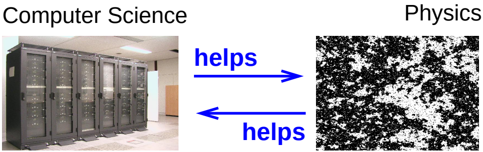
Blocking of motorways, guarding museums and other problems from computational physics

A.K. Hartmann

Institute for Physics, University of Oldenburg

Oldenburg, 12. November 2007

Outline



- How I got to Oldenburg
- Overview over research group
- Ground states of random-field systems
  “How to disrupt a motorway network”
- Phase transitions in the vertex-cover problem
  “How to guard a museum”

[AKH and H. Rieger, *Optimization Algorithms in Physics*, Wiley-VCH 2001]

[AKH and H. Rieger (eds.), *New Optimization Algorithms in Physics*, Wiley-VCH 2004]

[AKH and M. Weigt, *Phase Trans. in Combinatorial Opt. Problems*, Wiley-VCH 2005]

Were do I come from ?

1968 Heidelberg *

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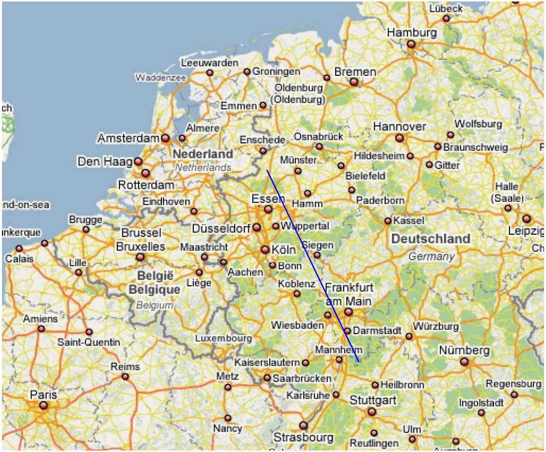

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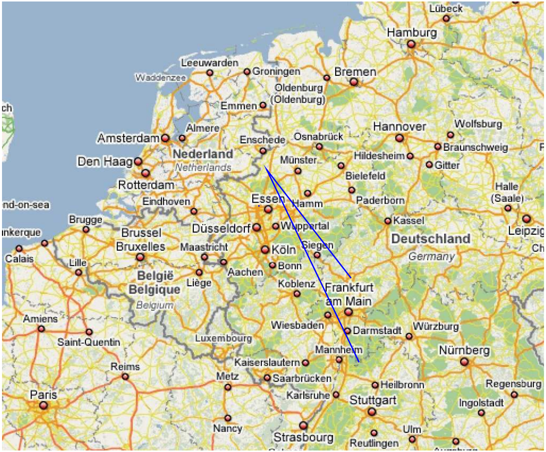

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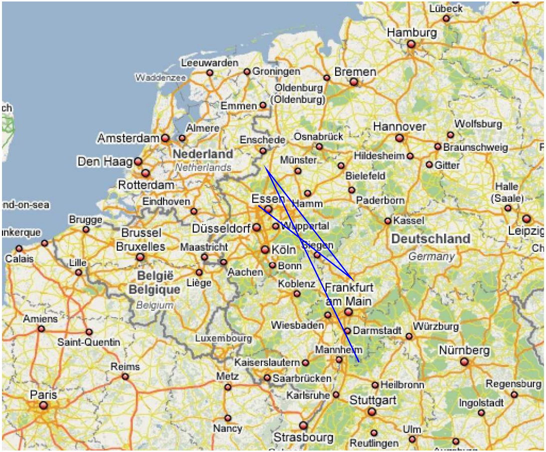

