Dagstuhl Seminar No. 9751

Algorithmic Techniques in Physics

organized by

Michael Jünger (Universität zu Köln)
Gerhard Reinelt (Universität Heidelberg)
Heiko Rieger (KFA Jülich)
Giovanni Rinaldi (IASI-CNR Roma)

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1 Preface

Traditionally, there has always been a strong scientific interaction between physicists and mathematicians in developing physics theories. However, even though numerical computations are now commonplace in physics, no comparable interaction between physicists and computer scientists has 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 scientist 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, extremal graph theory, etc.

For instance, when physicists talk about percolation theory, computer scientists would realize that they want to know when a graph has high probability of being connected. Invasion percolation, which occurs, e.g., by injection of a fluid material in a porous medium, and the problem of finding the minimal spanning-tree in a weighted random graph are also identical. Modern simulation methods in computational physics heavily rely on cluster identification, which means simply the detection of connected regions in a graph, or they are based on the construction and modification of hierarchical event trees. Finally, topics from the physics of stochastic processes like random walks play a role in recent algorithmic developments in computer science.

Thus it would be most fruitful to have a forum where physicists inform computer scientists about the problems they are dealing with. In the other direction it is important to keep physicists updated about the most recent algorithmic developments in computer science and in mathematical programming. In particular, in the study of ground states of strongly disordered, amorphous, and glassy materials many algorithms of combinatorial optimization have been applied: Random field systems, interfaces in random media, and diluted antiferromagnets are typical candidates for max-flow/min-cost algorithms; spin glasses are successfully dealt with via matching algorithms and branch-and-cut methods; for flux lines in type-II superconductors and random surface problems minimum-cost-flow algorithms can be applied. The list of interesting physical problems in this context ranges from structural glasses and superconductors over polymers, membranes, and proteins to neural networks. Here in most cases the computation of ground states turns out to be NP-hard or has unknown theoretical complexity. The search for an optimal solution also of these model Hamiltonians is an important task and a real challenge for a computer

scientist.

The predominant methods used by physicists to study these questions numerically are Monte Carlo simulations and/or simulated annealing. These methods are doomed to fail in the most interesting situations. But, as pointed out above, many useful results in optimization algorithms research never reach the physics community, and interesting computational problems in physics do not come to the attention of algorithm designers. There is a definite need to intensify the interaction between the computer science, mathematical programming, and physics communities.

Therefore, it appeared to be obvious to the organizers, that an exchange between these three groups has the potential of being fruitful for all sides: The computer scientists will recognize that computational physicists often deal with very similar problems, and try to solve them with a sometimes more pragmatic approach. And the physicists will profit from the most recent algorithmic development that are useful for them but usually reach their community only decades later. This workshop aimed at bringing together scientist of all three groups in the pursuit of establishing new interactions. We asked the participants to give presentations that are able to break scientific language barriers, and lay the foundations of new interdisciplinary work.

In retrospect, we believe that this seminar was a success. A good mix of tutorials and scientific talks on specific subjects created an atmosphere of lively discussions and interactions, inside and outside the lecture hall. A few new collaborations have indeed been initiated. Many participants stated that they enjoyed the seminar very much and learned a lot from the others. Many suggested a continuation of a new development started in Schloß Dagstuhl.

Due to slippery ice, the traditional Wednesday afternoon excursion had to be cancelled, however, we made up with the "Dagstuhl challenge", namely, computing a ground state of a specific ± 1-Ising-Spin-Glass. The participants competed with the aid of various quickly written computer programs and pure hand calculations. On Thursday evening, in a special ceremony, we could present the promised first prize (a spin glass full of Saarfürst Bier-Eiche) to Gérard Cornuéjols.

2 Final Program

Monday, 15 December 1997

9:00 – 9:15	Introduction
9:15 – 10:15	Rainer Schrader *Tutorial: Efficient Algorithms*
10:15 – 10:45	Coffee
10:45 – 11:45	Yefim Dinits *Tutorial: Network Flow Algorihms*
12:00 – 14:00	Lunch
14:00 – 15:00	Cristian Moukarzel *Tutorial: Percolation*
15:00 – 15:45	Mikko Alava *Application of the Max Flow Algorithm to the Random Field Ising Model*
15:45 – 16:30	Coffee
16:30 – 17:15	Wolfhard Janke *Multicanonical Monte Carlo Algorithms*
17:15 – 18:00	Uwe Täuber *The Coulomb Glass Problem*
18:00	Dinner

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9:00 – 10:00 Ewald Speckenmeyer
Tutorial: Parallel Algorithms

