OPTIMIZATION AND STATISTICAL MECHANICS

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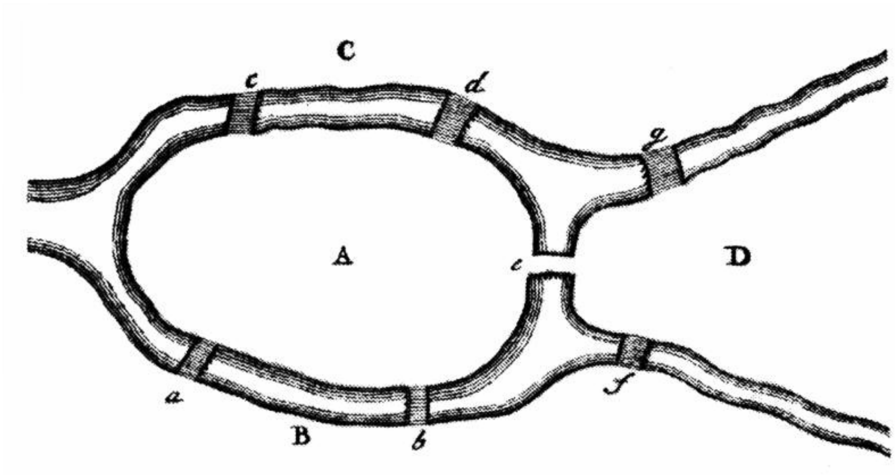
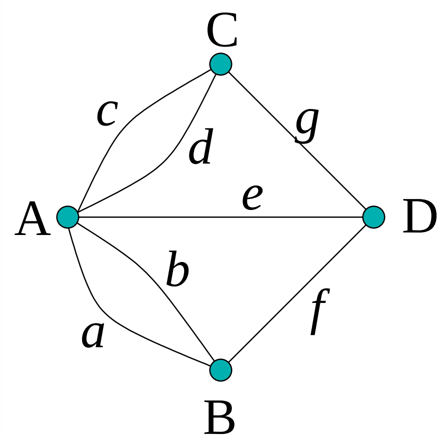
Two old decision problems

Eulerian circuits (1736)

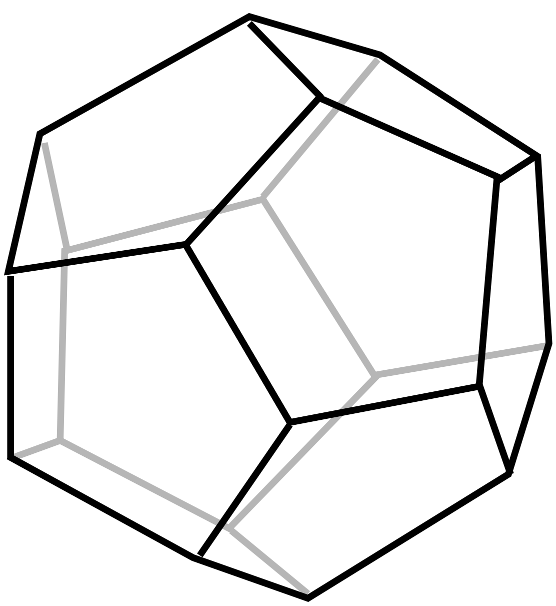


The seven bridges of Könisberg

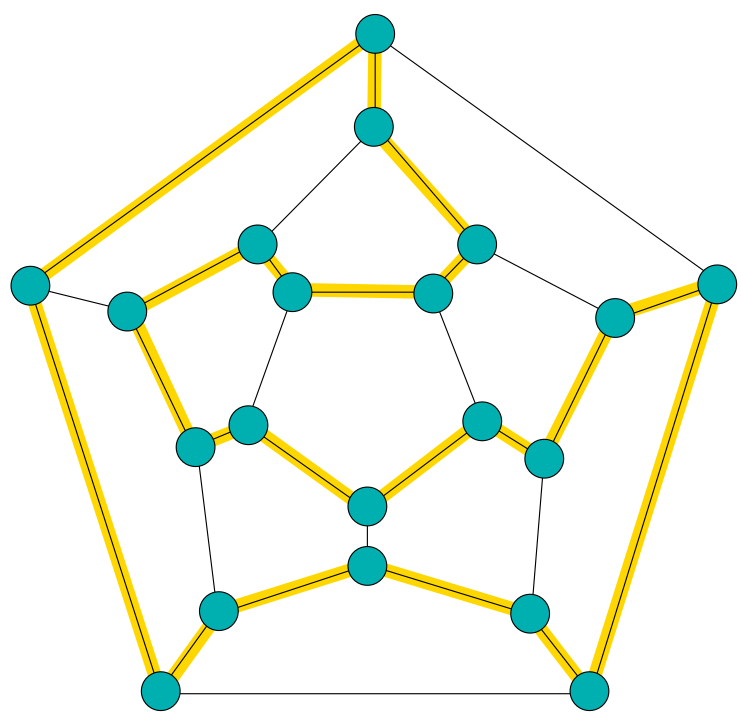


The equivalent graph

Hamiltonian cycles (1859)



The dodecahedron



The equivalent graph

Computer Science: computational complexity

Classifying problems according to the computational resources required for their solution (e.g. CPU time and memory) in the worst case.

tractable (in P) $\leftrightarrow$ sub-exponential: $\ln(N)$, N^α
intractable (in NP) $\leftrightarrow$ exponential: 2^N, $N!$

N is the number of variables in the problem.