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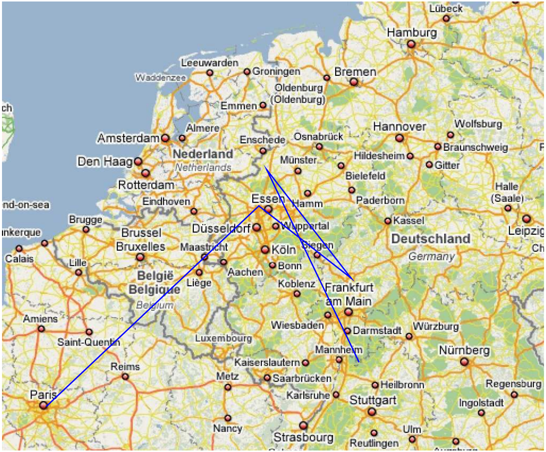

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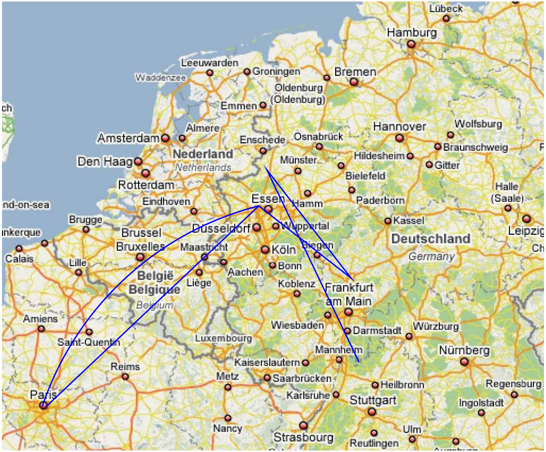

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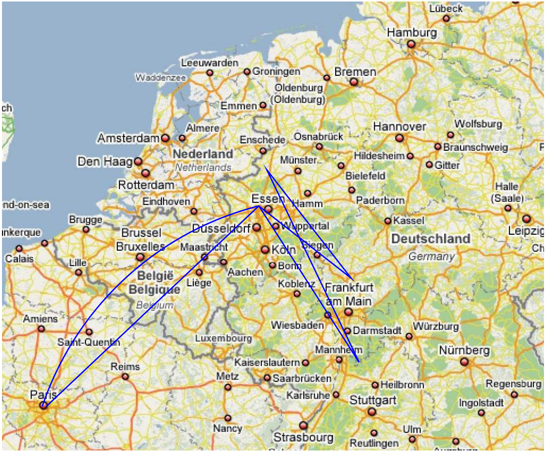

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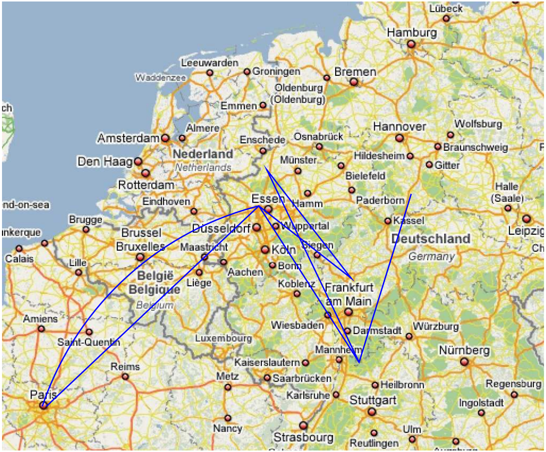

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2007 Oldenburg

Why studying physics?

- (1980)
  I want to be a film director!

  ⇒ save money for
  super 8 film camera

Why studying physics?

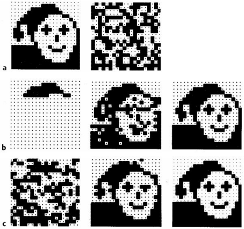
- (1980)
  I want to be a film director!

  $\Rightarrow$ save money for
  super 8 film camera

- (1982)
  Money is available!
  BUT: Computers are great!
  $\Rightarrow$ buy DRAGON 32

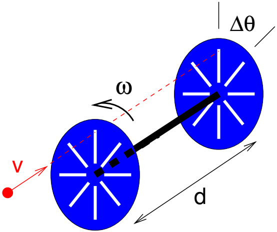
  almost NO games !
  $\Rightarrow$ write programs myself

- (1985) Spectrum der Wissenschaft: paper on neural networks
  Simulation on Dragon 32:
  works well!
  $\Rightarrow$ system $>$ Σ constituents!



