

Dagstuhl Seminar No. 01091  
**Algorithmic Techniques in Physics**

organized by

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# 1 Preface

Nearly three years earlier, in December 1997, the Dagstuhl Seminar “Algorithmic Techniques in Physics” took place. Researchers from Computer Science, Mathematics and Physics came together to discuss about algorithmic problems occurring in physics and physical concepts that might be useful in computer science. Bringing together people from three different areas was an experiment that, as all participants agreed in the end, turned out to be a success and, more importantly, should be repeated in the future.

The original seminar was motivated by the observation that traditionally, there has always been a strong scientific interaction between physicists and mathematicians in developing physical theories. However, even though numerical computations are now commonplace in physics, no comparable interaction between physicists and computer scientists had been developed. Since the last three decades the design and the analysis of algorithms for decision and optimization problems evolved rapidly. Simultaneously, computational methods in theoretical physics became a major research tool causing a fast growing challenge with regards to the underlying algorithmic concepts. The few interactions between physicists and computer scientists were often successful and provided new insights in both fields. For example, in one direction, the algorithmic community has profited from the introduction of general purpose optimization tools like the simulated annealing technique that originated in the physics community. In the opposite direction, algorithms in linear, nonlinear, and discrete optimization have turned out to be useful tools in physics. Surprisingly often physicists and computer scientists are concerned with very similar questions but use a different terminology disguising in this way the significant overlap and preventing fruitful collaboration. Many notions of physicists in particle physics the computer scientists call problems or algorithms in combinatorics and extremal graph theory.

During the first seminar it became clear that the communication that was intended by the organizers was indeed fruitful. The computer scientists realized rather quickly that computational physicists often deal with very similar problems and try to solve them with a sometimes more pragmatic approach. And the physicists profited from the most recent algorithmic development that were useful for them but usually reach their community only decades later. Actually a number of participants (including the organizers) took home various ideas that were later converted into scientific publications. Various algorithms from combinatorial optimization are now standard tools in the computational physics community that studies the properties of ground states of disordered and complex systems. Some problems have been solved, but new ones have emerged. On the other hand, new algorithmic techniques have been developed which might be useful in solving these new problems. The topics that we treated in the second seminar include:

- Applications of polynomial optimization algorithms, including their problem specific implementation, to random physical systems. Well established examples here are the max-flow/min-cut algorithm to disordered ferromagnets or the min-cost-flow-algorithm to ensembles of magnetic flux lines.

- New developments in exact and heuristic algorithms for NP-hard physical problems, like the Coulomb- or the spin glass as well as new approaches to stochastic optimization. This included simulated annealing, genetic algorithms, semidefinite programming, Lagrangean relaxation, branch and cut, the Pfaffian method etc.
- Results on the nature of disordered systems and networks
- Concrete physical realizations of various standard problems in combinatorial optimization.
- The computational complexity of various computationally hard physical problems as they occur in the physics of glassy systems.
- Statistical properties and phase transitions of various standard problems in computer science like  $k$ -Sat etc.
- Scaling behavior of various geometric properties of standard algorithms applied to grid graphs.
- And many more.

We found that since the last seminar many language barriers between physicists, mathematicians and computer scientists have been overcome. In a relaxed research atmosphere, the proposed problems were modeled and analyzed in consistent terminology understandable to all three groups. Therefore, an intensive information exchange was possible. This improvement became particularly apparent in the open forum discussions, where everybody was welcome to propose a problem and ask for possible solution methods.

Interestingly, it became clear that there is an increasing overlap in the research fields of both communities: physicists become more and more interested in combinatorial optimization problems and study their physical nature, whereas computer scientists realize the importance of studying physically relevant problems.

Our goal was to bring together the computer science, mathematical programming and physics communities in the pursuit of establishing new interactions and refreshing old ones, initiated in the '97 event. It turned out that we had chosen a good time for the second such Dagstuhl seminar.

## 2 Final Program

Monday, 26. February 2001

- 9:15 – 9:30 Introduction
- 9:30 – 10:15 Phil Duxbury  
*Are random systems universal?*  
*Is there a zero temperature fixed point?*
- 10:15 – 10:45 Coffee
- 10:45 – 11:30 Stephan Mertens  
*Random Costs in Combinatorial Optimization*
- 11:30 – 12:15 Werner Krauth  
*Absence of Thermodynamic Phase Transition in Model Glass Formers*
- 12:15 – 14:00 Lunch
- 14:00 – 14:45 Naoki Kawashima  
*Renormalization Group and Optimization*
- 14:45 – 15:30 Alan Middleton  
*Connections between Excitations in Physical Systems and Algorithms*
- 15:30 – 16:15 Coffee
- 16:15 – 17:00 Eira Seppälä  
*Serial and Parallel Maximum Flow-Minimum Cut Algorithms Applied to Random Bond and Random Field Ising Systems*
- 17:00 – 17:45 Viljo Petäjä  
*Entanglement of Directed Lines in Disordered Environment*
- 18:00 Dinner

