1059 (1985)`

- Random First Order Transition (RFOT) theory

  `Kirkpatrick, Thirumalai, Wolynes, PRA 40, 1045 (1989)`

- Mode Coupling Theory

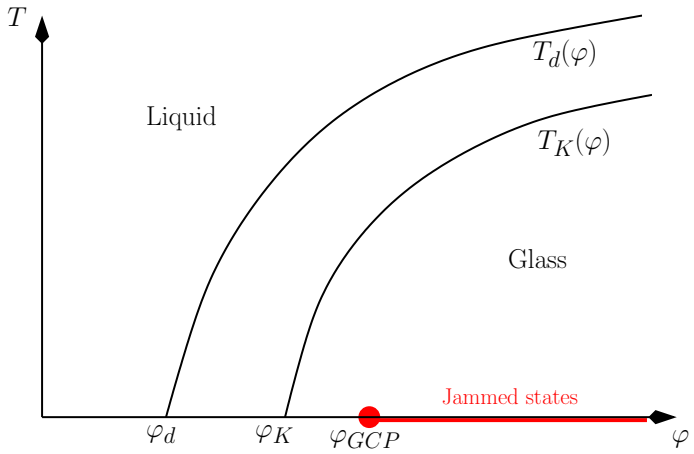
  `W. Gotze, Oxford University Press (2009)`

- Replica Theory

  `Mézard, Parisi, PRL 82, 747 (1999); Parisi, FZ, RMP 82, 789 (2010)`

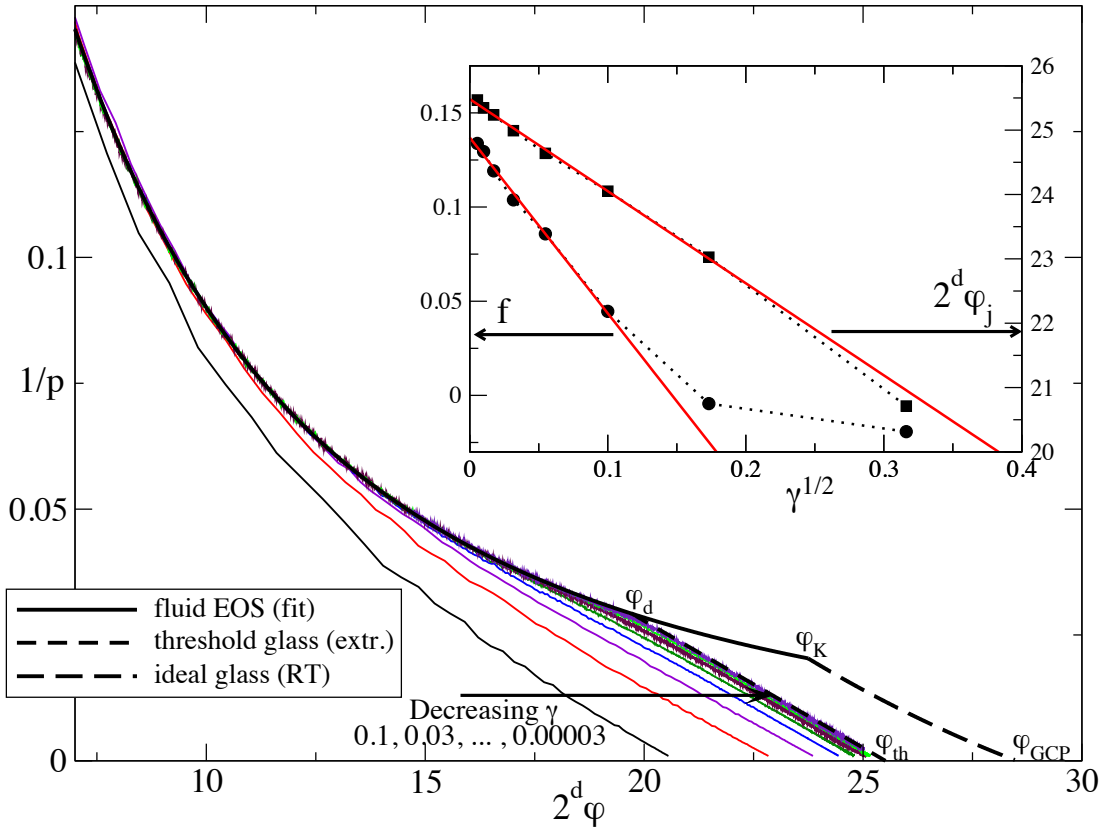
It might be exact for $d \to \infty$ and it is a reasonable approximation at finite d