10:00 – 10:30 Coffee

10:30 – 11:30 A. Peter Young
Tutorial: Disordered Systems

11:30 – 12:15 Peter Grassberger
Monte Carlo Simulations of Polymers
by Means of a Generalized Rosenbluth Method

12:15 – 14:00 Lunch

14:00 – 14:45 Jürgen Bendisch
Calculation of Exact Ground States
in 2D Ising Spin Glasses
Using a Matching Algorithm

14:45 – 15:30 Petra Mutzel
An Approach to Exact Ground State Calculation
in 2D Ising Spin Glasses
with Periodic Boundary Conditions

15:30 – 16:15 Coffee & Cake

16:15 – 17:00 Martin Loebl
Graph Theory of Crystal Structures

17:00 – 17:45 Sigismund Kobe
Branch and Bound Algorithm Applied to Problems
of Connectivity in the Low Temperature
Configuration Space of Ising Spin Glasses

18:00 Dinner

Wednesday, 17 December 1997

9:00 – 10:00 Martin Grötschel
Tutorial: Polyhedral Combinatorics

10:00 – 10:30 Coffee

10:30 – 11:30 Naoki Kawashima
Tutorial: Finite Size Scaling and Critical Phenomena

11:30 – 12:15 Cristian Moukarzel
Tutorial: Rigid Percolation

12:15 – 13:45 Lunch

13:45 – 17:45 Excursion to Trier

18:00 – 20:00 Dinner

20:00 – 20:45 Sigismund Kobe
Ernst Ising: Physicist and Teacher

Thursday, 18 December 1997

9:00 – 10:00 Paul Spirakis
Tutorial: Quantum Computing from a Computer Scientist's Point of View

10:00 – 10:30 Coffee

10:30 – 11:15 Matthias Müller & Serge Santos
Geometric Structure Calculations of Dense Macromolecular Systems

11:15 – 12:00 Denis Naddef
Branch and Cut

12:15 – 14:00 Lunch

14:00 – 15:00 Giovanni Rinaldi
Tutorial: Solving NP-hard Ising Spin Glass Problems

15:00 – 15:45 Alexander Hartmann
The Degenerate Ground State Structure of 3D Random Field Systems and 3D $\pm J$ Spin Glasses

15:45 – 16:30 Coffee & Cake

16:30 – 18:00 General Discussion & Working Groups

18:00 – 20:00 Dinner

20:00 – 20:15 The *Spin Glass Award* Ceremony

Friday, 19 December 1997

9:00 – 10:00 Jochem Zowe
Which Material is the Best One?
The Answer of a Mathematician

10:00 – 10:30 Coffee

10:30 – 11:15 Marcus Peinado
Dobrushin Uniqueness, Rapidly Mixing Markov Chains, and Molecular Modelling

11:15 – 12:00 Franz Rendl
Solving Large Scale Max Cut Problems Using Eigenvalue Optimization

12:15 Lunch

3 Abstract of Presentations

Rainer Schrader

Tutorial: Efficient Algorithms

In this introductory talk we focus on basic ideas for efficient algorithms for three problems on graphs: shortest paths, network flows and matchings. Without formally defining efficiency, the algorithms are both empirically as well as theoretically sufficiently fast in that the observed running times are acceptable and worst-case bounds are given by low-degree polynomials in the number of nodes and edges of the graphs. We sketch the idea of Dijkstra's algorithm for the calculation of shortest paths. We observe that the running time is essentially determined by the properties of the underlying data structure for the front nodes. We introduce the notion of augmenting paths for network flows and describe the Ford-Fulkerson algorithm. The optimality of the algorithm is shown via the max-flow-min-cut theorem. The techniques for network flows are transferred to matchings in bipartite graphs. We close by showing that the fundamental algorithmic idea of finding augmenting paths carries over to general graphs.

Yefim Dinitz

Tutorial: Network Flow Algorihms

The history of Discrete Algorithms in Theoretical Computer Science is presented on the example of Network Flow Algorithms. Main concepts: a problem, a provable solution, convergence, finiteness, worst case time bounds. A way to achieve time time efficiency: to use maximally any information obtained, on the example of Layered Network data structure. The method of amortized complexity for proving worst case efficiency bounds. Why shortest augmenting paths provide finiteness? Solvable generalizations of the max-flow problem. Reductions between problems. Equivalence classes of problems w.r.t. existence of a polynomial algorithm. A huge class of NP-complete and NP-hard problems covers almost all known hard problems. An approach in fashion: algorithms with bounded error of the solution found w.r.t. the optimum. Several approximation results for multicommodity flows, in particular, with a logarithmic multiplicative error. An example: the recent 2-approximation algorithm for the one-source unsplittable flow problem.