- (1986) Nice physics classes
  exam: find “new” velocity filters
  1. possible!
  2. derive equation
  3. equation is simple:

$$d/v = n \cdot \Delta\Theta/\omega$$



- Computer Sience $=$ data bases, operation systems, etc. ?
  $\Rightarrow$ no surprises $\Rightarrow$ study Physics (1987)

Computational Physics Group

Björn Ahrens

Taha Yasseri (Gö)

Kristian Marx (Gö)

some former members (also on picture):
Magnus Jungsbluth, Martin Zumsande, Emmanuel Yewande
guest (DAAD): Konstantin Nefedev (autumn 2007)

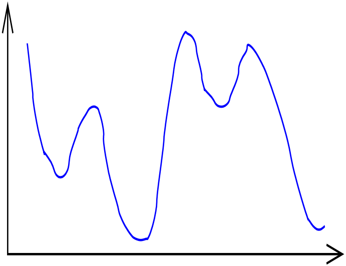
What are we doing?

"Computational Theoretical Physics"

Large scale computer simulations
new algorithms

[Paderborn Parallel Computing Center]

Optimization algorithms
development/applications
systems with 10^6 particles



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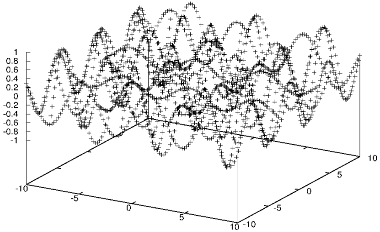


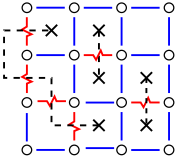
systems with 10^6 particles

Disordered magnets

Spin glasses

Random-field systems

(B. Ahrens, O. Melchert)

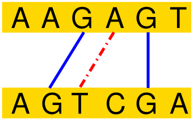


Bioinformatics

RNA secondary structures

Sequence alignment

(B. Burghardt, S. Wolfsheimer)

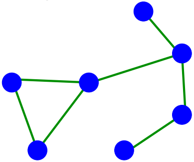


Phase transitions in optimization problems

Vertex cover

Satisfiability

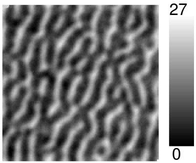
(A. Mann)



Surface Physics

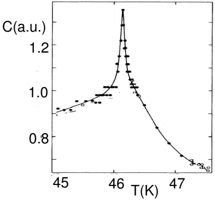
Sputtering

Pattern formation (T. Yasseri)



Random-field Ising magnets (RFIM)

- Ordered systems (lattices): well understood
  real world: disorder $\rightarrow$ make (sometimes) strong difference
- Experiments with DAFF
  specific heat $\rightarrow$ phase transition:
  $C(T) \sim \log|(T - T_c)/T_c|$
  ordered system ($d = 3$):
  $C(T) \sim |(T - T_c)/T_c|^{-\alpha}$ ($\alpha = 0.1$)



[D.P.Belanger et al., 1983]

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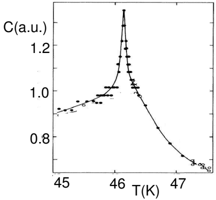
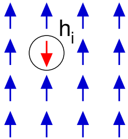


[D.P.Belanger et al., 1983]

- Model for random magnets (d-dim. lattice):
  Ising spins $\sigma_i = \pm 1$ with local fields h_i.
  $$H = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j - \sum_i h_i\sigma_i$$
  h_i: Gauss distributed (width h)



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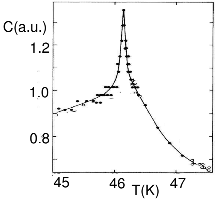