Tuesday, 27. February 2001

- 9:00 – 9:35** Jerome Houdayer  
*Computing the Ground State of a Spin Glass  
using Genetic Algorithms and Renormalization*
- 9:35 – 10:15** Olivier Martin  
*Spin Glasses: Ground States and Energy Landscapes*
- 10:15 – 10:45** Coffee
- 10:45 – 11:30** Frauke Liers  
*Studying the Spin Glass State by Combinatorial Optimization*
- 11:30 – 12:15** Guy Hed  
*Clustering Analysis of the Spin Glass Phase*
- 12:15 – 14:30** Lunch
- 14:30 – 15:30** Anna Gallucio  
*Optimization via enumeration:  
Pfaffian method for max-cut and Ising problems*
- 15:30 – 16:15** Coffee
- 16:15 – 17:00** R. Zecchina  
*1. Topological/combinatorial counting over non-planar lattices  
2. Exact results in diluted spin glasses and  
. NP-complete optimization problems*
- 17:00 – 17:45** Martin Loebel  
*An anti-algorithmic solution to three-dimensional problems*
- 18:00** Dinner

Wednesday, 28. February 2001

- 9:00 – 9:40**    Gerald Gruber  
*Lagrangian Relaxations for Max-Cut Using Bundle Methods*
- 9:40 – 10:30**   Kurt Mehlhorn  
*Recent Developments in LEDA*
- 10:30 – 11:00**   Coffee
- 11:00 – 11:45**   Alexander Hartmann  
*The Vertex-Cover Problem:  
Introduction and Experimental Results*
- 11:45 – 12:30**   Martin Weigt  
*Phase Transition and Typical Computational Complexity of  
Vertex Covering Sparse Random Graphs*
- 12:15 – 13:30**   Lunch
- 13:30 – 18:00**   **EXCURSION**
- 18:00**            Dinner



Thursday, 1. March 2001

- 9:00 – 9:45**    Kai Nagel  
*Iterative Relaxation for Network Optimization in  
Transportation Simulations*
- 9:45 – 10:30**    Hawoong Jeong  
*The Architecture of Complexity: From the Diameter of the  
WWW to the Structure of the Cell*
- 10:30 – 11:00**    Coffee
- 11:00 – 11:40**    Ingo Morgenstern  
*Optimization for Tone Playing and Production Lines*
- 11:40 – 12:15**    Jae-Dong Noh  
*Ground State Property Studies of Random Periodic  
Elastic Media with a Maxflow/Minicut Algorithm*
- 12:15 – 14:30**    Lunch
- 14:30 – 16:00**    “Open problem” forum / Discussion:  
H. Rieger / T. Hagerup:  
*Random Potts model / k-cut problem.*  
F. Pfeiffer:  
*Why physicist need minimal surfaces.*  
etc. ...
- 16:00**            Coffee
- 18:00**            Dinner

Friday, 2. March 2001

- 9:00 – 9:45 Miguel Anjos  
*Semidefinite Programming Relaxations for Max-Cut*
- 9:45 – 10:30 Christoph Helmberg  
*On Numerical Experiments with a  
Semidefinite Programming Bound for Spin Glasses*
- 10:30 – 11:00 Coffee
- 11:00 – 12:00 “Open problem” forum cont. / Discussion / Farewell
- 12:15 Lunch

### 3 Abstract of Presentations

#### Phil Duxbury

*Are random systems universal? Is there a zero temperature fixed point?*

In studies of scaling phenomena and phase transitions in random systems, the physics community often takes regular graphs and also idealised disordered distributions. It is important to know if the behavior of these idealised systems carries over to the behavior of disordered materials, such as random magnets and glasses, polycrystalline materials, flux lines in superconductors and diffusion in doped semiconductors. Only some aspects of the models apply to these real problems, namely scaling exponents and amplitude ratios near critical points. However we need these quantities to be *universal* to changes of many of the details in the lattice models.