Cristian Moukarzel

Tutorial: Percolation

A brief overview is given of the main phenomenology involved in a percolative transition. These are discussed in the context of a dilute lattice, that is one in which only a fraction p of the sites (site disorder) or bonds (bond disorder) is present.

Sets of sites connected by at least one path of occupied bonds form clusters, the size of which grows as p is increased. On large systems, there is a sharply defined value p_x

below which no cluster spans the system, and above which with probability one there is a spanning cluster. The density P_∞ of this spanning cluster is therefore zero below p_c, and behaves as $P_\infty \sim (p - p_c)^\beta$ above p_c.

The backbone is the subset of the spanning cluster through which current flows if a potential difference is applied between opposite ends of the system (occupied bonds are good conductors, and empty bonds are insulators), and its density behaves as $B \sim (p-p_c)^{\beta_B}$ above p_c.

A correlation length $\xi(p)$ can be defined as the typical size of finite connected clusters, and it is seen that it diverges on both sides of p_c as $\xi \sim |p - p_c|^{-\nu}$.

Over distances $r < \xi$, connected clusters are fractals, and their mass scales as $M(r) \sim r^{d_f}$ where $d_f = d - \beta/\nu$.

All critical exponents are universal, that is, they do not depend on microscopic details such as the type of lattice (as long as its dimensionality is fixed) or the type of disorder.

Mikko Alava

Application of the Max Flow Algorithm to the Random Field Ising Model

Finding the groundstate of the random field Ising model happens to be formally equivalent to finding the max-flow/ min-cut on a flow network. Moreover, the physics of the RFIM at low temperatures is governed by the groundstate properties so such applications hold much promise.

The best network flow algorithm for this particular problem turns out to be the push-relabel/preflow one with periodic global distance updates and a FIFO stack for the active vertices. The CPU-scaling turns out to be close to $N^{1.2}$. I also discuss a straightforward idea of parallelizing the preflow algorithm for MPP computers by taking advantage of the regular properties of the graphs via domain decomposition.

As a practical application I review recent studies of the groundstates and domain walls of the 2D RFIM. The possibility of studying systems up to $L = 1000$ makes it possible to both understand for the first time the theoretically predicted breakup of the groundstate and the consequences for domain walls. The former follows the expected exponential dependence of the length scale on random field strength. The domain walls are below this scale self-affine but the roughness exponent is about 5/4 and not unity as predicted. Around this length scale the walls break up along with the groundstate, and become fractal.

For all practical purposes the RFIM is now 'solved' in the sense that fast, polynomial algorithms allow the study of the groundstates except perhaps in $D > 2$ in which memory requirements might necessitate the development of efficient parallel network algorithms. There is however a large class of spin-models with discrete symmetry, like the N-state Potts-model, which do not seem to have easy solutions in the form of easy combinatorial algorithms.

Wolfhard Janke

Multicanonical Monte Carlo Algorithms

Canonical Monte Carlo simulations of many disordered systems such as spin glasses and systems undergoing first-order phase transitions are severely hampered by the occurrence of very rare states which lead to exponentially diverging autocorrelation times with increasing system size and hence to exponentially large statistical errors.

One possibility to overcome this problem is the multicanonical reweighting method. Using standard local update algorithms it could be demonstrated that the size dependence of autocorrelation times is then well described by a less divergent power law, $\tau \propto V^{\alpha}$, with $\alpha \approx 1.3$. After a review of the basic ideas, combinations of multicanonical reweighting with *non-local* update algorithms are briefly discussed.

It is first shown that multigrid update techniques further improve the performance of multicanonical simulations by roughly one order of magnitude, uniformly for all system sizes. Then the multibondic algorithm is discussed which combines cluster updates with the reweighting idea. In this way the dynamical exponent α can be reduced to unity, the optimal value one would expect from a random walk argument. Asymptotically for large system sizes the multibondic algorithm therefore always performs better than the standard multicanonical method.

Uwe Täuber

The Coulomb Glass Problem

Investigating the physical properties of localized, interacting particles leads to the *Coulomb glass problem*, which is defined as follows: Distribute N "pinning" sites x_i on $[0, L]^D$, e.g., randomly, then assign a random variable t_i to each site, and to each link the weight function (interaction energy) $V_{ij} = V(|x_i - x_j|)$, which depends on the Euclidean distance $|x_i - x_j|$ only. The task is to find the optimal configuration of site occupation numbers $n_i = 0, 1$ such that the cost function (Hamiltonian) $H = \sum_{i=1}^{N} n_i t_i + \frac{1}{2} \sum_{i \neq j}^{N} n_i n_j V_{ij}$ is minimized, subject to the constraint $\sum_{i=1}^{N} n_i = fN$, with $f < 1$.