Mean field theory should be exact in large d



$$p_{\rm fluid}(\varphi) = 1 + 2^{d-1}\varphi\,\frac{1-A_{\rm d}\,\varphi}{(1-\varphi)^d}$$

$$p_{\rm fv}(\gamma,\varphi) = \frac{d\,\varphi_{\rm j}(\gamma)[1-f(\gamma)]}{\varphi_{\rm j}(\gamma)-\varphi}$$

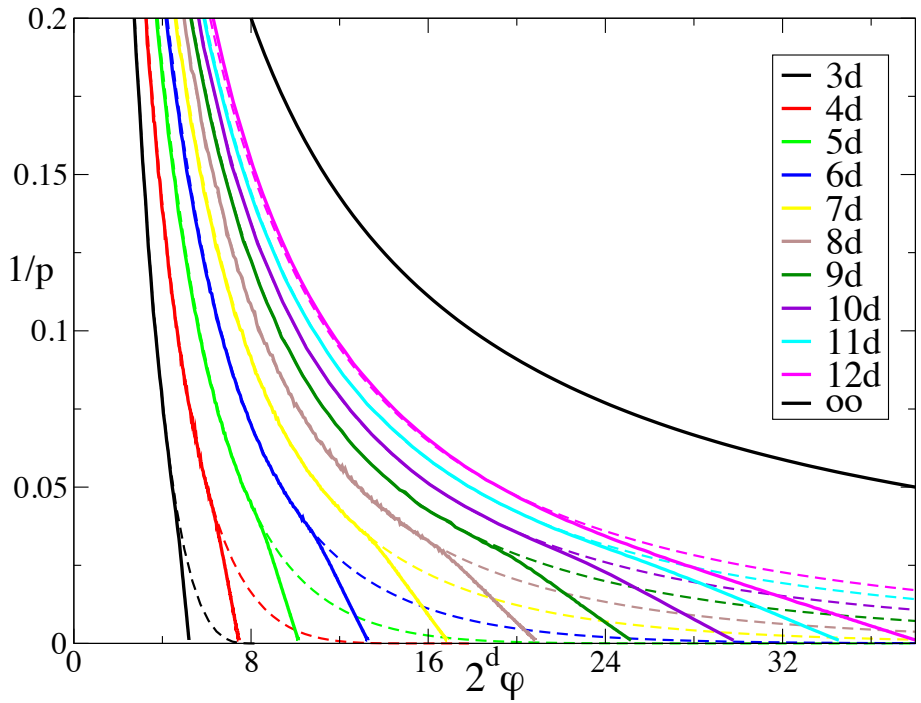


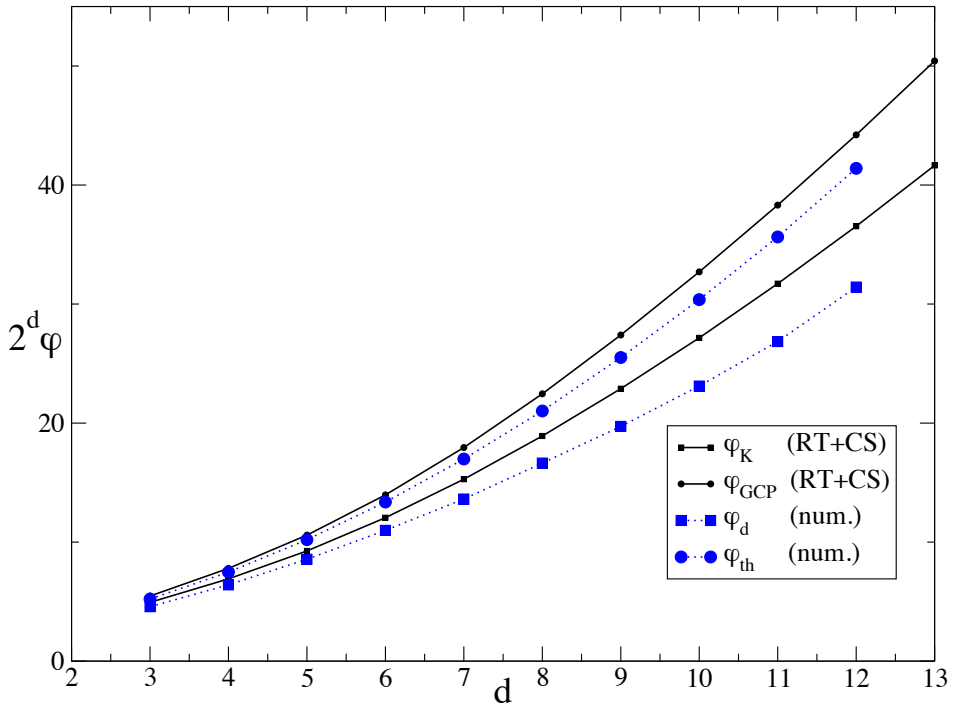
Compression of 9-dimensional hard spheres at constant rate
while doing local moves (event-driven collisions)