Specifically, in disordered systems we hope that the scaling behavior at zero temperature is typical of that at finite temperature (i.e. there is a zero temperature fixed point) and that the scaling behavior does not depend on the details of the disorder distribution or lattice structure (though we expect dimensionality to be important). We have shown that the minimum spanning tree (MST) geometry is universal for all disorder distributions, while the shortest path tree has two known universality classes. The DPRM class for weak disorder and the MST class at strong disorder. In contrast the random field Ising model on a complete graph is non-universal in the ground state. However universality is restored at finite temperature. Thus either the RFIM ground state is not characteristic of the behavior

at finite temperature or the RFIM mean-field theory is pathological. We are studying the effect of different disorder distributions on the three-dimensional RFIM to see which of these conclusions is correct.

## **Stephan Mertens**

### *Random Costs in Combinatorial Optimization*

The random cost problem is the problem of indentifying the minimum in a list of random numbers. By definition, this problem cannot be solved faster than by exhaustive search. It is shown that a classical NP-hard optimization problem, number partitioning, is essentially equivalent to the random cost problem. On the one hand this explains the bad performance of heuristic approaches to the number partitioning problem but on the other hand allows to calculate the probability distributions of the optimum and sub-optimum costs.

## **Werner Krauth**

### *Absence of Thermodynamic Phase Transitions in Model Glass Formers*

The nature of the glass transition has been a subject of much controversy for at least the last 50 years. It is clear (from a phenomenological point of view) that it corresponds to the point at which the viscosity of a structurally disordered liquid reaches a value typical for a crystal. But it is not clear whether the glass transition is a purely dynamical phenomenon or whether an underlying thermodynamic transition is responsible for the pronounced slowdown of the system. In this talk, the viscosity of the liquid is related to the equilibration time of a particular (local) Monte Carlo algorithm. However, we can also perform Monte Carlo simulations with a new Cluster Algorithm which remains ergodic even far within the glassy phase. In a system of polydisperse hard disks in two dimensions, we find no evidence for a thermodynamic phase transition up to very high densities; the glass is thus indistinguishable from the liquid on purely thermodynamic grounds.

Work done in collaboration with L. Santen (Paris).

## **Naoki Kawashima**

### *Renormalization Group and Optimization*

Renormalization group is one of the most essential ideas in recent developments of statistical physics. It gives a microscopic foundation for scaling and universality. It is pointed out that a procedure similar to Kadanoff's real space renormalization transformation can be quite useful to construct an efficient heuristic algorithm for a class of optimization problems. In contrast to its application to uniform systems, it turns out to be advantageous to define block spins in such a way that the underlying structure of the system may be taken into account. This is accomplished by taking a few replicas of the system, partially optimizing them using any known algorithm, and then comparing them. The efficiency of the method is demonstrated in the application of it to the 2d Ising spin glass model. As a result, we observe

fractal nature of the low-lying excitations of the model, i.e., droplets, which dominates the system behavior at low temperature.

## **Alan Middleton**

### *Excitations in Physics and Challenges in Algorithms*

This talk emphasized the importance and challenge of studying excitations in disordered materials using combinatorial optimization and the relation between physical properties and time bounds on algorithms. A list of applications of combinatorial optimization was reviewed and two problems in P, the random field Ising magnet (RFIM) and the two dimensional elastic medium (solved using bipartite matching) were introduced. Excitations correspond to the physical degrees of freedom at each scale and are used to describe the dynamics of a system. The uniqueness of the optimal solution in the interior of a large graph in the limit of large graphs corresponds to the physical notion of one or two ground states in the thermodynamic limit. As presented for the case of the random field Ising model, this uniqueness gives bounds on the time needed to find a ground state; critical slowing down of the push-relabel flow algorithm is evident at the physical phase transition. Excitations can be found in the planar bipartite matching (elastic medium) by detecting negative cycles in a modified graph. Open questions remain about the (worst case or typical) complexity of finding certain excitations.

## **Eira Sepälä**

### *Serial and Parallel Maximum Flow-Minimum Cut Algorithm Applied to Random Bond and Random Field Ising Systems*

The random field Ising model and domain walls in random bond Ising systems are studied using a maximum flow - minimum cut algorithm. The mapping of the random Ising systems to flow graphs is shown. The method, Push-and-Relabel algorithm, is presented and the technical details of the implementation are reported. A parallel version of Push-and-Relabel algorithm using domain decomposition is presented and shown to be useful for increasing the memory available, but not for reducing CPU-time. Using the parallel algorithm the system sizes  $400^3$  and  $200^3$  for random bond and random field systems, respectively, are achieved. The use of residual graphs when studying sensitivity of the ground state structure to a perturbation is introduced. As examples some results of the problems studied are shown:  $\{11\}$  and  $\{111\}$  oriented random bond domain walls with a periodic potential in the limit of large amplitude of the potential move by discrete jumps between potential valleys and finally roughen over the potential barriers. Domain walls in random bond magnets with an applied field change by discrete jumps. In two-dimensional random field Ising magnets a percolation phenomenon is studied. The sensitivity of percolation clusters is calculated using the residual graph method and the number of so called “red clusters” is shown to scale as the red sites in standard percolation.