Physical implementations have so far employed variants of the Efros/Shklovskii algorithm, which finds approximate, locally stable minima of H by testing with respect to all possible single-particle transfers. Defining site energies $\epsilon_i = t_i + \sum_{j \neq i}^{N} n_j V_{ij}$, this amounts to ensuring that $\Delta_{i \to j} = \epsilon_j - \epsilon_i - V_{ij} > 0$ for all pairs (i, j) with $n_i = 1$ and $n_j = 0$. After taking the ensemble average over many different pin distributions, the output is an estimate for the total ground state energy H, as well as the site energy histogram (density of states) $g(\epsilon)$, as functions of f and the interaction range λ/d, where d is the average site distance. In physical applications, $V(r) = e^{-r/\lambda}/r$ for charge carriers in doped semiconductors, $V(r) = K_0(r/\lambda)$ for magnetic flux lines in type-II superconductors, pinned to columnar defects, with $K_0(x) \sim -\ln x$ for $x \ll 1$, and $K_0(x) \sim x^{-1/2} e^{-x}$ for $x \gg 1$.

The resulting configuration represents topologically strongly disordered, amorphous spatial structure ("glass"), as a consequence of the competition between randomness and interaction-induced correlations. In addition, there appears a dramatic depletion in the

density of states $g(\epsilon)$ in the vicinity of the chemical potential μ, which separates the empty and filled states, of the form $g(\epsilon) \sim |\epsilon - \mu|^s$, where s is a positive, perhaps universal gap exponent. This "Coulomb gap" implies a strong reduction of low-energy transport processes in such systems.

Ewald Speckenmeyer

Tutorial: Parallel Algorithms

The problem of designing a good parallel algorithm is discussed for the warmup example of prefix sum computation. Next models of parallel computation are introduced. Because of their relevance for solving NP-hard problems different load balancing strategies are presented: diffusion type load balancing, load balancing on hypercube and grid networks, and finally a precomputation based load balancing approach of type global information/local migration. Analytical results of the latter load balancing strategy are presented. It is shown that the amount of load moved through a complete binary processor tree is at most four times as high as in an optimal clique network in the average.

A. Peter Young

Tutorial: Disordered Systems

The talk surveyed some basic concepts in the theory of phase transitions in random systems. After explaining why random systems are interesting, and not merely "dirt", some of the popular models, based on the Ising mode, were introduced. The concept of "frustration" was explained, along with a description of two important frustrated models, which have been studied by combinatorial optimization methods, the random field Ising model and the spin glass. The necessity for averaging in random systems and the concept of "self averaging" were discussed next. The talk went on to emphasize the importance of the "defect energy", which can be calculated by combinatorial optimization methods, in determining universal propertied in the vianity of the phase transition. Finally, an unusual feature of spin glasses, which does not occur in "clean" systems, the "chaotic" dependence of the spin configuration on temperature was discussed.

Peter Grassberger

Monte Carlo Simulations of Polymers by Means of a Generalized Rosenbluth Method

We present simulations of long (ca. 100 to 1,000,000 monomers) polymer chains. In the simplest case, the chains are modelled by self avoiding random walks on a regular d-dimensional lattice, with an additional attractive energy between each non-bonded nearest neighbor pair. At infinite temperature, this is the well known excluded volume problem in highly diluted solvents. At low temperature the attraction makes the chains collapse via the so-called 'theta-transition'. Typical observables like the end-to-end distance show

scaling laws with anomalous and 'universal' critical exponents. More complicated models, some with different phase transitions & critical exponents, are obtained by adding walls, porous media, stiff chains, finite dilution, or heterogeneity along the chain as e.g. in heteropolymers.

In most of these cases we can achieve very high efficiency by NOT following the usual Metropolis strategy where the statistical sample is obtained from a Markov process with the Boltzmann distribution as stationary state. Instead, we follow an old idea by Rosenbluth & Rosenbluth who suggested to sacrifice importance sampling by selecting biased configurations. This leads to a weighted sample, unfortunately. Our "Pruned-Enriched Rosenbluth Method" (PERM) is based on the observation] that, in all hard problems, constructing a configuration involves many single steps. Thus we can intervene during the build-up of a configuration by making copies of very successful ones, and killing those with too low weight. This can be done without introducing systematic errors. It leads to a recursive (depth-first) implementation of the "go-with-the-winners" strategy. It gains its efficiency by the great freedom one has in choosing the original bias, the thresholds W^+ and W^-, and the number k of copies.