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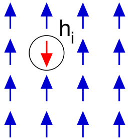
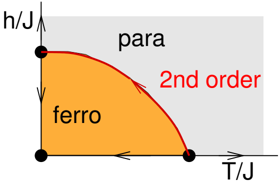


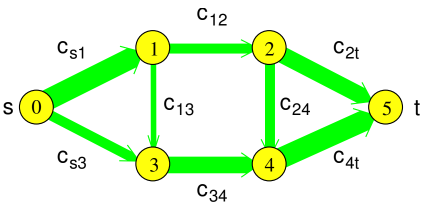
- Phase diagram →

Aim:
Calculate ground states ($T = 0$)
of large systems



Networks

- Idea: mapping of RFIM $\leftrightarrow$ network



- Network = graph + edge capacities:
  $G = (V, E)$, $E \subset V \times V$
  $c_{ij} > 0$, $s, t \in V$
- Now: network $\rightarrow$ RFIM

- Much transit traffic in Austria
$\longrightarrow$ blockade 25. October 2002

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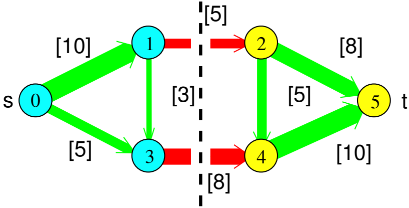
  $\rightarrow$ blockade 25. October 2002

- Cut street network into $(S, \overline{S})$
  $S \cup \overline{S} = V, S \cap \overline{S} = \emptyset,$
  $s \in S, \quad t \in \overline{S}$



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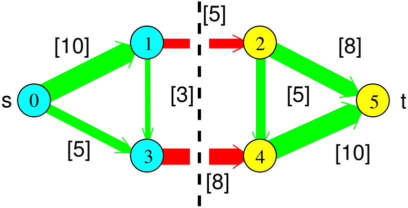

- People needed to block:
  $\sim$ capacity of cut

$$C(S, \overline{S}) = \sum_{i \in S, j \in \overline{S}} c_{ij} \, .$$

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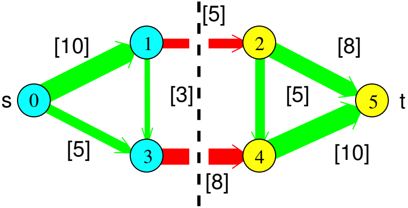

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- With $\underline{X} = (x_0, \ldots, x_{n+1})$, $x_i = 0/1$, $x_i = 1 \Leftrightarrow i \in S$
  [J.-C. Picard and H.D. Ratliff, Networks 1975]

$$C(\underline{X}) = \sum_{ij} c_{ij} x_i (1 - x_j) = -\sum_{ij} c_{ij} x_i x_j + \sum_i (\sum_j c_{ij}) x_i$$

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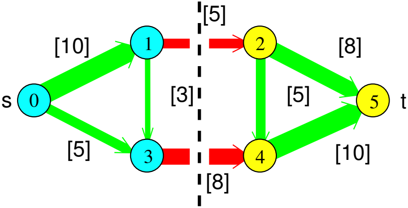

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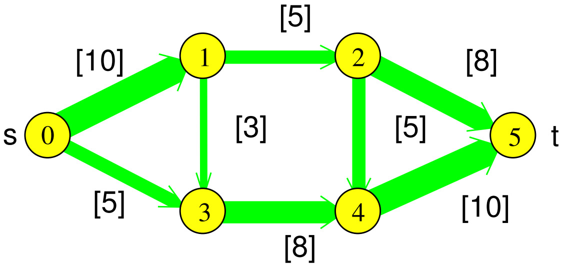
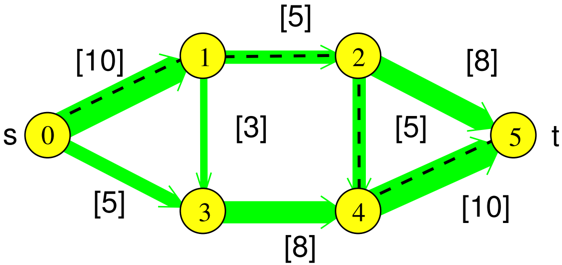
- Minimum energy = capacity of min. cut = max. flow