This work is done in collaboration with M. Alava, P. Duxbury, C. Moukarzel, and V. Petäjä.

## Viljo Petäjä

### *Entanglement of Directed Lines in Disordered Environment*

During the recent years an intensive theoretical research has been carried out to clarify the effects of thermal fluctuations, disorder and defects on the properties of flux line systems [1]. This research is heavily motivated by the experimental connection to dirty type-II superconductors, in which vortices (flux lines) interact with disorder. The disorder gives a rise to a complicated phase diagram [2]. At low temperatures with a strong point disorder flux lines form a vortex glass. This phase is characterized by a topologically complicated geometric configuration of entangled flux lines.

We investigate entanglement of flux lines or directed polymers in disordered media (DPRM) with an exact numerical method [3]. The algorithm finds a joint ground state for  $N$  lines in three dimensions. In the case of a single line system the roughness exponent is well known [4] but for the roughening of a  $N$ -line system there is not yet found any satisfactory scaling relation. This demonstrates the non-triviality of  $N$ -line systems.

In [5] Drossel and Kardar calculated distributions of winding angles in the case of a single line and also investigated the winding of a random walker. We generalize the calculations to  $N$ -line systems. We investigate the scaling of winding angle and the formation of flux line bundles. We find scaling relation for the winding angle.

This work has been done in collaboration with H. Rieger, University of Saarbrücken.

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## Jérôme Houdayer

### *Simulating Spin Glasses*

*Computing the ground state of a spin glass* A genetic algorithm is presented which is able to find a spin glass ground state with high probability up to sizes as large as  $14^3$  in reasonable time. A renormalization procedure (first introduced by N. Kawashima) is used which given a set of spin configurations produces a smaller spin glass problem with the common parts of the

given configurations frozen. This procedure is implemented recursively together with a local search to optimize on all scales. Moreover, in opposition to standard genetic algorithms, the population is always forced towards smaller energy, which assures convergence and efficiency. *Cluster Monte Carlo for 2-d spin glasses* A new Monte Carlo algorithm for 2-d spin glasses is presented. This algorithm uses clusters defined as in the renormalization procedure. The use of clusters together with parallel tempering make this algorithm more than one thousand time faster than previous methods. Using this tool one can equilibrate  $100^2$  spin systems down to  $T = 0.1$ . Numerical simulations shows that for the 2-d  $\pm 1$  spin glass, the correlation length diverges as  $\xi \sim e^{-2\beta J}$  in contradiction to standards lore.

## Olivier C. Martin

### *Spin Glasses: Ground States and Energy Landscapes*

We examine excited states in spin glasses on grid graphs (3 dimensional cubic lattices, up to sizes  $12 \times 12 \times 12$ ). Our algorithm for finding ground states is the genetic renormalization algorithm (cf. previous talk by J. Houdayer). The edge weights are Gaussian independent random variables, and we study this system with both free and with periodic boundary conditions. Now, given an instance (set of weights),

- compute the ground state
- choose two spins at random and impose the constraint that their relative orientation changes
- compute the new ground state including this constraint

The two ground states differ by a connected cluster of spins containing say  $V$  spins. By considering both the distribution of  $V$  and the topology of the connected cluster, we give numerical evidence that the Fisher Huse exponent  $\theta$  (defined from  $\Delta E$  goes as  $r^\theta$ ) is zero. Numerous open questions remain, in particular concerning the geometric nature of these system-size excitations. We suggest that ground state solvers capable of handling  $15 \times 15 \times 15$  grids would have a high impact in the spin glass community.

In collaboration with J. Houdayer and F. Krzakala

## Frauke Liers

### *Studying the Spin Glass State by Combinatorial Optimization*

Spin glasses are certain alloys, e.g. CuMn. We are interested in the nature of the spin glass phase that might occur while cooling down the alloy to deepest temperatures. We are considering the Hamiltonian in the Edwards Andersen model. By a branch and cut algorithm we can determine exact ground states of spin glasses, i.e., the global minimum of the Hamiltonian. By applying a weak perturbation to the bulk of the system we study low lying excited states. With extensive statistics and state of the art system sizes we test different models suggested and discussed for the nature of the spin glass state, i.e., the

droplet scaling, mean field and some intermediate picture. The preliminary results up to  $L = 10$  do not support clearly one of these pictures since finite size effects may be large.