[Skoge, Donev, Stillinger, Torquato, PRE 74, 041127 (2006)]

[Charbonneau, Ikeda, Parisi, FZ, arXiv:1107.4666]

Mean field theory should be exact in large d





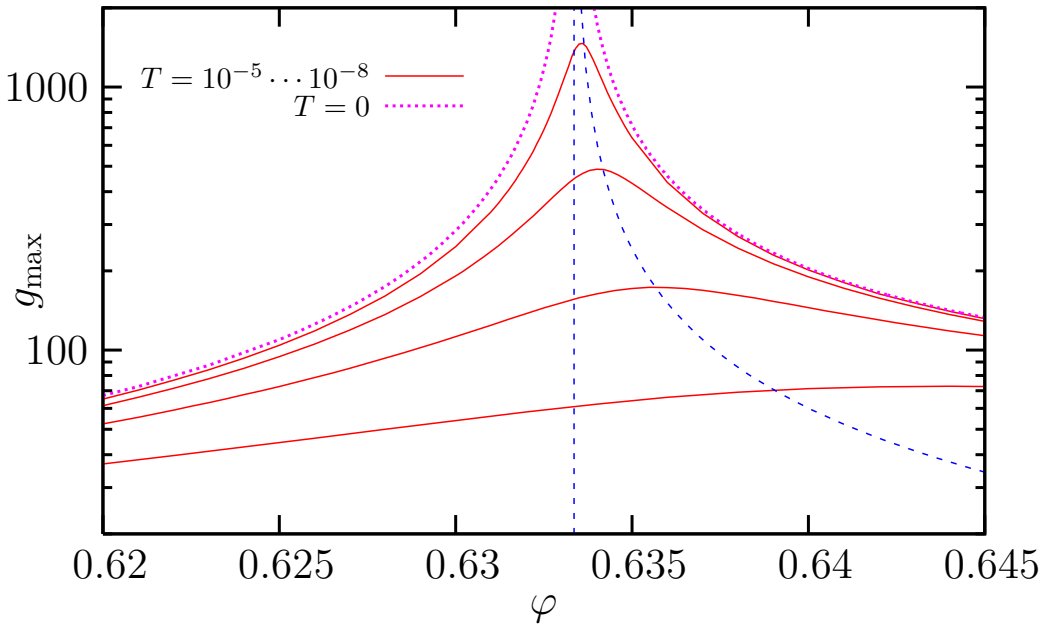
Large d scaling: $\varphi_{GCP} \sim 2^{-d} d \log d$