Jürgen Bendisch

Calculation of Exact Ground States in 2D Ising Spin Glasses Using a Matching Algorithm

In the field of Statistical Physics, building minimal matchings of frustrated plaquettes in random square (sq), honeycomb (hc) and triangular (tr) $\pm J$ Ising models (with mixed boundary conditions) by means of an efficient matching algorithm (by U. Derigs and A. Metz, Univ. of Cologne), exact groundstate-energies and -spin configurations can be calculated. A Fortran 77 program produces, for lattices of a size up to 300×300 plaquettes, average magnetizations, in dependence of given concentrations p of antiferromagnetic bonds. Using the inflection points of the produced empirical curves, one can extrapolate to the wanted groundstate threshold p_c which marks the phase transition between ferro- and para-magnetism. We obtain the estimates $p_{c,hc} \approx 0.065$, $p_{c,sq} \approx 0.10$, $p_{c,tr} \approx 0.15$. Our conjecture is that $p_{c,hc} = 1/15$, $p_{c,sq} = 1/10$, $p_{c,tr} = 3/20$. (The 11) Archimedean and their dual tilings are presented as lattices which are relevant for further investigation on groundstate p_c, in order to obtain a deeper understanding of interrelations among these p_c. So, in particular, as a missing link between square and honeycomb lattices, 3 types of pentagonal lattices are generated, just as the duals of certain Archimedean tilings. We give a conjecture on groundstate p_c for Archimedean tilings and their duals.

Petra Mutzel

An Approach to Exact Ground State Calculation in 2D Ising Spin Glasses with Periodic Boundary Conditions

We consider the problem of exact ground state calculation in 2-dimensional Ising spin glasses with periodic boundary conditions. This problem can be transformed to a max-cut problem in a toroidal grid graph, which can be solved in polynomial time. However, the running time is in the order of $O(L^6)$ for grids of size $L \times L$, and it seems not to be practical for grids of sizes 300×300. When relaxing the periodic boundary conditions, the problem (now, a max-cut problem on a planar grid graph) can be transformed into a minimum perfect matching problem, which can be solved for instances of sizes up to 300×300 (see abstract of J. Bendisch). We like to find a similar algorithm for the toroidal max-cut problem.

We consider a planar embedding of the grid graph $G = (V, E)$ on the torus and its geometric dual graph $G_D = (V_D, E_D)$. We will show that every cut $F \subseteq E$ in the original graph corresponds to an Eulerian subgraph $F_D \subseteq E_D$ in G_D that satisfies certain evenness conditions. Hence, the problem results in searching for a minimum T-Join in G_D on the "odd" vertices of V_D satisfying certain parity constraints. This problem can, e.g., be transformed to a minimum perfect matching problem with parity constraints. Unfortunately, we do not know how to solve this problem (or the constrained T-Join problem) efficiently.

For computational studies, we suggest a 2-step approach. First, we solve the unconstrained minimum perfect matching problem. If the parity constraints are satisfied, we have found the optimum solution to the problem. If not, we suggest to solve a minimum T-Join problem on a graph G'_D. If the solution value is zero, we have found the optimum solution of our original problem in the second step. Our computational studies on 2D-Ising spin glasses with $\pm J$ interactions and $p = 0.5$ show that the second step increases the percentage of solved instances (from previously around 20%) to 60%. (This work has started at the meetings of the max-cut group within an ESPRIT project. The group consists of I. Gierens, M. Jünger, G. Reinelt, G. Rinaldi, C. De Simone and myself).

Martin Loebl

Graph Theory of Crystal Structures

It is shown that the partition function of Ising problem may be written as a linear combination of Pfaffians. The number of terms of the linear combination equals 4^g, where g is the genus of the underlying lattice.

