

Blockierung von Autobahnen, Bewachung von Museen und andere Problemstellungen der computerorientierten Physik

A.K. Hartmann

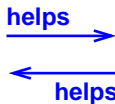
Institute for Physics, University of Oldenburg

Oldenburg, 12. November 2007

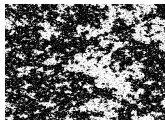


Outline

Computer Science



Physics



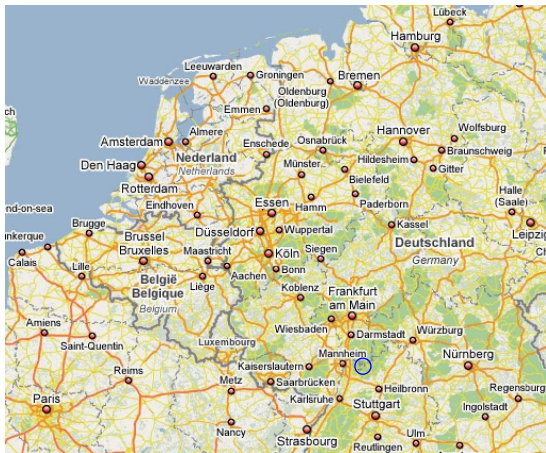
- How I got to Oldenburg
- Overview over research group
- Ground states of random-field systems
“How to disrupt a motorway network”
- Phase transitions in the vertex-cover problem
“How to guard a museum”

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

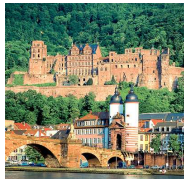
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[AKH and M. Weigt, *Phase Trans. in Combinatorial Opt. Problems*, Wiley-VCH 2005]

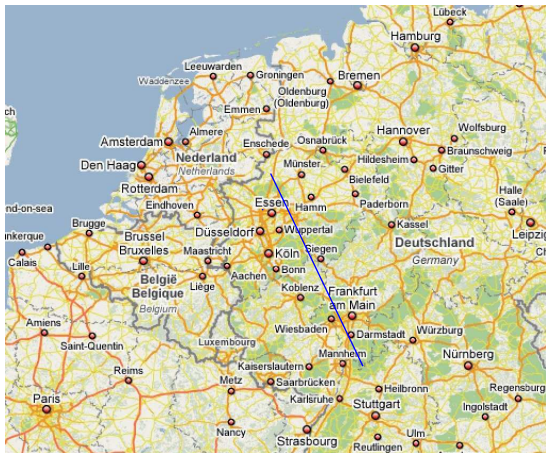
Were do I come from ?