This work is done in cooperation with M. Jünger, M. Palassini, A.P. Young. Ideas from M. Diehl, G. Reinelt and G. Rinaldi contributed much to the algorithm.

## Guy Hed

### *Clustering analysis of the spin glass phase*

Clustering is a procedure in which a set of objects is partitioned into groups or clusters, so that objects that are more ‘similar’ are grouped together.

We generate an unbiased sample of states for a 3d spin glass at  $T < T_c$ . In order to investigate the nature of the state space we cluster the states. The states are separated into two clusters,  $\mathcal{C}$  and  $\bar{\mathcal{C}}$ , related by spin-flip symmetry. Each of these is partitioned into two clusters:  $\mathcal{C}$  into  $\mathcal{C}_1$  and  $\mathcal{C}_2$ ;  $\bar{\mathcal{C}}$  into  $\bar{\mathcal{C}}_1$  and  $\bar{\mathcal{C}}_2$ . We relate each state cluster to a Gibbs state – a free energy valley.

In order to investigate the micro-structure of the system we cluster the spins. We find at least two macroscopic spin domains in which the spins are highly correlated. These spin domains determine the state space landscape. The free energy barrier separating the Gibbs states  $\mathcal{C}$  and  $\bar{\mathcal{C}}$  is related to the largest spin domain. The barrier between the Gibbs states  $\mathcal{C}_1$  and  $\mathcal{C}_2$  (as well as between  $\bar{\mathcal{C}}_1$  and  $\bar{\mathcal{C}}_2$ ) is related to the second largest spin domain.

We can use the above mapping of the phase space to improve the analysis of different observables, such as the overlap distribution, by calculating them only for the relevant part of the phase space, in which they take a non-trivial value.

This work was done in collaboration with: E. Domany, A. K. Hartmann, D. Stauffer, M. Palassini and A. P. Young.

## Anna Gallucio

### *Optimization via enumeration: Pfaffian method for Max-cut and for Ising problem.*

The theory of Pfaffian orientations has been introduced in statistical physics as a useful technique to solve problems having a pure combinatorial flavour. Using this theory, Kasteleyn proved in early sixties that the number of perfect matchings of planar graphs may be computed efficiently by evaluating the Pfaffian of an antisymmetric matrix. He also stated that the result might be extended to graphs of higher genus  $g$  using a linear combination of  $4^g$  Pfaffians instead of a single one. He did not give a rigorous mathematical proof of his statement since the method was considered of little practical use. So, a close analysis was carried out by Kasteleyn only for the case of toroidal grids, or, equivalently, square lattices with periodic boundary conditions.

In an earlier joint paper with M. Loebbl, we gave a rigorous proof of Kasteleyn’s statement for general graphs embeddable on orientable surfaces of genus  $g$  and provided an explicit description of the  $4^g$  coefficients used in the linear combination of Pfaffians (partial results for graphs of genus  $g > 1$  were obtained independently by T. Regge and R. Zecchina).

Using the enumeration duality for the generating function of cuts, or, in more physical terms, the high-temperature expansion of the partition function of the Ising model, we proved the existence of a polynomial time algorithm to solve the *max-cut* problem in the class of graphs of bounded genus  $g$ .

In the lecture, we overviewed the algorithm and presented an implementation developed to compute the *partition function* of a two-dimensional  $\pm J$  Ising spin glass. The use of modular arithmetics joint with the chinese remainder theorem allowed us to obtain an exact integer algorithm which solves instances up to  $40 \times 40$  in reasonable time. The overall complexity of the algorithm is  $O(n^{3.5})$  where  $n$  is the size of the lattice, but the computation of the Pfaffians can be easily decomposed into  $O(n)$  independent computations, so that a faster, parallel implementation of the algorithm is possible.

(joint work with M. Loeb and J. Vondřak)

## **Riccardo Zecchina**

*Part I: Combinatorial/Topological approach to non-planar lattice statistics*

*Part II: Exact results in diluted spin glasses and random NP-complete combinatorial problems*