Sigismund Kobe

Branch and Bound Algorithm Applied to Problems of Connectivity in the Low Temperature Configuration Space of Ising Spin Glasses

All ground states and low-lying excitations of a finite Ising spin glass model

$$E_0 = \min \ (- \sum_{i<j}^{1...N} J_{ij} S_i S_j) \quad \text{with} \quad S_i = 1 \vee -1$$

can be found by a branch-and-bound algorithm [1]. The method is illustrated using an example with N = 7 spins (nodes) and arbitrary antiferromagnetic coupling constants $J_{ij} < 0$ (edges). Results for a $4 \times 4 \times 4$ cubic lattice with periodical boundary conditions and random couplings of the strengths $+J$ or $-J$ with $p = 0.5$ are discussed, where p is the concentration of antiferromagnetic couplings. The structure of the states in the configuration space is englightened by a representation by means of 'clusters' in the configuration space and their connectivity. The relaxation behaviour of the system can be described by random walks in this high-dimensional space. Rewriting this task as an eigenvalue problem the influence of 'entropic barriers' in comparison with an unstructured system can be studied, leading to a better understanding of the anomalous slow dynamic behaviour. Finally, based on the knowledge of the cluster structure for energetically low-lying states approximations are proposed to describe the long-time relaxation behaviour of glassy systems.

[1] S. Kobe, A. Hartwig, Comput. Phys. Commun. 16 (1978) 1

Martin Grötschel

Tutorial: Polyhedral Combinatorics

This tutorial presentation aims at introducing the basic concepts of polyhedral combinatorics and outlining the algorithmic aspects of the polyhedral theory of combinatorial optimization problems. Employing the problem of a wolfe, a goat and a bunch of cabbages (known to every child) which was invented more than 1200 years ago by Alcuin of York I describe how real problems are modeled as integer programs. The LP relaxation of Alcuin's problem turns out to reveal all the difficulties that one encounters in practice when trying to solve IP's by LP techniques. I use the issues coming up here to explain some fundamental results of polyhedral theory (the Weyl-Minkowski Theorem, nonredundant representations, characterization of facets and vertices), I outline why it is important to know and use these theoretical concepts for the solution of combinatorial optimization problems by means of cutting plane algorithms. The talk concludes with a discussion of the separation problem for systems of inequalities. Algorithms for this problem form the backbone of all successful branch & cut algorithms of combinatorial optimization.

Naoki Kawashima

Tutorial: Finite Size Scaling and Critical Phenomena

Different materials in different situations sometimes exhibit a similar behavior in the vicinity of critical points. A critical point usually appears as an end point of a phase transition line – a line in a phase diagram at which a phase transition such as the ones from the gas phase to the liquid phase, takes place. As one approaches a critical point, various macro scopic quantities show singular behaviour, usually power-law behaviour with some fractional exponents, which are called critical indices. The type of a critical point determines a global feature of the phase diagram to a certain extent analogous to singular points in the catastrophe theory. Therefore, estimating critical indices is one of the main goals in statistical physics. In order to do this based on computation of finite-sized systems, physicists almost always resort to finite-size-scaling. The key idea is, roughly speaking, that if one takes the correlation length as unit of scale, two systems with the same system size measured in this unit should look the same regardless of other physical parameters. This idea results in a functional form into which most of macroscopic quantities should fit as a function of all the physically relevant parameters and system size. An example of its application is presented for the percolation transition in two-dimensional Ising spin glass model at zero temperature.

Cristian Moukarzel

Tutorial: Rigid Percolation

Central-force rigidity percolation occurs when a diluted lattice composed of points (nodes) joined by bars (edges) is able to transmit stresses on a macroscopic scale. Since bars can freely rotate around their ends (forces are purely central), simple connectivity is not enough for rigidity, so that identifying rigid clusters is not an easy task. This problem of graph rigidity has been studied by mathematicians for a long time and is related to other problems such as the unicity of graph realizations (See for example B. Hendrickson, SIAM J. Comput, 21 (1992), 65). The assumption of generic graph realizations allows one to discuss (generic) rigidity in terms of connectivity properties alone. Of central importance is the concept of constraint redundance. A constraint (a bar) is redundant when it connects two points that where already rigidly linked. Therefore a redundant constraint can be removed without increasing the number of degrees of freedom of the system. Once redundant bars have been removed, the remaining ones (independent bars) cancel one degree of freedom each. On a two-dimensional system composed of n points joined by bars we will then have $2n - \hat{E}$ remaining degrees of freedom, where $\hat{E}$ is the number of independent edges on the system. If the number of remaining degrees of freedom equals 3 the system is said to be *rigid*. It is clear then that all we need is a procedure to identify redundant constraints. In two dimensions the basic theoretical tool for this is given by Laman's theorem:

> A graph $G(n, E)$ with n nodes and E edges contains no redundant edges in two dimensions **iff**

$E' \leq 2n' - 3$, for all subgraphs $G'(n', E')$

Testing this condition in a naive way would require one to look at the 2^n different subgraphs. But it is possible to see that this graph property can be mapped into a property of matchings on an associated bipartite graph, from which a matching algorithm for rigidity can be constructed that runs in $O(n^2)$ worst-case and $\sim O(n)$ on practical cases

(See reference above and: C. Moukarzel, J. Phys. A **29** (1996), 8097).