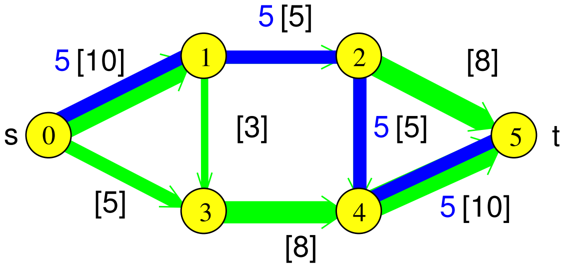
- Calculate maximum flow: Ford-Fulkerson algorithm (1956)



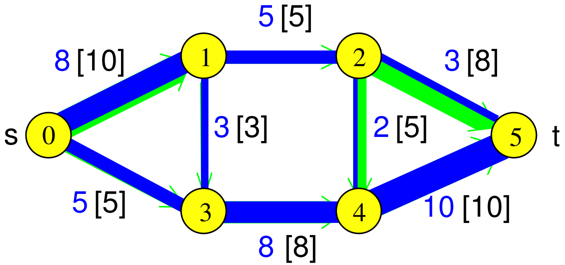
- Calculate maximum flow: Ford-Fulkerson algorithm (1956)



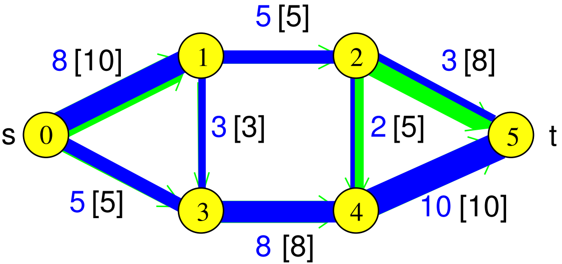
- Calculate maximum flow: Ford-Fulkerson algorithm (1956)



- Calculate maximum flow: Ford-Fulkerson algorithm (1956)



- Calculate maximum flow: Ford-Fulkerson algorithm (1956)



- Modern algorithms (computer science): concurrent flow increments

  [R.E. Tarjan, *Data Struc. + Netw. Algorithms* 1983]

  [A.V. Goldberg, 1988-1998]

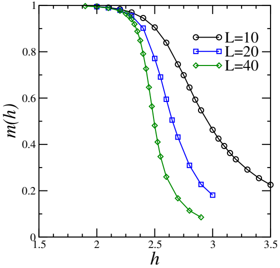
  parallel algorithms

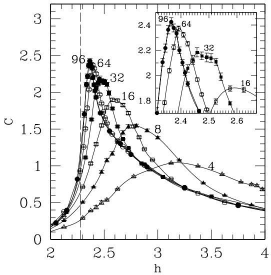
  [R. Anderson and J.C. Setubal, J.Parall.Distr.Comp. 1995]

- Exact ground state of large systeme, e.g. with 100^3 spins.

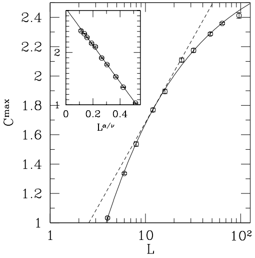
Results

- New methods to calculate physical quantities ↓
- Average Magnetization   Specific heat



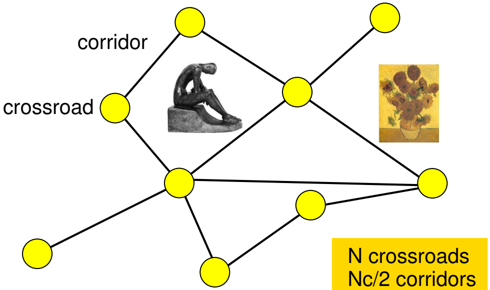


- Height of maxima
  no divergence
  $C^{\max}(L) = C_{\max} + a_2 L^{\alpha^\star/\nu}$
  $\rightarrow \alpha = 0$ $(\alpha^\star = -0.6)$
  $C_{\max} = 2.84(5)$
  [AKH & A.P. Young, Phys. Rev. B, 2001]
  but from experiments: $\log L$