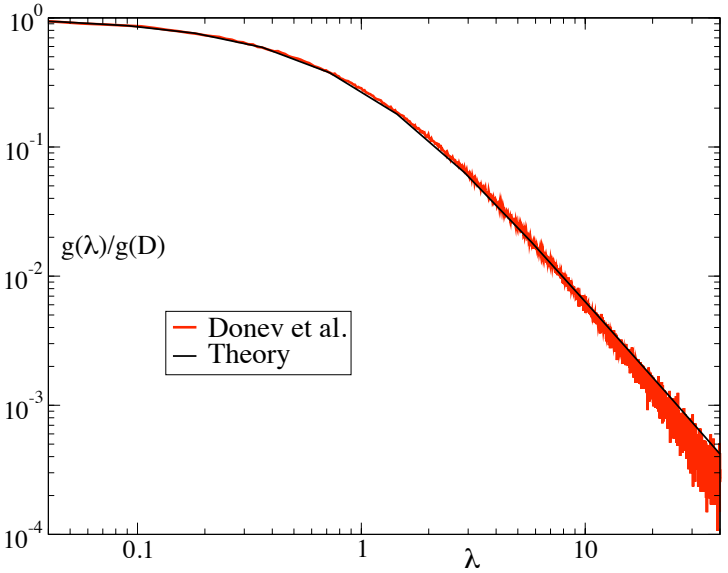
The liquid equation of state approaches the mean field one upon increasing d
Replica theory captures well the trend with increasing dimension
There is a discrepancy with Mode-Coupling Theory (Miyazaki's talk)

[Charbonneau, Ikeda, Parisi, FZ, arXiv:1107.4666]

Mean field theory is not so bad in $d = 3$

Scaling around jamming:





$$p \sim g(D) \sim (\varphi_j - \varphi)^{-1}$$

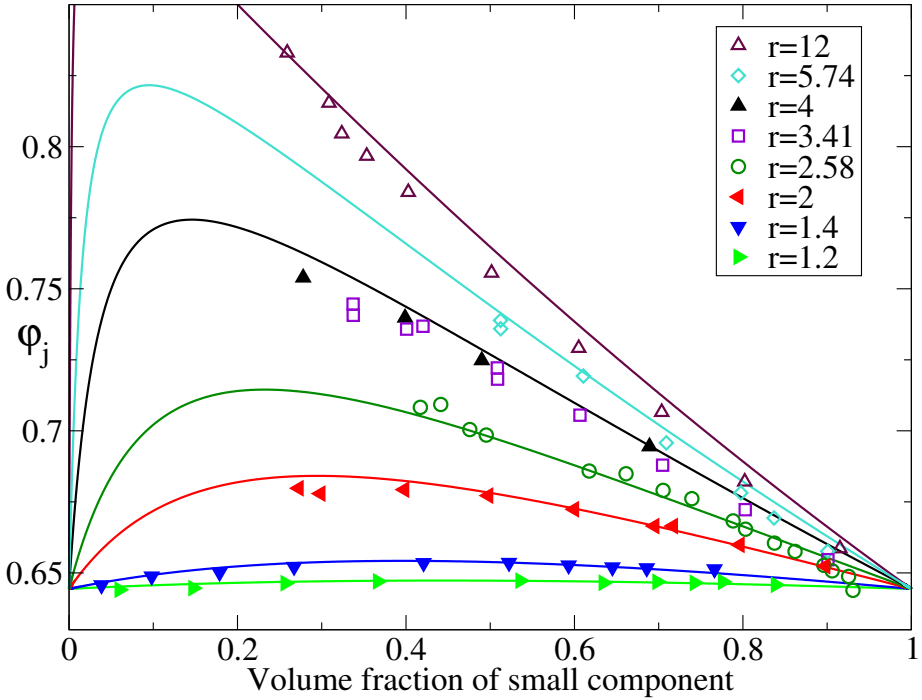
$$\frac{g(r)}{g(D)} = \Delta\left(\frac{r-D}{D}p\right) = \Delta(\lambda)$$