1968 Heidelberg *



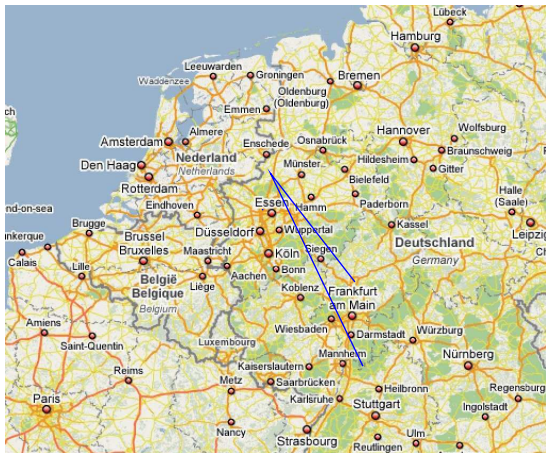
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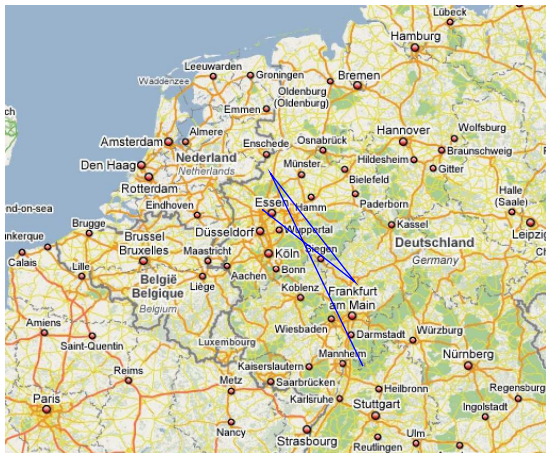
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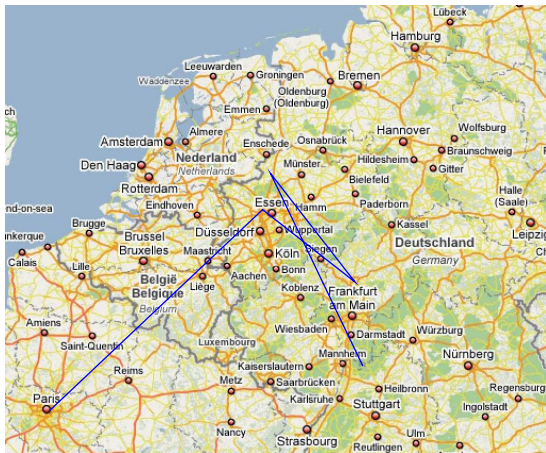
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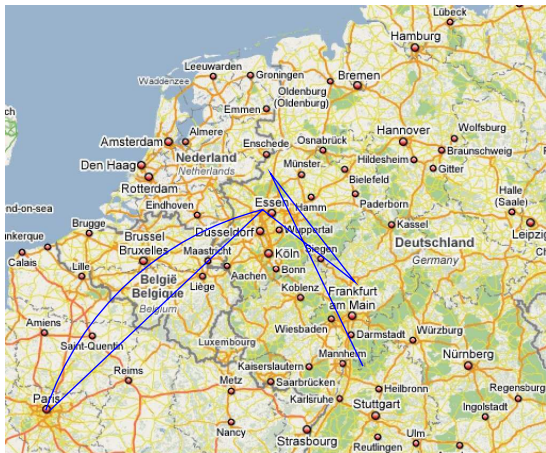
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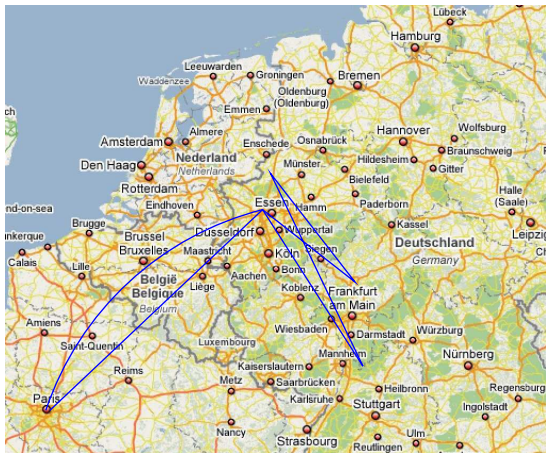
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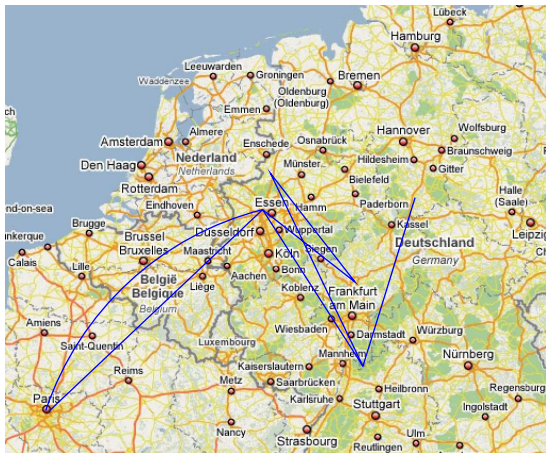