Main Complexity Classes

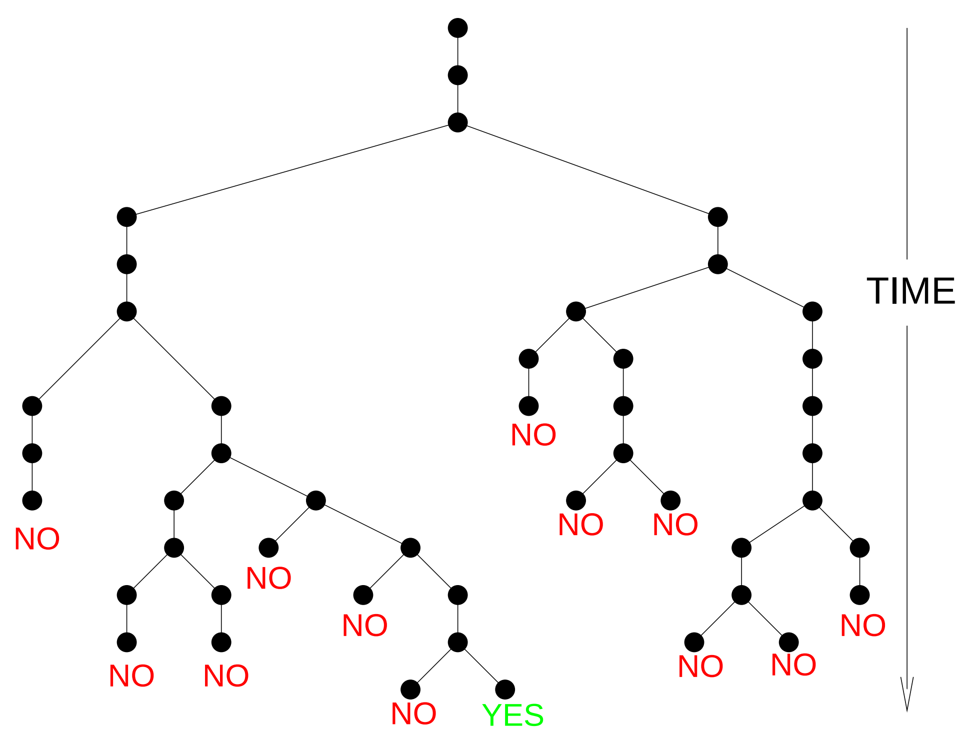
P = polynomial
NP = non-deterministic polynomial

$\Downarrow$

- non-determ. algorithms: `goto both`
- succinct certificate

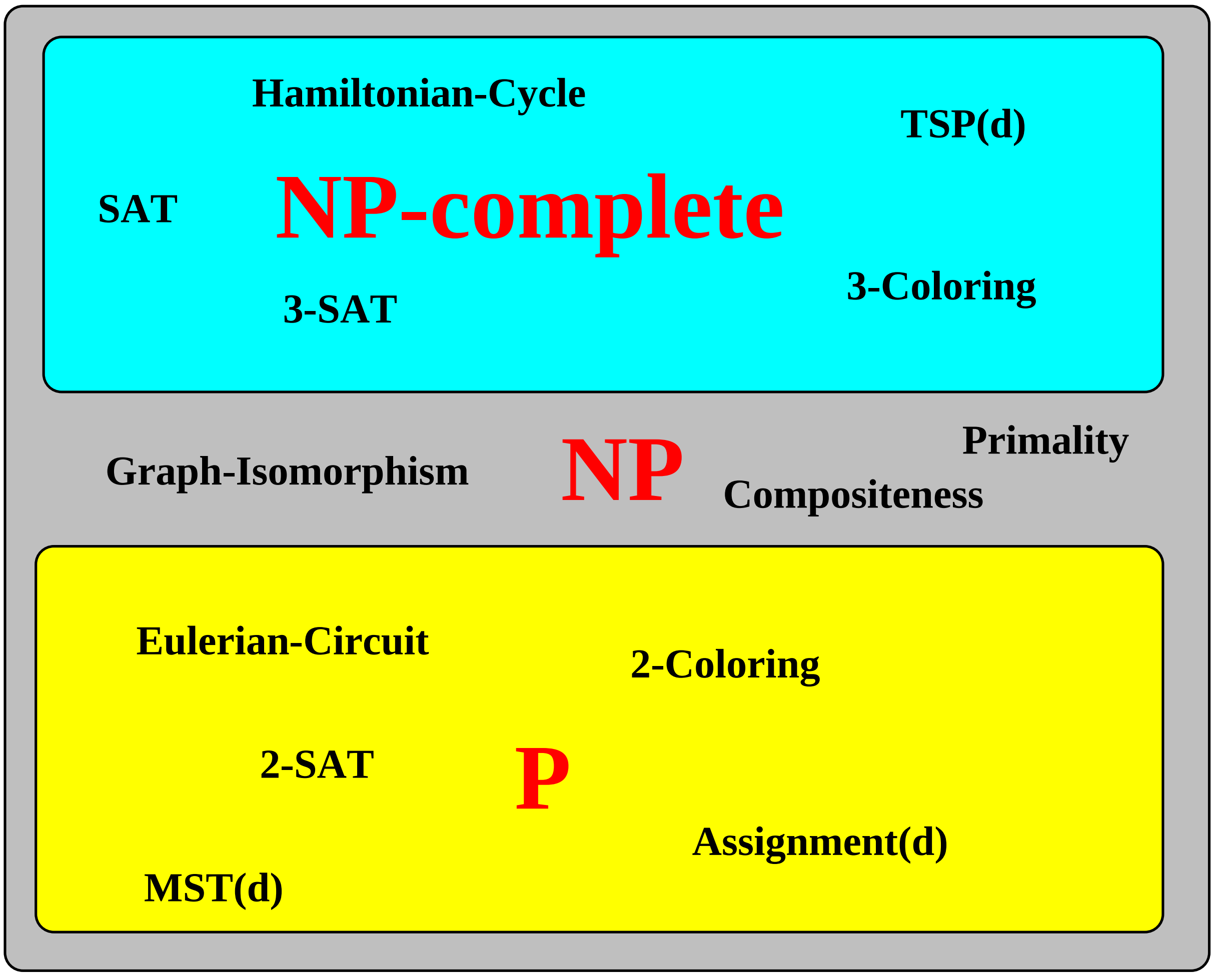
P = NP ?
First Millennium Prize Problem

Quantum computation !