Sigismund Kobe

Ernst Ising: Physicist and Teacher

The Ising model is a widely used standard model of statistical physics. Every year about 800 papers which apply this model are published; problems regarding neural networks, protein folding, biological membranes, social imitations, social impact in human societies and frustration are among them. Ernst Ising was born on May 10, 1900 in Köln. In his dissertation he studied a model of ferromagnetism which his supervisor Wilhelm Lenz (1988 - 1957) had introduced in 1920 [1, 2]. Milestones of the development of the Ising model are given. The biography of Ernst Ising reflects the life of a Jewish physicist and teacher under the Nazi rule in Germany [3].

[1] W. Lenz, Phys. Zeitschrift 21 (1920) 613
[2] E. Ising, Zeitschrift f. Physik 31 (1925) 253
[3] S. Kobe, J. Stat. Phys. 88 (1997) 991

Paul Spirakis

Tutorial: Quantum Computing from a Computer Scientist's Point of View

This tutorial lecture discusses the differences between a new model of computation (the quantum Turing Machine) and the classical abstract computation models. We examine and demonstrate through examples the natives of quantum interference, quantum parallelism and entanglement and we survey the theoretical construction of a universal quantum Turing Machine. We then define a new class, the Quantum NC, which combines quantum and classical parallelism. We show that the problems of discrete logarithm and factoring both belong to this class, i.e. they can be solved in only polylog time given a polynomial number of quantum processors. We show this by suitable transforming Shor's proof of the inclusion of discrete log in quantum polynomial time.

Matthias Müller & Serge Santos

Geometric Structure Calculations of Dense Macromolecular Systems

A fundamental goal of Material Science is to relate the microscopic structure of a material to its macroscopic properties and to be able to predict the change of these macroscopic properties upon the introduction of chemical modifications at the microscopic level. In its solution, computer simulation, has been established as a powerful tool.

Polymers are an important class of modern materials. Computer simulation plays an ever-expanding role in the design of new polymers, and the understanding of the properties of existing polymers.

In dense polymer systems, the goal of efficient phase-space sampling is a most difficult one, since it is very difficult in polymer MC simulations to change from one configuration to the successive one, especially at high densities. To date, no conventional sampling techniques robust and efficient enough to serve the purpose of ensemble sampling are available.

In our work, we introduce a novel off-lattice sampling technique that aims at enhancing the efficiency of existing MC methods. We focus our attention on three currently incompatible aspects essential for the new algorithm to be a prerequisite for a promising sampling technique: the computational efficiency and robustness, the ability to treat long polymer chains, and the applicability to chemically realistic polymer structures with bulky side-groups.

The novel Parallel-Rotation (ParRot) method is suitable for simulation of glassy polymers, especially for long chains. ParRot operates on the entire chain in contrast to most continuum MC methods that operate only on chain ends or the chain interior.

ParRot also promises to be very suitable for solving the packing problem that consists in constructing "reasonable" amorphous packings starting from atomistic models of single polymer chains. This difficult problem has always been of utmost interest for simulation, since it is very difficult to completely change the starting structure during the simulation of dense atomistically detailed polymer system.

The ParRot move constitutes a basic and essential contribution to the success of this novel approach. Preliminary results have shown that it is possible to generate very large structures of "good" quality for simulation purposes. Advantages of the the ParRot move include the universality of its application to systems of chains of arbitrary length, bond lengths, and angles, monomer-unit size, pendant group structure, and branching structure.

Denis Naddef

Branch and Cut

Branch-and-Cut is a method used in Combinatorial Optimization to solve NP-hard problems. The problem, which is described relatively to a ground set E, is first translated into an Integer Linear Program with in general superexponentially many inequalities.

In a first step this Integer Linear Program is attacked by using a cutting plane algorithm: One starts with a subset of the constraint set, solves it with an LP solver, add violated inequalities which were left out repeat as long as needed. If one fails to obtain an integer solution one splits the problem into two parts and solves each part by the same method.

In the last part of the talk we showed how to augment the probability of success of the method.