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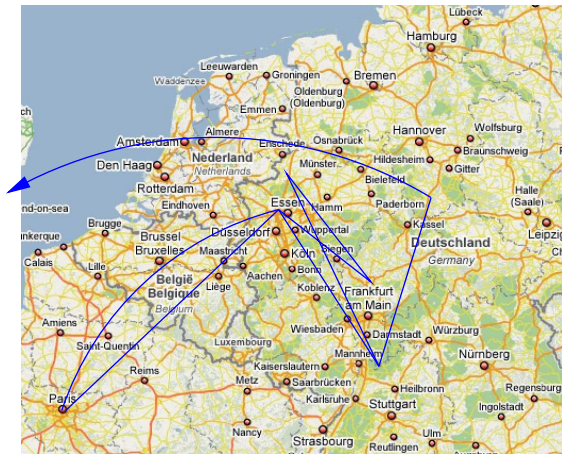
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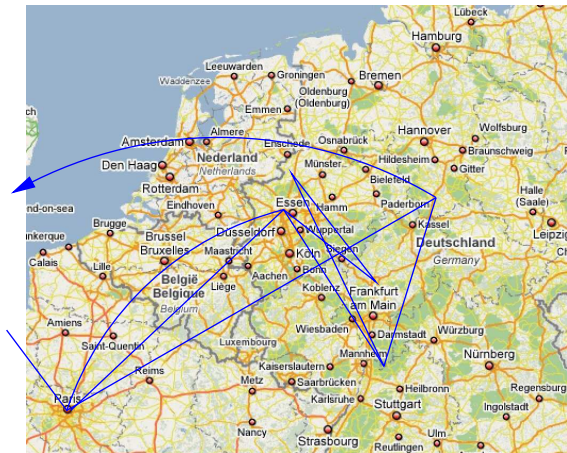
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Why studying physics?

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

⇒ save money for
super 8 film camera



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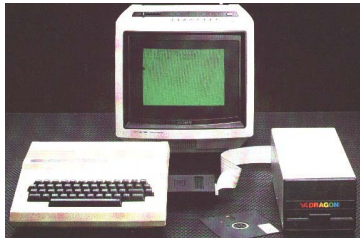


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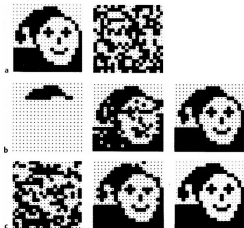


- (1982)
Money is available!
BUT: Computers are great!
⇒ buy **DRAGON 32**

- almost NO games !
⇒ write programs myself

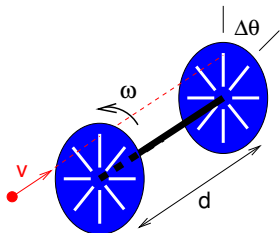


- (1985) Spectrum der Wissenschaft:
 paper on neural networks
 Simulation on Dragon 32:
 works well!
 ⇒ system > Σ constituents!



- (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 Science = data bases, operation systems, etc. ?
 ⇒ no surprises ⇒ study Physics (1987)

Computational Physics Group

Oliver Melchert

Stefan Wolfsheimer



Bernd Burghardt (Gö)

Alexander Mann (Gö)

Alexander Hartmann



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?

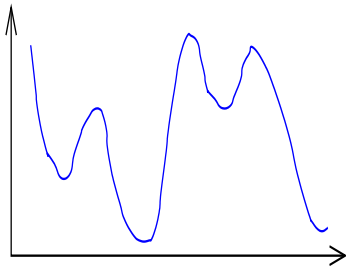
“Computational Theoretical Physics”

Large scale computer
simulations
new algorithms



[Paderborn Parallel Computing Center]

Optimization algorithms
development/applications
systems with 10^6 particles



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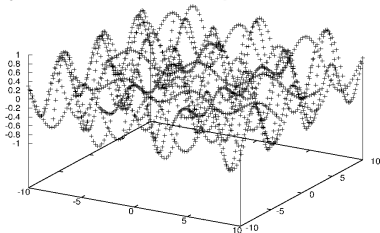
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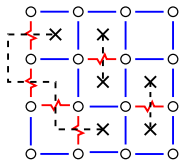
systems with 10^6 particles