THEOREM: All problems in NP are polynomially reducible to K-SAT ($K > 2$). (Cook, 1971)

NP-complete are the hardest **NP** problems.



Beyond NP

- $\left\{ \begin{array}{l} \text{decision} \\ \text{evaluation} \\ \text{optimization} \end{array} \right\}$ problems (NP-hardness)
- counting problems (#P,#P-complete): e.g. #SAT counts the entropy of SAT.

Some interesting problems

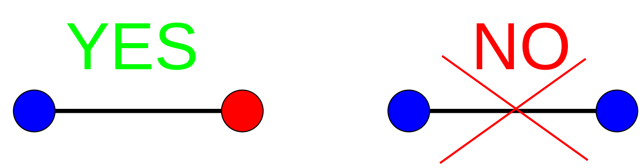
SAT

Boolean variables: $x_i \in \{0,1\} \quad i = 1,\ldots,N$
Logical operators: $\bar{\cdot}$ = NOT, $\vee$ = OR, $\wedge$ = AND
Given a Boolean formula like
$(x_1 \vee x_{27} \vee \bar{x}_3) \wedge (\bar{x}_{11} \vee x_2) \wedge \ldots \wedge (\bar{x}_{21} \vee x_9 \vee \bar{x}_8 \vee \bar{x}_{30})$
decide if a satisfying truth assignment exist

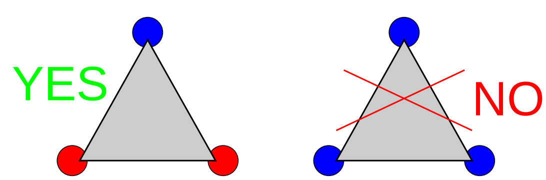
Random 3-SAT: 3 random literals per clause
clauses = αN

Coloring

q-coloring on graphs:
2-coloring $\in$ P
3-coloring $\in$ NP-c



Bicoloring on hypergraphs:
NP-complete



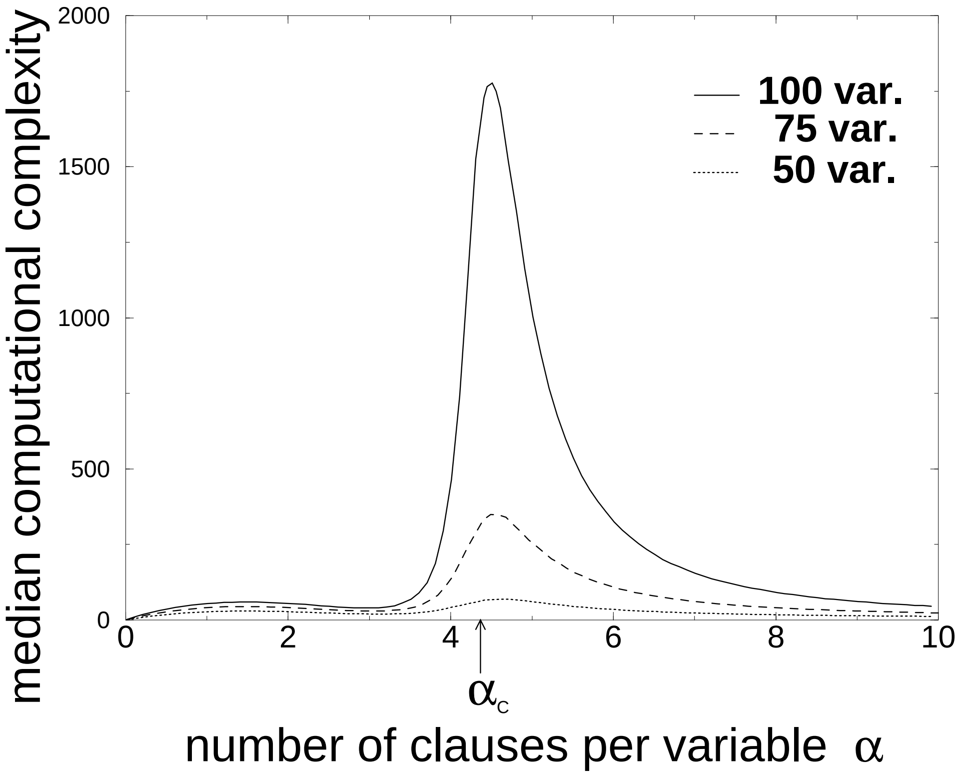
Computer Science	Physics
K-SAT	Diluted Ising Spin Glasses
Graph Coloring	Potts Models
Vertex Cover	Hard Spheres
...	...

Worst-case vs. Typical-case

Real-world NP-complete and #P-complete problems may have many easy instances

Ensemble of random NP-complete problems hard on average (e.g. random 3-SAT)

Random models: phase transitions, NP-hardness



Onset of complexity $\leftrightarrow$ Phase transition

SAT/UNSAT transition: $E = \#$ violated clauses becomes greater than zero.

What makes problems hard close to α_c?

Mapping to a Statistical Mechanics problem

Zero temperature limit of a diluted mean-field spin model. Much harder than usual fully connected!