*Part I:* Among the known approaches to the evaluation of the D=2 Ising partition function which have followed the celebrated Onsager solution, the Pfaffian method fully exploits the combinatorial and topological properties of the lattices (or graphs) by relating the partition function to the generating function of close-packed dimer configurations. Though the method is in principle independent from the dimensionality of the lattice, the corresponding analysis in three dimensions has never been developed, due to the difficulty of extending Kasteleyn's Orientation Theorem to the case of non-planar lattices. We have dealt with the issue of extending such a combinatorial approach to general lattices of non-trivial topological genus (T.Regge and R.Zecchina, J.Math.Phys. 37, 2796 (1996)). The partition function (i.e. the weighted matching polynomial) is given by the sum of  $2^{2g}$  Pfaffians and the chief result consists in a general rule that determines the sign with which each Pfaffian appears in the expansion of the partition function. Indeed, such signs can be computed explicitly by a simple topological argument based on the structure of the intersection and orientation of the homology cycles that can be defined on the lattice. For the case of group lattices, we have also shown that the computation of the partition function is greatly simplified by the use of symmetries of an extended group which greatly reduces the number of distinct Pfaffians. As a representative example we have obtained the complete solution for the Ising model on a finite lattice (N=168) of genus  $g=3$  known as the Klein lattice group. Successively, we have further generalized the above results to lattices of high topological genus ( $g$  proportional to the number N of vertices) and to the general problem of evaluating the permanent of 0-1 matrices (T. Regge and R. Zecchina, J.Phys.A 33, 741-761 (2000)). The 3D Ising model and the dimer coverings problem on a cubic lattice, where  $g = 1 + N/4$ , have been discussed in detail. As expected, the expansion of the partition function is shown to be given by  $2^{2g} = 2^{2+N/2}$  Pfaffians classified by the oriented homology cycles of the lattice. Correct counting is guaranteed by a signature term which depends on the topological intersection of



the oriented cycles through a simple bilinear formula. Finally, the same formalism has been applied to the counting problem of perfect matchings over general lattices and provides a determinant expansion of the permanent of 0-1 matrices.

Note: An alternative derivation of similar results can be found in the work of Galluccio and Loeb1.

*Part II:* We study the low temperature properties of spin glass models with finite connectivity and optimization problems. In the context of one-step replica symmetry breaking theory, we study a simple functional Ansatz which is exact for  $p$ -spin like models over random hypergraphs of uniform degree. The ground state energy can be computed as a function of the connectivity. The results for two representative cases, the  $p$ -spin model and the Bicoloring optimization problem, are given. For fluctuating connectivity, the same Ansatz can be used in a variational way: for  $p$ -spin models (also known as  $p$ -XOR-SAT in computer science) it provides the exact configurational entropy together with the dynamical and static critical connectivities (for  $p = 3$ ,  $\gamma_d = 0.818$  and  $\gamma_s = 0.918$  resp.), whereas for hard optimization problems like 3-SAT or Bicoloring it provides the lowest known upper bounds for their critical thresholds ( $\gamma_c^{var} = 4.396$  and  $\gamma_c^{var} = 2.149$  resp.). (S.Franz, M.Leone, F.Ricci-Tersenghi, R.Zecchina, submitted 2001)

## Martin Loeb1

### *An anti-algorithmic solution to 3-dimensional problems*

A new expression for the partition function of the dimer arrangements and the Ising partition function of the 3-dimensional cubic lattice is presented. The partition functions are expressed by means of expectations of determinants of matrices naturally associated with the cubic lattice. Determinants and spectral properties of random matrices are extensively studied and there is a hope that these new expressions open up a possibility to apply fundamentally different statistical methods and Monte carlo simulations to study the 3-dimensional problems. The principal method used is the theory of Pfaffian orientations developed recently by Galluccio and Loeb1 (and independently by Regge and Zecchina). Regge and Zecchina (2000) also provide an expression for the 3-dimensional problems based on Pfaffian orientations. The two expressions are different: the one presented in my lecture has a strong statistical character while the expression of Regge and Zecchina is topological.

## Gerald Gruber

### *Lagrangean Relaxation for Max-Cut Using Bundle Methods*

We consider the problem of maximising a concave function  $c : \mathcal{R}^n \rightarrow \mathcal{R}$  subject to finitely many constraints. In particular, given  $c : \mathcal{R}^n \rightarrow \mathcal{R}$ ,  $A \in \mathcal{R}^{m \times n}$ ,  $b \in \mathcal{R}^m$  and a convex set  $X$  we deal with

$$\begin{aligned}
(\text{P}) \quad & \max c(x) \\
& \text{s.t. } x \in X \\
& Ax \leq b
\end{aligned}$$

The number of constraints  $m$  could be very large, hence solving (P) is still too difficult. The goal is selecting important inequalities of  $Ax \leq b$  to get a good approximation of the original problem. We present a method which leads to such an approximation in reasonable time. This work was done with I. Fischer, F. Rendl, R. Sotirov.

## Kurt Mehlhorn

### *Recent Advances in the LEDA System*

We report about three recent advances:

- a hierarchy of graph classes: the new graph classes allow one to customize the graph data structure. This saves space and hence increases speed.
- an implementation of an  $\mathcal{O}(nm \log n)$  weighted matching algorithm for general graphs.
- the average case analysis of a heuristic for weighted matchings.