Disordered magnets

Spin glasses

Random-field systems

(B. Ahrens, O. Melchert)

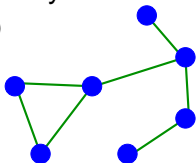


Phase transitions in optimization problems

Vertex cover

Satisfiability

(A. Mann)

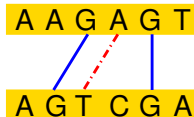


Bioinformatics

RNA secondary structures

Sequence alignment

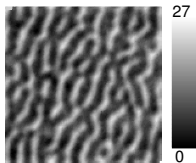
(B. Burghardt, S. Wolfsheimer)



Surface Physics

Sputtering

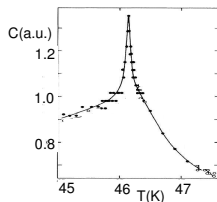
Pattern formation (T. Yasseri)



Random-field Ising magnets (RFIM)

- Ordered systems (lattices): well understood
real world: **disorder** → make (sometimes) strong difference

- Experiments** with DAFF
specific heat → 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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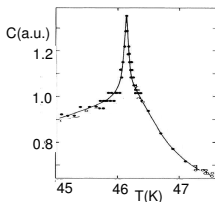
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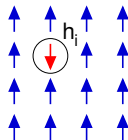


[D.P. Belanger et al., 1983]

- 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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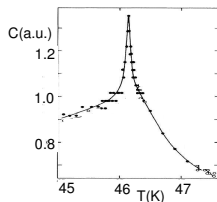
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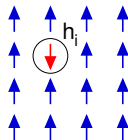


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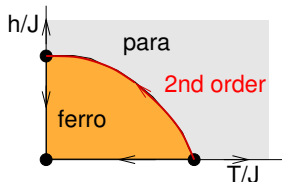
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- Phase diagram →

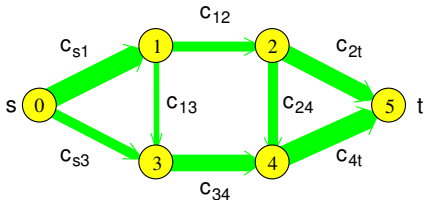
Aim:

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



Networks

- Idea: mapping of RFIM \leftrightarrow network



- Network = graph + edge capacities:

$$G = (V, E), E \subset V \times V$$

$$c_{ij} > 0, s, t \in V$$

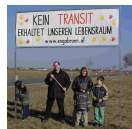
- Now: network \rightarrow RFIM



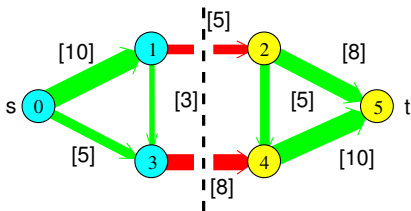
- Much transit traffic in Austria
→ blockade 25. October 2022



- Much transit traffic in Austria
→ blockade 25. October 2002



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

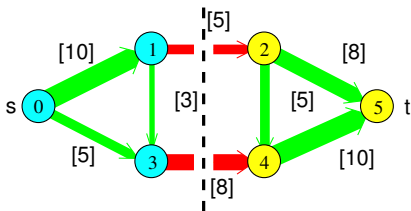


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 \sim **capacity** of cut

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



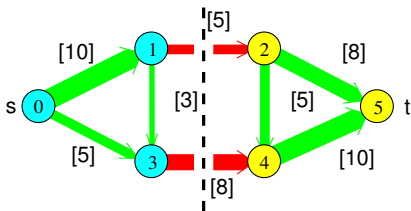
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- With $\underline{X} = (x_0, \dots, x_{n+1})$, $x_i = 0/1$, $x_i = 1 \Leftrightarrow i \in S$
[J.-C. Picard and H.D. Ratliff, Networks 1975]