For random 3-SAT, with $s_i = (-1)^{x_i}$,

$$\mathcal{H} = \frac{1}{8}\left(\alpha N - \sum_{i=1}^{N} H_i s_i + \sum_{i<j} T_{ij} s_i s_j - \sum_{i<j<k} J_{ijk} s_i s_j s_k\right)$$

$$\begin{aligned} H_i &= \textstyle\sum_\ell \Delta_{\ell,i} \\ T_{ij} &= \textstyle\sum_\ell \Delta_{\ell,i}\Delta_{\ell,j} \\ J_{ijk} &= \textstyle\sum_\ell \Delta_{\ell,i}\Delta_{\ell,j}\Delta_{\ell,k} \end{aligned} \qquad \Delta_{\ell,i} = \begin{cases} 1 & \text{if} \quad \bar{x}_i \in C_\ell \\ -1 & \text{if} \quad x_i \in C_\ell \\ 0 & \text{otherwise} \end{cases}$$

For 3-hyper-SAT also known as 3-XOR-SAT

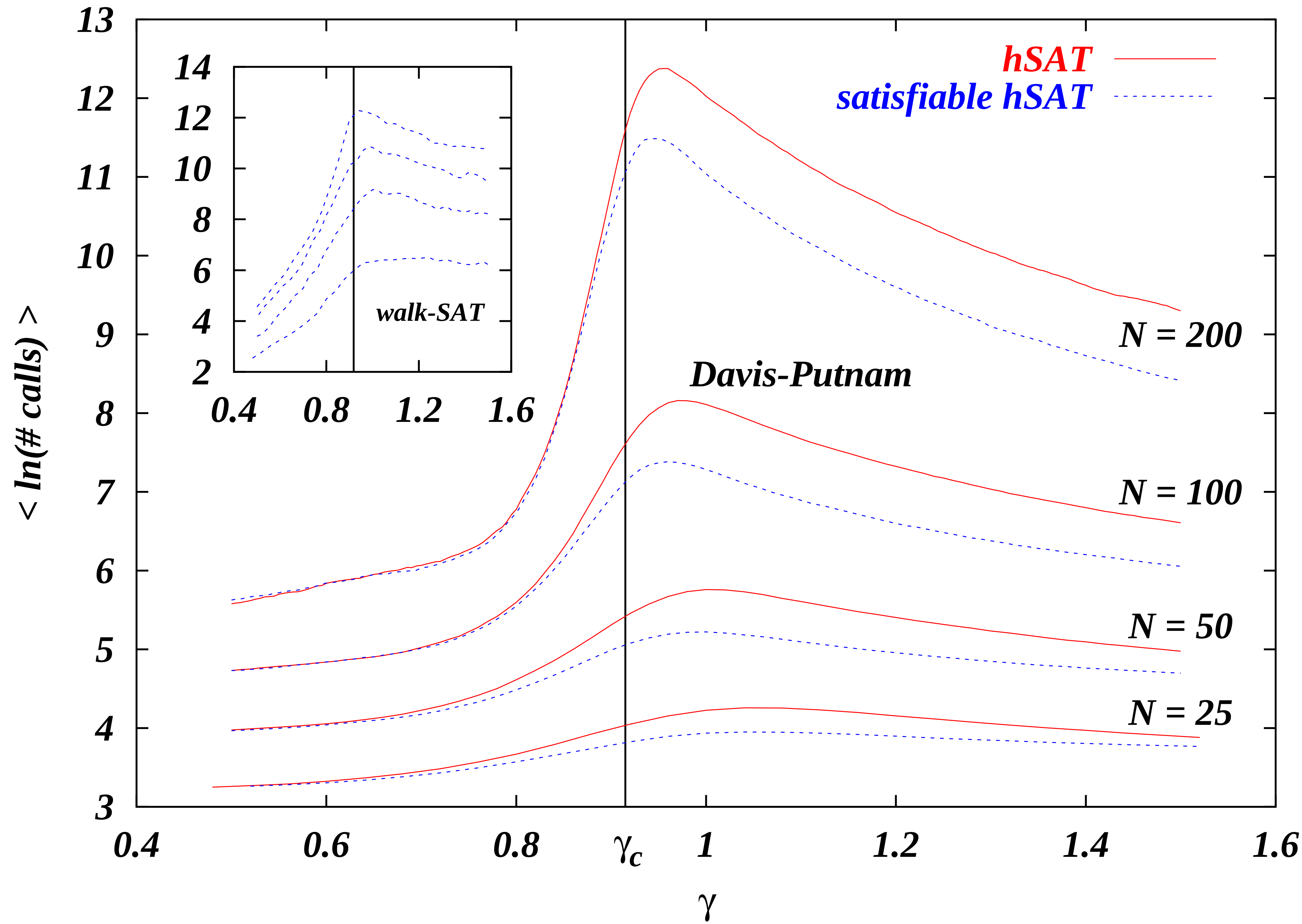
$$F = (x_2 \oplus x_{15} \oplus x_{33}) \wedge \ldots \wedge (\bar{x}_4 \oplus \bar{x}_{21} \oplus \bar{x}_9)$$

$$\mathcal{H} = \frac{1}{2}\left(\gamma N - \sum_{\{i,j,k\}\in G} J_{ijk}\, s_i\, s_j\, s_k\right)$$

$$G = \{\text{set of } \gamma N \text{ random triples}\}$$

Two versions:

- unfrustrated, ferromagnetic: $J_{ijk} = 1$
  $\rightarrow$ 1st order ferromagnetic transition
- frustrated, 3-spin glass: $J_{ijk} = \pm 1$
  $\rightarrow$ SAT/UNSAT transition



hSAT
satisfiable hSAT
Davis-Putnam
walk-SAT
N = 200
N = 100
N = 50
N = 25
< ln(# calls) >
γ
γc

Diluted 3-spin models

Defined by the following Hamiltonian

$$\mathcal{H} = \frac{1}{2}\left(\gamma N - \sum_{\{i,j,k\}\in G} J_{ijk}\, s_i\, s_j\, s_k\right)$$

G is a set of γN random triples (**the hypergraph**).

Two kinds of hypergraphs:

- fixed connectivity C
  every index must appear C times and $\gamma = \frac{C}{3}$
- fluctuating connectivity (Poisson distrib.)
  every plaquette is chosen with prob. $\frac{\gamma N}{\binom{N}{3}}$

The model and the results can be generalized to any connectivity distribution and to any p-spin interacting terms (with $p > 2$).