Vertex-Cover Problem

- Prototypical problem of theoretical Computer Science
- Museum



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  ARE
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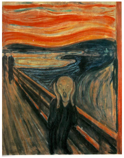
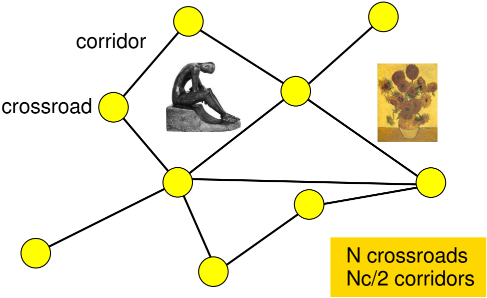


Edvard Munch's "Der Schrei" stolen in Oslo August 2004



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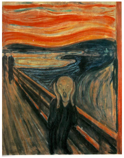

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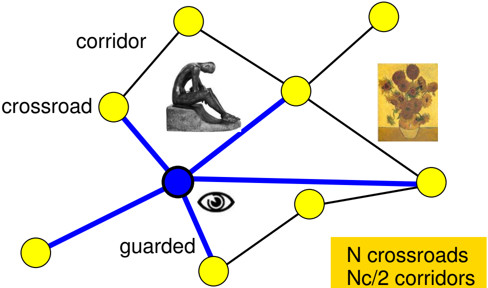

$X = xN$ guards
guard only adjacent corridors

Vertex-Cover Problem

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- Museum
  ARE
  THEY
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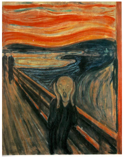

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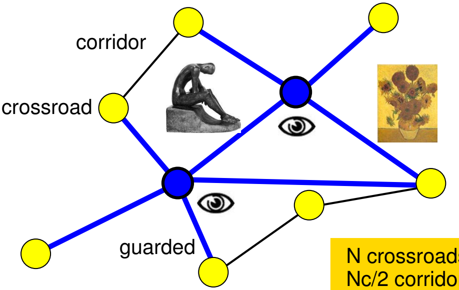
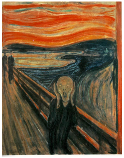


N crossroads
Nc/2 corridors

$X = xN$ guards
guard only adjacent corridors

Vertex-Cover Problem

- Prototypical problem of theoretical Computer Science
- Museum ARE THEY SAFE?



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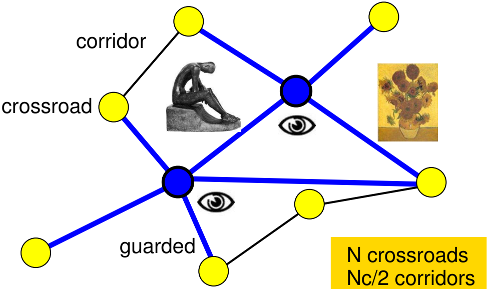


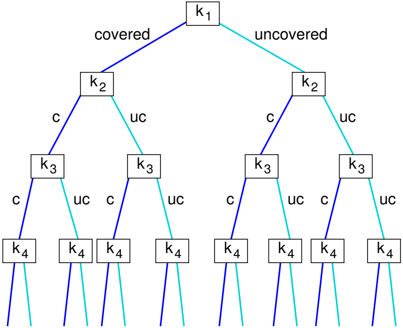
$X = xN$ guards
guard only adjacent corridors

- Mathematically: museum = graph $G = (V, E)$
  Vertex cover $A \subset V : \forall (i, j) \in E : (i \in A) \vee (j \in A)$
- Decision problem: all corridors guardable w. X guards?
  Optimization problem: minimize number of unguarded corr.
- Vertex-cover problem = NP-complete