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

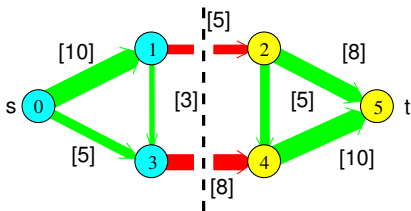
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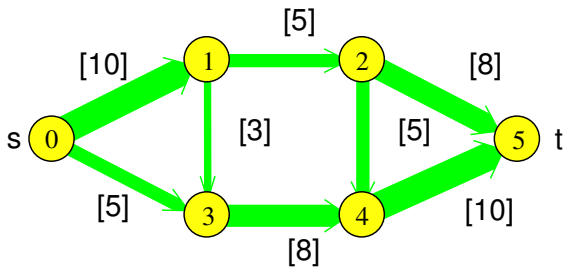


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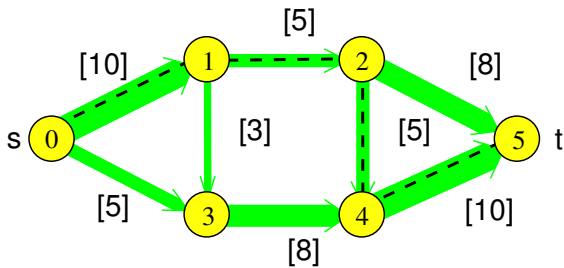
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- Minimum energy = capacity of min. cut = max. flow

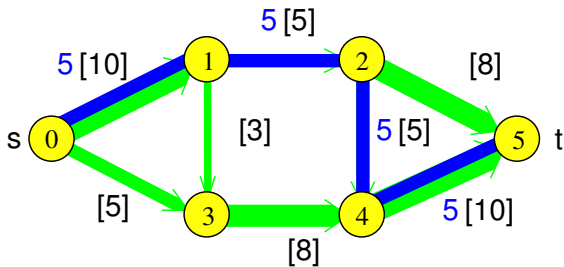
■ Calculate maximum flow: **Ford-Fulkerson algorithm** (1956)



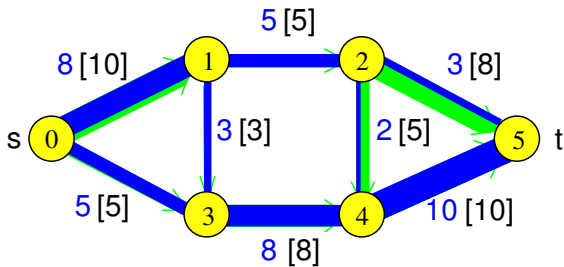
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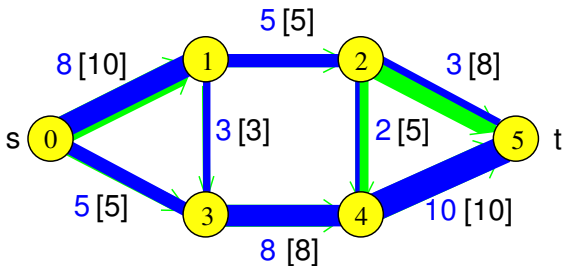
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- Modern algorithms (computer science):
concurrent flow increments

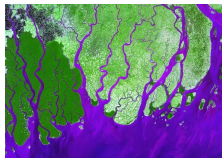
[R.E. Tarjan, *Data Struct. + Netw. Algorithms* 1983]

[A.V. Goldberg, 1988-1998]

parallel algorithms

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

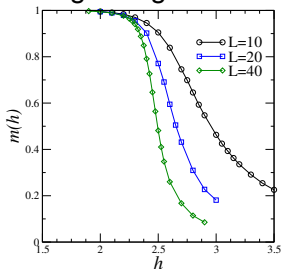
- Exact ground state of large systeme, e.g. with 100^3 spins.