Two versions of the model:

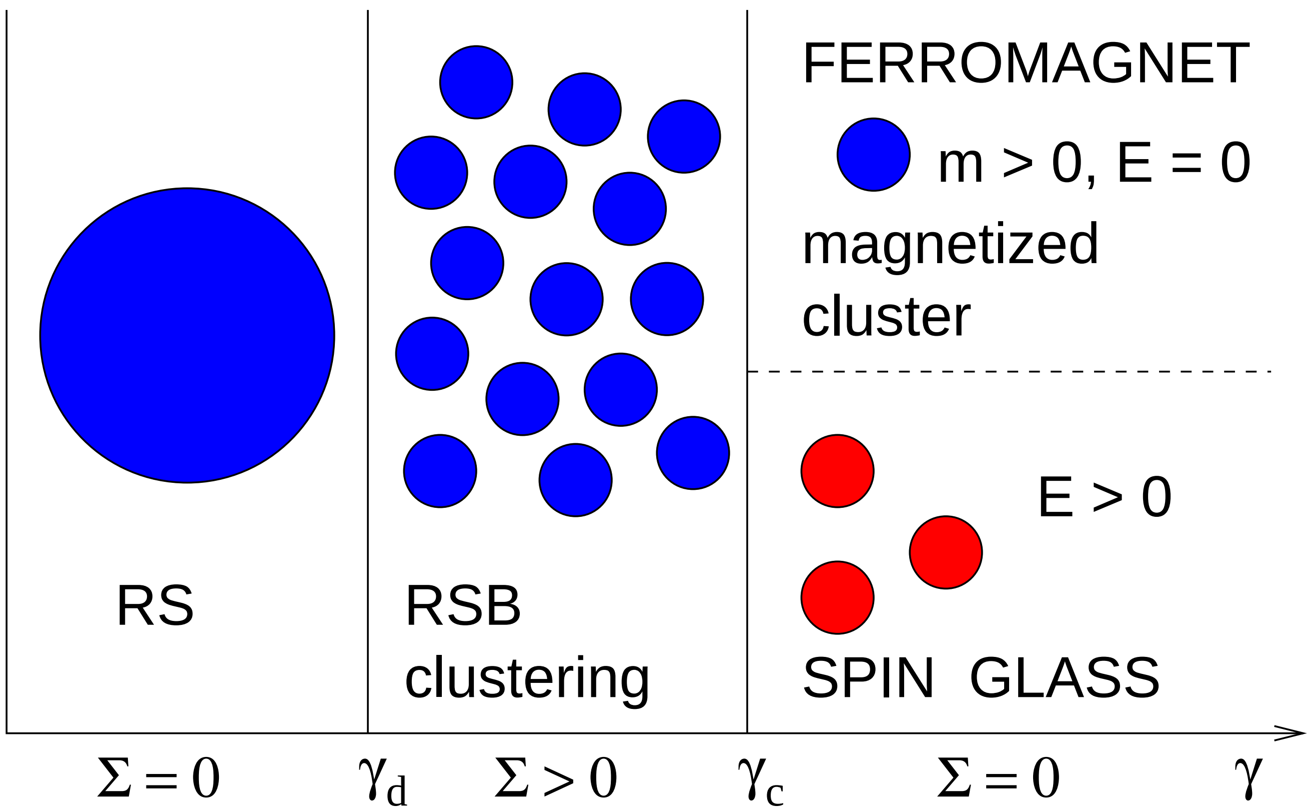
- unfrustrated, ferromagnetic: $J_{ijk} = 1$
  $\rightarrow$ 1$^{\text{st}}$ order ferromagnetic transition
- frustrated, spin glass: $J_{ijk} = \pm 1$
  $\rightarrow$ SAT/UNSAT transition

Both versions have a glassy phase!

Zero-temperature phase diagram

Any $p > 2$ and fluctuating connectivity hypegraphs.

Analytic solution and numerics:
if $E = 0$ (no frustration) $\rightarrow$ Gaussian elimination
if $E > 0$ $\rightarrow$ exhaustive enumerations