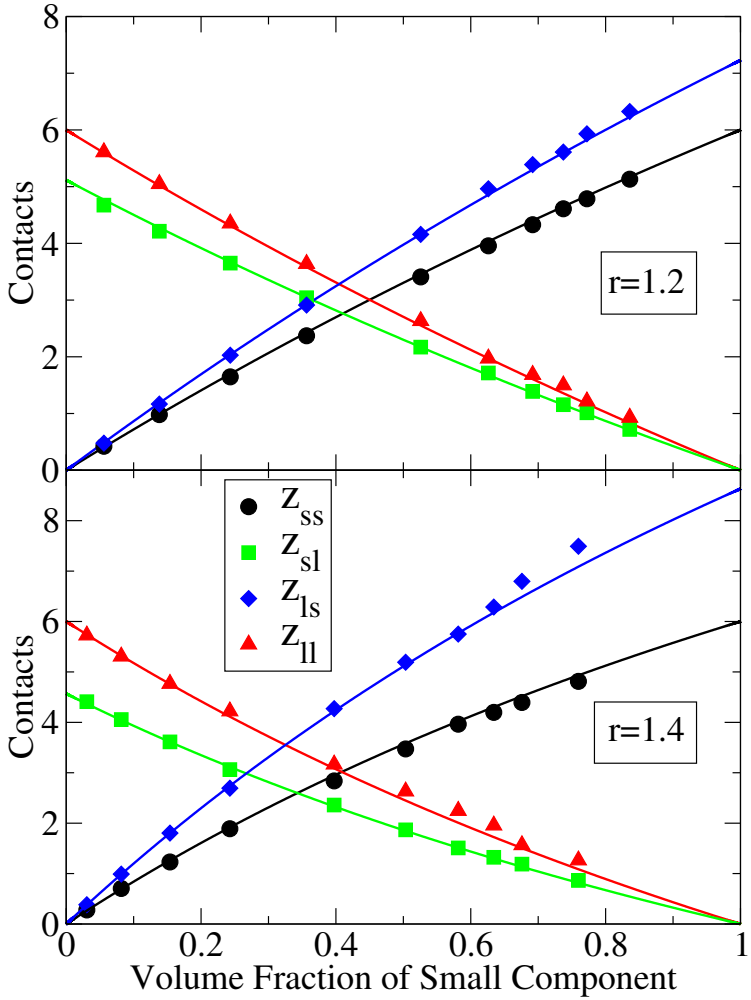
[Parisi, FZ, RMP 82, 789 (2010)]

[Berthier, Jacquin and FZ, PRL 106, 135702 (2011) and arXiv:1106.4663]

Mean field theory is not so bad in $d = 3$

Binary mixtures: jamming density and interparticle contacts



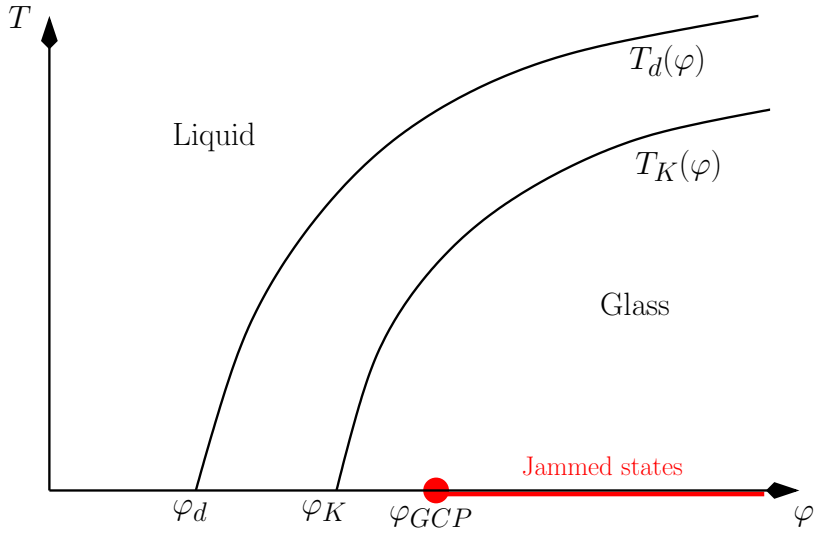


$r = D_A/D_B$

All packings are predicted to be globally isostatic.
Partial contact numbers are almost independent of φ_j.

[Biazzo, Caltagirone, Parisi, FZ, PRL 102, 195701 (2009)]

Conclusions



- A glass transition temperature $T_d(\varphi)$. Below it, history dependence and lack of equilibration.
- Jamming happens inside the glass region. The "random close packing" point depends on the algorithm used to create amorphous packings.
- Mean field theory predicts the existence of a "glass close packing", that would be reached only through an infinitely slow annealing. This is an upper bound to any amorphous jammed state.
- In large d, $\varphi_{GCP} \sim 2^{-d} d \log d$. Amorphous packings seem to evolve smoothly with dimension.
- Mean field theory might be exact at large d, and it is a reasonable approximation in low d.
- Still at low d crystallization is important.