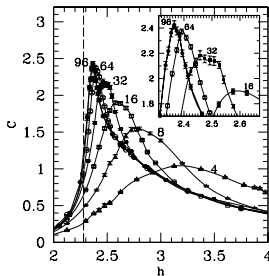
Results

- New methods to calculate physical quantities ↓

- Average Magnetization



- Specific heat



- Height of maxima
no divergence

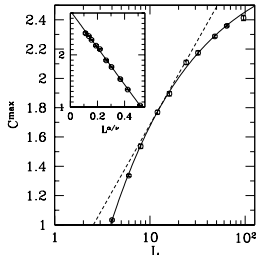
$$C^{\max}(L) = C_{\max} + a_2 L^{\alpha^* / \nu}$$

$$\rightarrow \alpha = 0 \quad (\alpha^* = -0.6)$$

$$C_{\max} = 2.84(5)$$

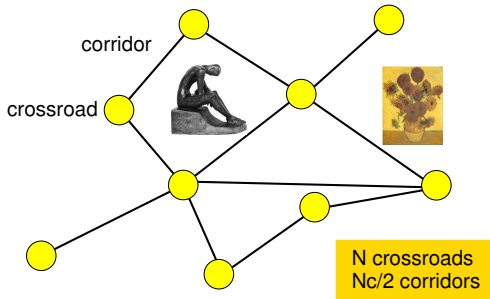
[AKH & A.P. Young, Phys. Rev. B, 2001]

but from experiments: $\log L$



Vertex-Cover Problem

- Prototypical problem of theoretical Computer Science
- **Museum**



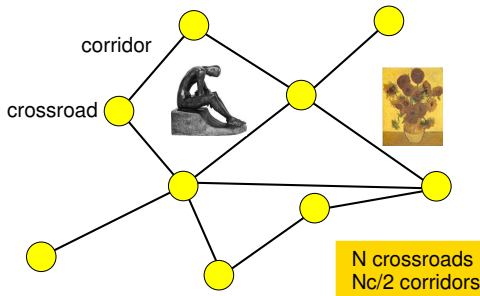
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Edvard Munch's "Der Schrei" stolen in Oslo August 2004



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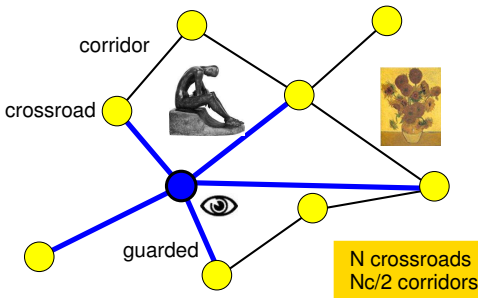
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$X = xN$ guards
guard only adjacent corridors



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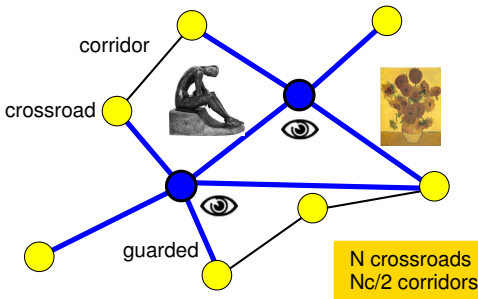
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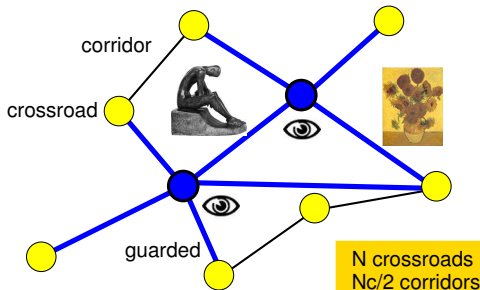
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guard only adjacent corridors