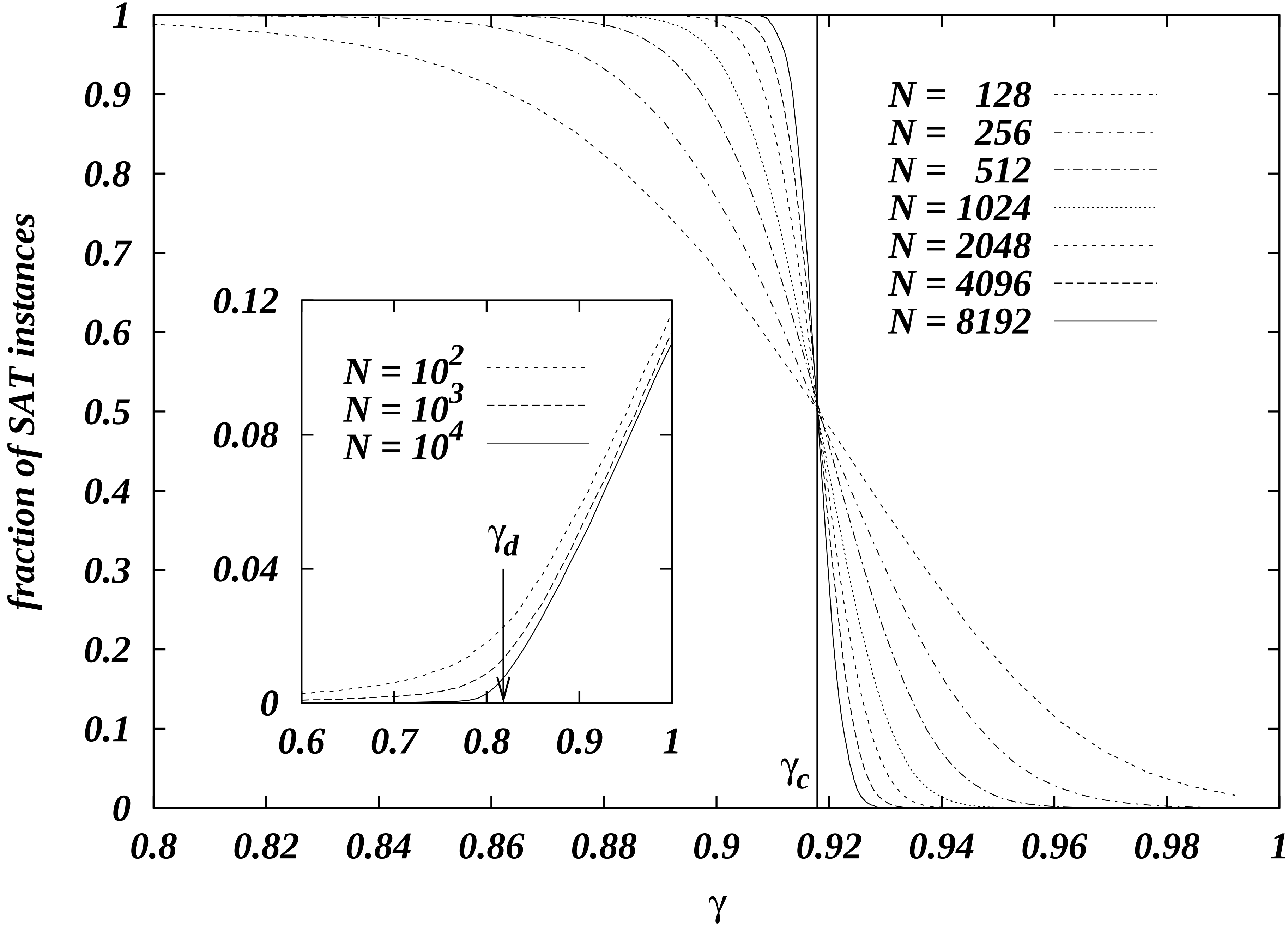


Configurational entropy: $\Sigma(\gamma) = \frac{1}{N} \ln(\#\ \text{clusters})$

A common problem

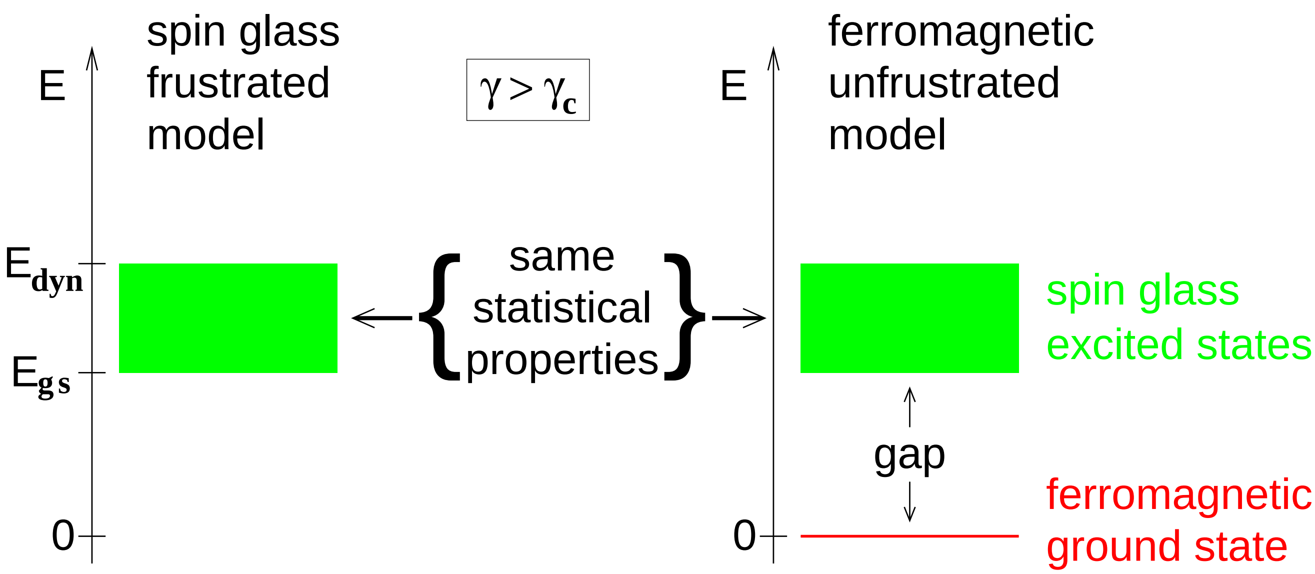
- diluted p-spin glass at $T = 0$
- random p-XOR-SAT §
- low density Parity Check codes
- random linear systems in finite fields (GF[2])