Branch-and-bound algorithm

Task: min. # of uncov. edges

Complete algorithm:
(basically) enumerate all states



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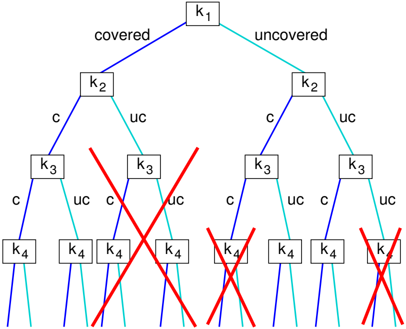
Complete algorithm:
(basically) enumerate all states



Avoid subtrees w/o solutions

$best$ $=$ minimum so far

X' $=$ # of curr. covered vertices

$\Rightarrow$ cover $F := X - X'$ vertices

List F vertices with highest current degrees. Ex. ($F = 3$):

n_1: 5 edges
n_2: 3 edges
n_3: 3 edges

---

n_4: 2 edges
n_5: 2 edges
$\dots$

$d_{\max} \equiv \sum_{i=1}^{F} d(n_i)$

If (#(uncovered edges)$-d_{\max}$ $>$best) $\rightarrow$ bound!

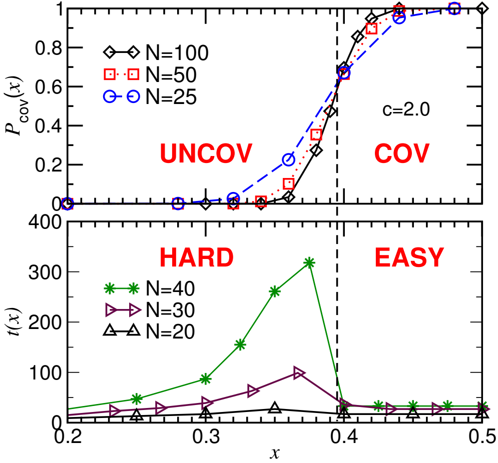
Phase transition

- Ensemble: Erdös-Rényi random graphs:
  N vertices and $cN/2$ random edges
- Numerically: averaging over different realizations
- $c = 2$

  Probability to cover

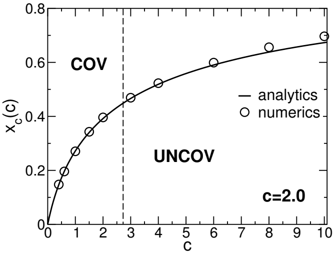
  Running time = number of nodes in branching tree

  [M. Weigt and AKH, Phys. Rev. Lett. 2000]



Phase diagram

- Analytical treatment: $\Leftrightarrow$ spin-glass or hard-core gas
  Stat. Mech. methods:
  replica trick/cavity approach
  $\rightarrow$ phase diagram $x_c(c)$,
  exact for $c \leq e \approx 2.718$
  [M. Weigt & AKH, PRE 2001]



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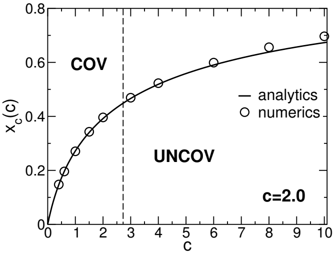
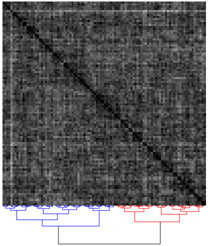
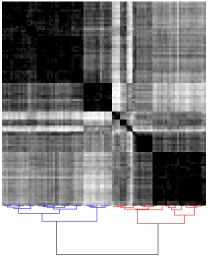


- Many solutions $\rightarrow$ cluster structure ?