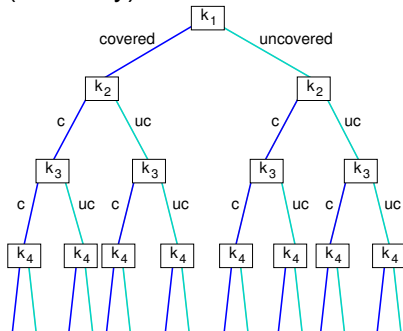
- Mathematically: museum = graph $G = (V, E)$
Vertex cover $A \subset V : \forall (i, j) \in E : (i \in A) \vee (j \in A)$
- **Decision problem**: all corridors guardable w. X guards?
Optimization problem: minimize number of unguarded corr.
- Vertex-cover problem = NP-complete

Branch-and-bound algorithm

Task: min. # of uncov. edges

Complete algorithm:

(basically) enumerate all states



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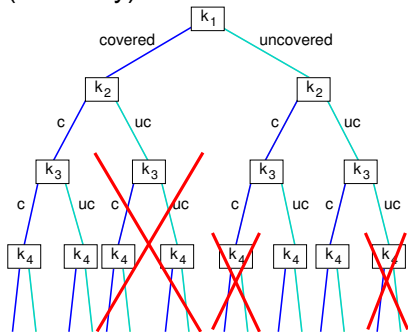
Avoid subtrees w/o solutions

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

...

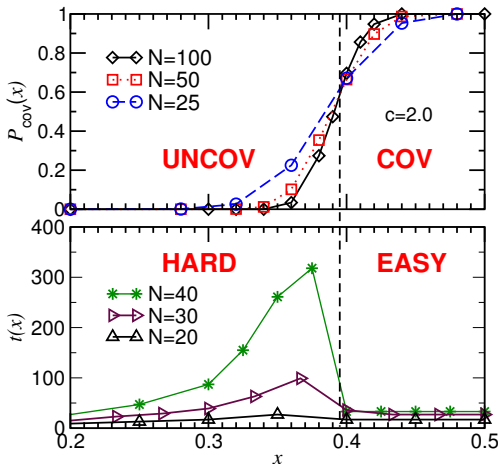
$$d_{\max} \equiv \sum_{i=1}^F d(n_i)$$

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

Phase transition

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

Probability to cover

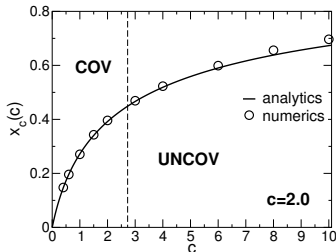


Running time =
number of nodes
in branching tree

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

Phase diagram

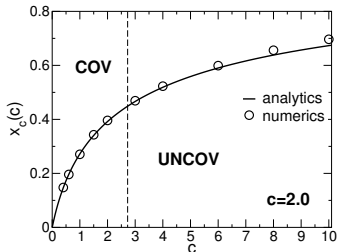
- Analytical treatment: \Leftrightarrow spin-glass or hard-core gas
- Stat. Mech. methods: replica trick/cavity approach
- \rightarrow phase diagram $x_c(c)$, exact for $c \leq e \approx 2.718$
- [M. Weigt & AKH, PRE 2001]



Phase diagram

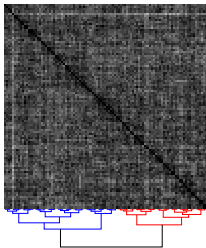
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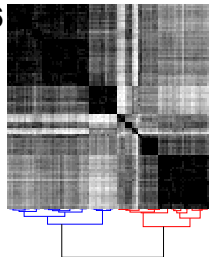
- Many solutions \rightarrow cluster structure ?

$c = 2$



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

$c = 6$

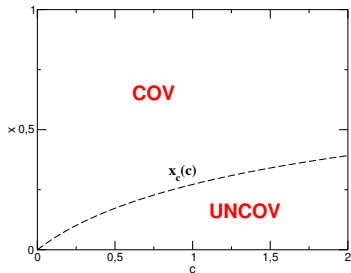


Number of clusters grows with N for $c > e$.