§ considered an open problem in theoretical computer science



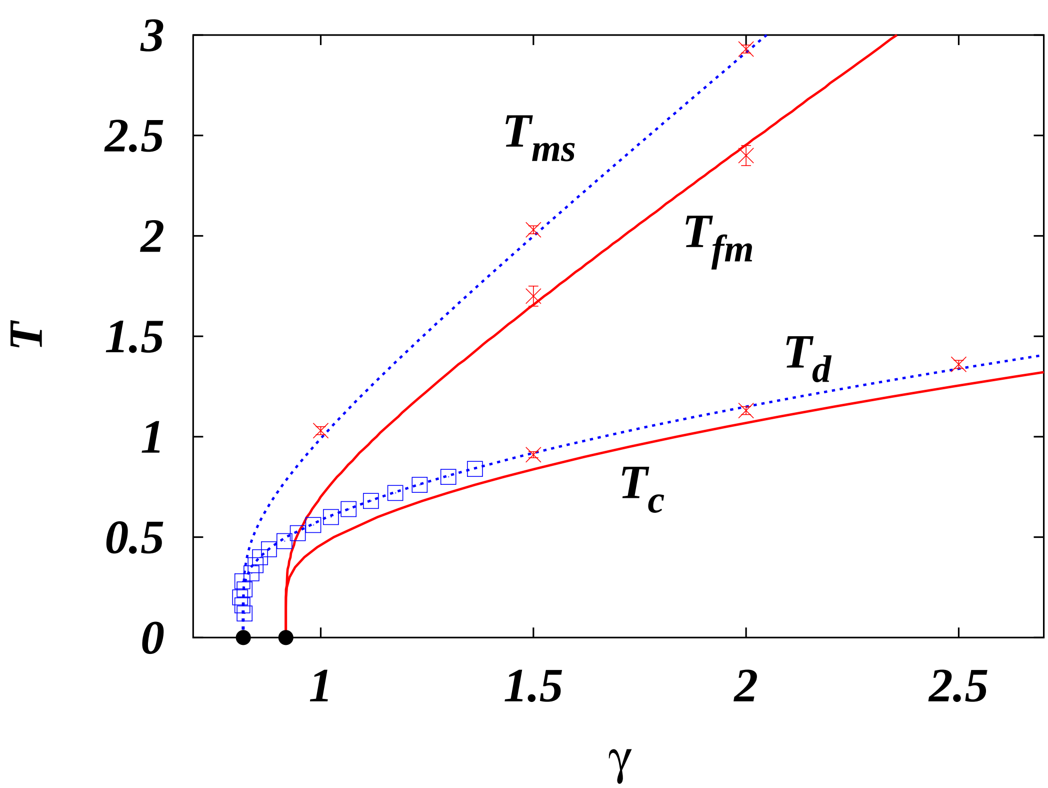
fraction of SAT instances
γ
γ_c
γ_d
N = 128
N = 256
N = 512
N = 1024
N = 2048
N = 4096
N = 8192
$N = 10^2$
$N = 10^3$
$N = 10^4$

The structure of the configurational space



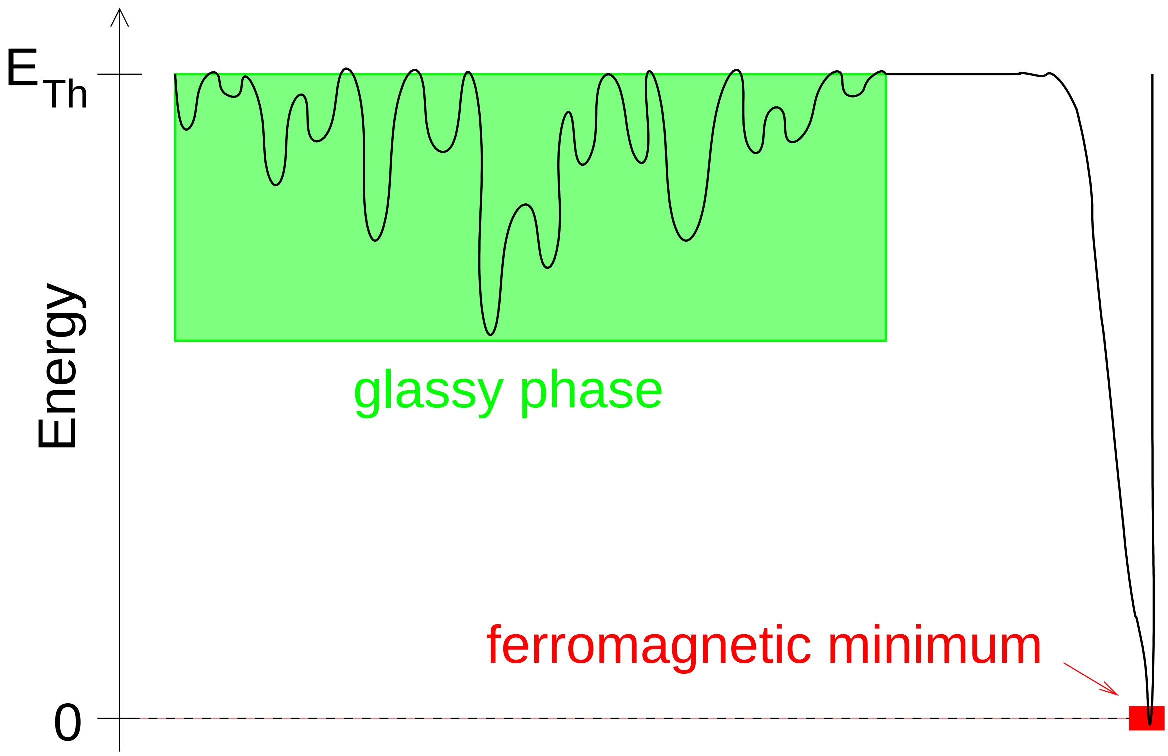
Starting from a random configuration, both models have the same off-equilibrium dynamics

Phase diagram



T is the temperature and 3γ is the average connectivity

Static and dynamic limits do not coincide!