Giovanni Rinaldi

Tutorial: Solving NP-hard Ising Spin Glass Problems

The minimum of the Hamiltonian of an Ising system can be computed by finding a maximum cut in a graph. The techniques provided by Polyhedral Combinatorics seem to be the most suitable to solve these problems to optimality for the large sparse instances that derive from the Ising systems of interest in numerical simulations. The first part of the talk is devoted to describing the basic properties of the polytope associated with the maximum cut problem. It is shown how a basic relaxation of the problem can be solved in polynomial time. Using this relaxation in a branch-and-cut framework, it is actually possible to find the exact Hamiltonian of a large number of 2D toroidal systems with up to 10,000 spins. For 3D system this relaxation is unfortunately quite weak to be of practical use. A stronger relaxation is provided by a contraction/lifting procedure. With this procedure it is show how 3D instances of moderate size can be solved to optimality in a reasonable amount of time. Finally, a sensitivity analysis technique is described that can be used for the exact computation of the magnetization of an Ising system as a function of the external field. The relevant parameters estimated via numerical simulations based on these exact techniques seem to disagree with the values predicted by the scaling theory.

Joint work with C. De Simone, M. Diehl, M. Jünger, P. Mutzel, R. Reinelt, H. Rieger.

Alexander Hartmann

The Degenerate Ground State Structure of 3D Random Field Systems and 3D $\Sigma\mathcal{J}$ Spin Glasses

The ground state structure of three dimensional diluted Ising antiferromagnets in a field (DAFF), random field Ising magnets (RFIM) and $\pm J$ Ising spin glasses (SG) are compared. A ground state is the state a system takes at zero temperature (T=0), it is the global minimum at the Energy Function. Ground state structure means that for each realisation of given system there are many different ground states, which all have the same energy. The structure describes how these different ground states are related to each other.

All ground states of DAFF and RFIM system can be calculated at once in polynomial time. Most of the spins ($> 95\%$) have in all ground states always the same orientation, they are signed. The rest of the spins are collected in many small clusters, which interact only rarely. So these clusters can take almost independently two orientations. That means that the number of ground states per system increases exponentially in the system size, but their structure is rather simple.

The ground state calculation for the SG is NP-hard. Using an approximation method called cluster-exact approximation in connection with a genetic algorithm, different ground states are generated. The ground states differ very much, and they are related to each other in an ultrametric way. So we get a very complex structure.

Jochem Zowe

Which Material is the Best One? The Answer of a Mathematician

The talk deals with a central question of structural optimization which is formulated as the problem of finding the stiffest structure which can be made when both the distribution of material as well as the material itself can be freely varied. Our emphasis is on a mathematical formulation which leads to numerical procedures for the problem, and we show that the problem after discretization can be rewritten as a mathematical programming problem of special form. We propose iterative optimization algorithms based on interior-point methods and on semidefinite programming and show a broad range of numerical examples that demonstrates the efficiency of our approach.

Marcus Peinado

Dobrushin Uniqueness, Rapidly Mixing Markov Chains, and Molecular Modelling

We consider the problem of generating random elements from an (exponentially) large set. Problems of this type are of fundamental importance in computer science and in statistical physics. For example, the set could be the set of configurations of a physical system, and the task could be to produce 'typical' configurations. The most successful approach to finding algorithms for such generation problems is based on rapidly-mixing Markov chains. The algorithm designer defines an ergodic Markov chain whose stationary distribution is the desired output distribution. The Markov chain is called rapidly-mixing if it approaches this distribution 'rapidly'. In practice, the main problem is to prove that a given Markov chain is indeed rapidly mixing. We discuss the technique of Dobrushin uniqueness which originates in mathematical physics. Finally, we extend the basic technique and obtain a rapidly mixing Markov chain for a problem from computational chemistry whose irregular structure had, until now, eluded analysis.

Franz Rendl

Solving Large Scale Max Cut Problems Using Eigenvalue Optimization

Recently, semidefinite relaxations for the max-cut problem have found increased interest, due to their theoretical approximation properties. From a computational point of view, interior point methods turn out to be very efficient to solve problems of medium size, say $n \approx 200$. On the other hand, these methods become impractical for larger instances, because one has to deal with dense linear algebra.

As alternative, we propose to study the dual of the semidefinite program, and reformulate it as eigenvalue optimization problem. We present a modification of the bundle method to deal with this problem. The key ingredients are a nonpolyhedral approximation of the ε subdifferential to build a local model. The computation of the step direction thus reduces to a quadratic but convex semidefinite program of small size. The approach has

been tested on a variety of large (but sparse) instances, and seems to provide a practical method for larger size problems.

4 Appendix

The Dagstuhl Spin Glass Challenge

The Winner's Entry