Physics: Replica Symmetry Breaking

Running Time

- Aim: analytical calculation of running time
- Phase diagram



Running Time

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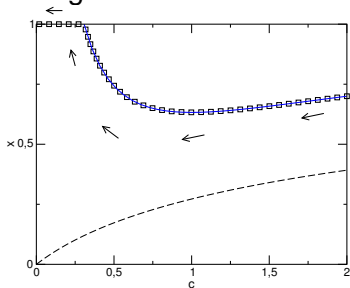
algorithm picks vertices:

moves ($T = 0 \dots N$)

→ effective

$$x(t = \frac{T}{N}) = \dots$$

$$c(t = \frac{T}{N}) = \dots$$



Running Time

- Aim: analytical calculation of running time
- Phase diagram

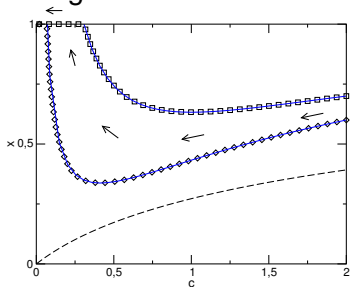
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→ effective

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Running Time

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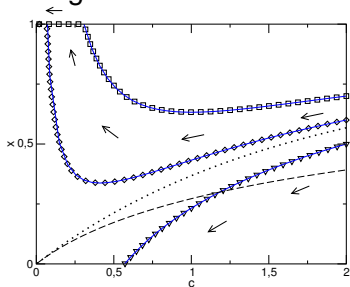
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Running Time

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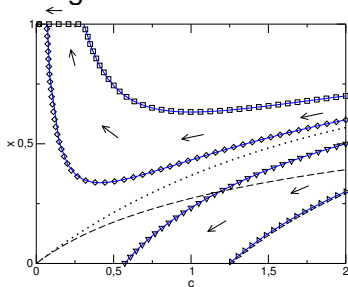
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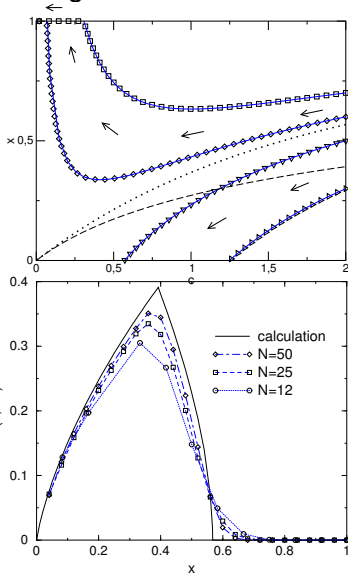
→ effective

$$x(t = \frac{T}{N}) = \dots$$

$$c(t = \frac{T}{N}) = \dots$$

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

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



Summary

Computer Science



Physics

- Ground states of disordered magnets
 - disorder makes a difference
 - Random-field Ising magnet
 - mapping to max-flow problem → 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!

- Audience
- Family
- Collaborators: S. Alder, B. Ahrens, C. Amoruso, T. Aspelmeier, W. Barthel, B. Blasius, S. Boettcher, A.J. Bray, K. Broderix, B. Burghardt, I.A. Campbell, A.C. Carter, R. Cuerno, E. Domany, A. Engel, M. Feix, R. Fisch, U. Geyer, T. Gross, M.B. Hastings, G. Hed, D.W. Heermann, J. Houdayer, M. Jünger, M. Jungsbluth, H.G. Katzgraber, S. Kobe, M. Koelbel, M. Körner, W. Krauth, R. Kree, M. Leone, F. Liers, A. Mann, K. Marx, O. Melchert, R. Monasson, M.A. Moore, A. Morales, J.J. Moreno, J. Munoz-Garcia, U. Nowak, M. Palassini, M. Pelikan, A. Rosso, F. Ricci-Tersenghi, H. Rieger, K. Sastry, D. Stauffer, R. Steuer, S. Trebst, M. Troyer, K.D. Usadel, M. Weigt, T. Yasserli, O.E. Yewande, A.P. Young, R. Zecchina, A. Zippelius
- Financial support: VolkswagenStiftung, DFG