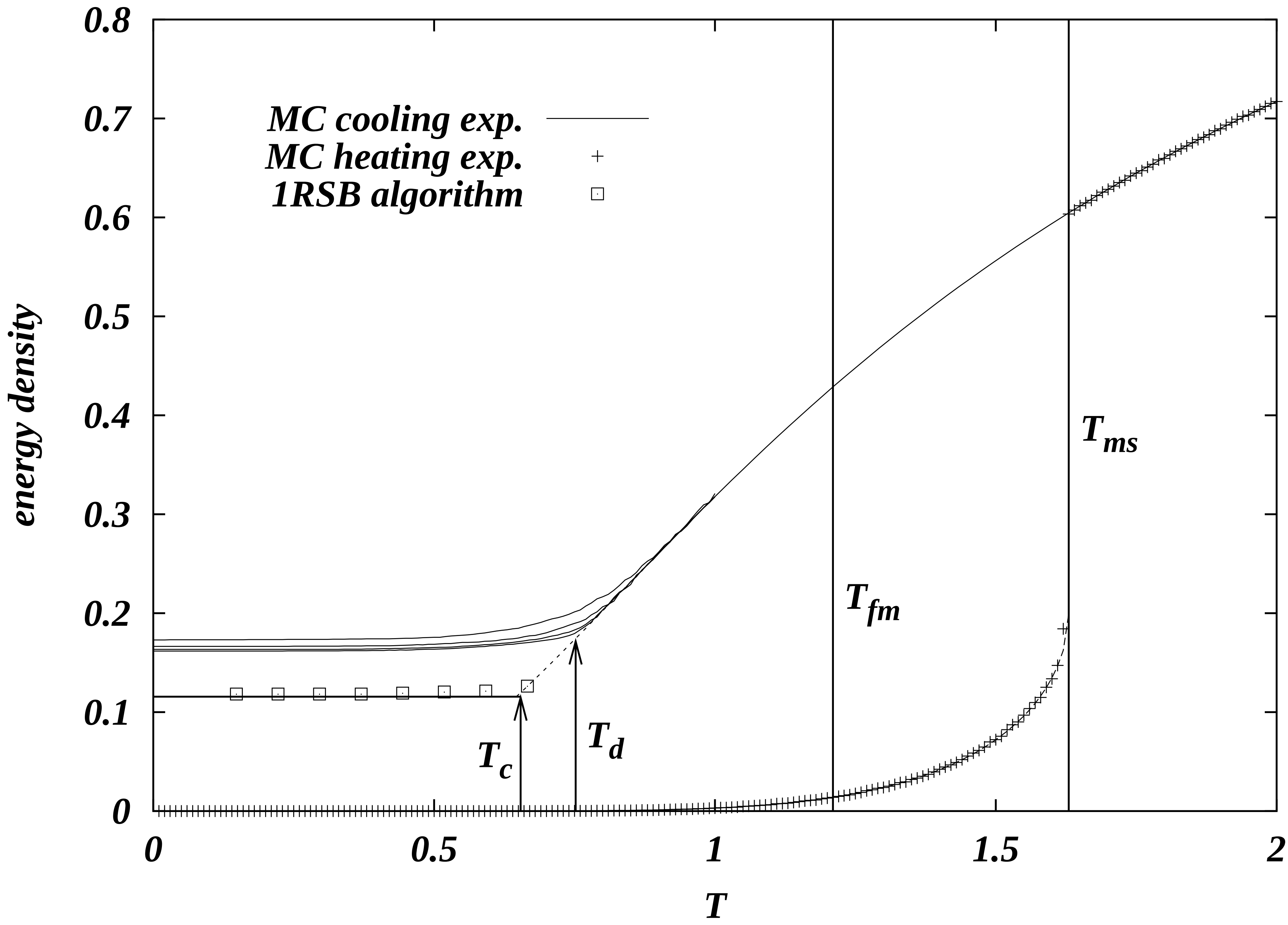


- Static limit: $t \to \infty$ before $N \to \infty$

For any finite size and for any ergodic dynamics the system relaxes to the ferromagnetic minimum (in a time which is exponentially large in N).

- Dynamic limit: $t \to \infty$ after $N \to \infty$

For an infinite sized system the time to escape from a metastable state is infinite and thus the system relaxes to the higher energy (E_{Th}) metastable state and get trapped there forever.



MC cooling exp.
MC heating exp.
1RSB algorithm
energy density
T
T_c
T_d
T_fm
T_ms
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0
0.5
1
1.5
2

Conclusions and perspectives

New results

• p-spin ($p > 2$) with fluctuating connectivity

→ structure of the configurational space: γ_d, γ_c and $\Sigma(\gamma)$

→ γ_c is the exact threshold for random p-XOR-SAT

→ new transitions in random hypergraphs

• p-spin ($p > 2$) and Bicoloring with fixed connectivity

→ exact 1-RSB solution: GS energy

• K-SAT and Bicoloring

→ variational bounds for α_c (at present the best!)

→ very good benchmark for SAT solvers

Some applications

• test-bed for heuristic algorithms: GS energy

• dynamical transitions in Coding and Cryptography

• solvable models for glassy systems and granular matter

Examples of open issues

• complete 1-RSB and FRSB theories (with correlations)

• out of equilibrium dynamics

• analysis of randomized algorithms

• better analysis of the configurational space in K-SAT

Some references

- Simplest introduction to Computational Complexity:
  S. Mertens, *"Computational Complexity for Physicists"*, cond-mat/0012185.

- NP-completeness and Computational Complexity:
  M.R. Garey and D.S. Johnson, *"Computers and Intractability. A guide to the theory of NP-completeness"* (Freeman, San Francisco, 1979).
  C.H. Papadimitriou, *"Computational Complexity"* (Addison-Wesley, Reading, MA, 1994).

- Phase transition in K-SAT:
  S. Kirkpatrick and B. Selman, Science **264**, 1297 (1994).

- Statistical Mechanics of K-SAT:
  R. Monasson and R. Zecchina, Phys. Rev. Lett. **76**, 3881 (1996); Phys. Rev. E **56**, 1357 (1997).

- Typical-case complexity:
  R. Monasson, R. Zecchina, S. Kirkpatrick, B. Selman and L. Troyansky, Nature **400**, 133 (1999).

- Hyper-SAT:
  F. Ricci-Tersenghi, M. Weigt and R. Zecchina, Phys. Rev. E **63**, 026702 (2001).

- 3-spin at finite temperatures:
  S. Franz, M. Mézard, F. Ricci-Tersenghi, M. Weigt and R. Zecchina, Europhys. Lett. **55**, 465 (2001).

- Exact solution for 3-spin at $T = 0$:
  S. Franz, M. Leone, F. Ricci-Tersenghi and R. Zecchina, Phys. Rev. Lett. **87**, 127209 (2001).