$c = 2$



$c = 6$

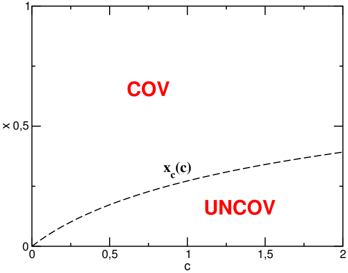


[W. Barthel & AKH,
Phys. Rev. B 2004]

Number of clusters grows with N for $c > e$.
Physics: Replica Symmetry Breaking

Running Time

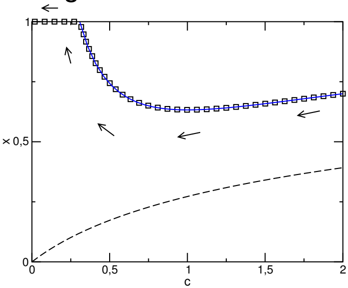
- Aim: analytical calculation of running time
- Phase diagram



Running Time

- Aim: analytical calculation of running time
- Phase diagram

algorithm picks vertices:
moves ($T = 0 \dots N$)
$\longrightarrow$ effective
$x(t = \frac{T}{N}) = \dots$
$c(t = \frac{T}{N}) = \dots$



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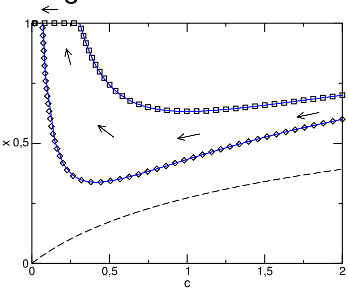

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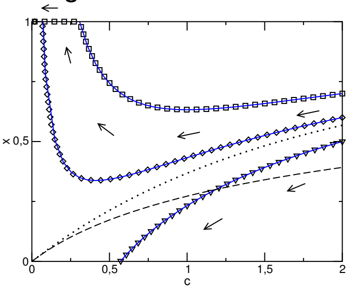

Running Time

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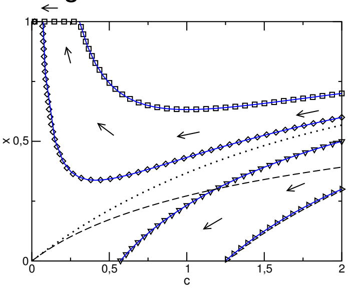

Running Time

- Aim: analytical calculation of running time
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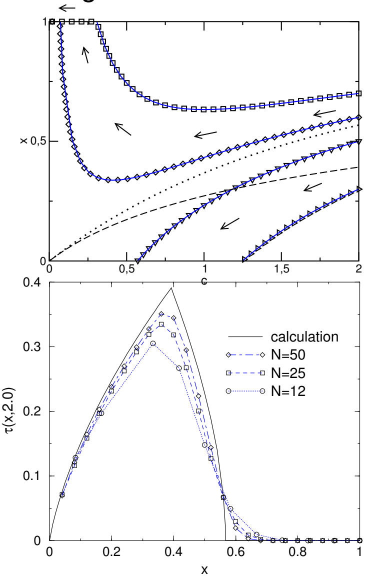
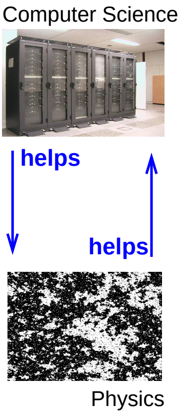


- Uncoverable subproblems:
  full backtracking
  saddle point: entropy
  $\rightarrow$ estimation of running time
  $$t \sim \exp(\tau N)$$

[M.Weigt and AKH,
Phys. Rev. Lett. 2001]

Summary



- Ground states of disordered magnets
  - disorder makes a difference
  - Random-field Ising magnet
  - mapping to max-flow problem $\longrightarrow$ ground state of large systems
  - characterize phase transition
- Vertex-cover problem
  - NP-complete
  - Branch-and-bound algorithm
  - phase-transition in solvability/running time
  - analytical calculation of typical running time

Thank You!

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- Family
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