## Alexander Hartmann

### *Phase transition in the vertex-cover problem*

The vertex-cover problem (VC) is a classical NP-complete problem in theoretical computer science. For a graph, a vertex cover  $V_{VC}$  is a subset of vertices, such that all edges are incident to at least one member of  $V_{VC}$ . On an ensemble of random graphs (with  $N$  vertices and  $cN/2$  edges), VC exhibits a phase transition controlled by the size of the vertex cover  $x = |V_{VC}|/N$ : For small values  $x$  it is impossible for almost all graphs to find a vertex cover, regardless which vertices are chosen to belong to it, while for  $x$  larger a critical value  $x_c = x_c(c)$  a vertex cover can be found almost surely. This transition coincides with a change of the typical time complexity of algorithms which solve VC. The instances which are the hardest to solve appear in the vicinity of the transition.

Here, the problem is treated by means of computer simulations and analytical calculations. Different algorithms (heuristic and exact) for solving VC are presented. The replica symmetric phase diagram is in excellent agreement with numerical findings up to average connectivity  $c = e$ .

Usually the covers of random graphs are highly degenerate. A quantity which allows to study the structure of the covers is the backbone, which is the subset of all vertices which have in all degenerate covers the same state (i.e. covered or uncovered). The behavior of VC on the  $x = x_c(c)$  phase boundary can be partly understood in terms of percolation transitions appearing at different connectivities  $c$  for the graphs, the non-backbone subgraph and the backbone subgraph and the core.

## **Martin Weight**

### *Typical solution time for a vertex-covering algorithm on finite-connectivity random systems*

Over the last few years, the analysis of phase transition phenomena in combinatorial optimization has increasingly attracted statistical physics. Many methods developed in statistical mechanics of disordered systems can be applied directly to describe the location of such phase transitions, the statistical properties of the solutions, or the behavior of algorithms. Here we analytically describe the typical solution time needed by a backtracking algorithm to solve the vertex-cover decision problem on random graphs. We find two transitions: The first one is algorithm dependent and marks the dynamical transition from linear linear to exponential solution times. The second one gives the maximal computational complexity and is situated exactly at the algorithm-independent phase transition in its solvability. Analytical results are found to agree perfectly with numerical simulations.

This work is done in collaboration with A. K. Hartmann.

## **Kai Nagel**

### *Iterative Relaxation for Network Optimization in Transportation Simulations*

In real transportation systems, people adapt to congestion, that is, they select modes, routes, starting times, etc. such that the effect of congestion is anticipated. In simulations, this is modelled via day-to-day replanning, that is, in each iteration a fraction of the simulated travellers changes plans based on information from the previous iteration. This is thus similar to a standard relaxation technique, where an approximate solution is computed, then behavior of this approximate solution is tested, and then the approximate solution is improved. Also, the questions are similar, for example: Does a given relaxation method converge? Is this solution unique? The simulations are stochastic, what does that mean? Corresponding results for large scale transportation simulations are as of now mostly computational; they indicate that for current scenarios the situation is well-behaved, that is, there is only one basin of attraction and all relaxation methods generate similar traffic patterns. This situation may however change with the inclusion of more degrees of freedom for the agent. – Another set of questions concerns the validity of such relaxed results. If real traffic is “relaxed”, then we have a purely computational problem to find that relaxed state fast. If real traffic however is not relaxed, then we need to model the adaptation process realistically.

## **Hawoong Jeong**

### *The Architecture of Complexity: From the Diameter of the WWW to the Structure of the Cell*

Systems as diverse as the world wide web or the cell are described by networks with complex topology. Traditionally it has been assumed that these networks are random. However, recent studies indicate that such complex systems emerge as a result of self-organizing processes governed by simple but generic laws, resulting in topologies strikingly different from those predicted by random networks. Such studies also lead to a paradigm shift regarding

our approach to complex networks, allowing us to view them as dynamical systems rather than static graphs. I will discuss the implications of these findings on the error and attack tolerance of the Internet, the robustness of the cells.

## Jae-Dong Noh

### *Ground State Property Studies of Random Periodic Elastic Media with a Maxflow/Minicut Algorithm*

Exact combinatorial algorithms developed by computer scientists are useful in studying ground state properties of physical systems with disorder. We apply the Maxflow/Minicut algorithm to study the ground state properties of random periodic elastic media. In periodic elastic media like charge density wave systems or flux line lattices frozen-in disorder (like point defects or other impurities) often competes with the periodic crystal potential. The former tries to roughen the elastic media whereas the latter increases the tendency to keep it flat. We study a lattice model for such a system in three space dimensions at zero temperature by computing their exact ground states using the Maxflow/Minicut algorithm. At a critical ratio between disorder strength and potential depth we find a roughening transition from a flat to a rough phase and characterize it by determining its critical exponents via finite size scaling. They turn out to be close to those of the three-dimensional random field Ising model, the implications are discussed. This work is done in collaboration with H. Rieger.

## Torben Hagerup, Heiko Rieger

### *The $q \rightarrow \infty$ random bond Potts model at criticality as a combinatorial optimization problem*

We consider the  $q$ -state Potts model at the critical temperature  $T_c(q)$  on a square lattice or 2d grid graph  $G = (N, E)$  with random bonds. It is defined by the Hamiltonian  $\mathcal{H} = -\sum_{e \in E} J_e \cdot \delta(S_{s(e)}, S_{t(e)})$  with  $J_e \geq 0$  fixed random variables,  $S_i \in \{1, \dots, q\} \forall i \in N$  and  $\delta(S, S') = 1$  for  $S = S'$  and  $\delta(S, S') = 0$  for  $S \neq S'$ . With the Fortuin-Kasteleyn transformation the partition function can be written as  $\mathcal{Z} = \sum_{x \subset E} q^{n(x) + \sum_{e \in x} (1/2 + w_e)}$ , where the sum is over all subsets  $x$  of the edge set  $E$  of  $G$ ,  $n(x)$  the number of connected components of  $G' = (N, x)$  and  $w_e(J_e)$  random weights symmetrically distributed around 0, e.g.  $w_e = \pm\omega$  with equal probability. In the limit  $q \rightarrow \infty$  the thermodynamic properties are determined by those configurations that maximize the exponent of  $q$  in  $\mathcal{Z}$ , i.e. the solutions to the combinatorial optimization task

$$\max_{x \subset E} \left\{ n(x) + \sum_{e \in x} \left( \frac{1}{2} + w_e \right) \right\}.$$

We discuss a 2/3-approximation to the optimal configuration of this maximization problem utilizing the Gomory-Hu tree of the graph  $G$  (with edge weights  $1/2 + w_e$ ). We compare it with approximate solutions obtained via simulated annealing and extract in this way

estimates for the critical exponents of the  $q \rightarrow \infty$  limit of the random bond Potts model. The exact solution to this combinatorial optimization problem is still an open question. This work has been performed in collaboration with R. Juhász and F. Iglói.

## Miguel Anjos

### *Semidefinite Relaxations for the Max-Cut Problem*

Semidefinite programming (SDP) has become an area of intense research in recent years. One reason for this is its application in computing bounds for quadratic boolean optimization. In this talk we consider the Max-Cut problem for a general graph. We begin by describing the Max-Cut problem and presenting different ways to formulate it as an optimization problem. We then use Lagrangian duality, together with appropriate redundant quadratic constraints, to derive an SDP relaxation that improves on the SDP relaxation studied by Goemans and Williamson. We present theoretical and computational results for this new strengthened relaxation.

This is joint work with H. Wolkowicz.

## Christoph Helmberg

### *Numerical experiments with a semidefinite programming bound for spin glasses*

The task of locating a maximum cut in a weighted graph or finding the ground state in an Ising model of a spin glass may be formulated as a quadratic programming problem in variables  $x_i \in \{+1, -1\}$  for  $i = 1, \dots, n$ . Well known relaxations for the convex hull of all possible interactions between these variables (vectors  $[x_i x_j]_{1 \leq i < j \leq n}$ ) are the metric polytope (the set of all points satisfying all triangle inequalities) in linear programming and a semidefinite relaxation going back to Shor. Both relaxations have provably good properties. For complete graphs, the combination of triangle inequalities and the semidefinite relaxation proved to yield a very strong relaxation in practice. The approach, however, was limited to instances of small size because early semidefinite programming solvers were not able to exploit structure. The new spectral bundle method offers this possibility. Short range models of Ising spin glasses correspond to grid graphs. For these instances the support of the cost matrix is extremely sparse. The metric polytope restricted to this support is described by the so called odd cycle inequalities. In order to approximate for some larger instances the bound obtained from the intersection of the semidefinite relaxation with the odd-cycle polytope we implemented a cutting plane approach based on the spectral bundle method. Even though the spectral bundle method is a subgradient method, the new approach seems to work well. Unfortunately, our preliminary results indicate that on instances arising from Ising spin models with short range interaction the bound is not significantly better than the one obtained by the pure linear programming approach using odd-cycle inequalities exclusively. For the future we consider artificially enlarging the support. This may help to improve the bound because of the coupling effect of the semidefiniteness constraint.