Tagungsbericht 9/1995

Large Discrete Systems

26.02. – 04.03.1995

The workshop on "Large Discrete Systems" was planned by Thomas Beth (Karlsruhe) and Martin Grötschel (Berlin). It was intended as a meeting of people from different areas of science and mathematics to talk to each other, to learn, and to provide information that others may benefit from. The traditionally spontaneous and flexible schedule of Oberwolfach Conferences was especially advantageous for this interdisciplinary workshop. Many talks had an additional computer demonstration or discussion in the evening. In contrast to usual Oberwolfach Conferences we had more survey talks which lead to rather specialized discussions. Due to collisions with some other important conferences it was not possible to get together representatives of all sciences that are connected to large discrete systems. But in reviewing the workshop we had the impression that it was just the right number of participants to really profit from all the different areas that were discussed. For more detailed information on the aims and scopes of the workshop see the abstract of the general introduction by Th. Beth.

The positive atmosphere of Mathematisches Forschungsinstitut was supported by the well known hospitality of the staff and the dedication of Matthias Kreck, the director of the institute. It is largely owing to them that all participants left with a positive feeling.

Vortragsauszüge

Th. Beth

Large Discrete Systems - An Attempt towards Synergy

In setting the stage of our Workshop, it is briefly described what has been envisaged by the organizers by combining the many different areas which are to be represented at this conference. Using the classical epistemological hierarchy of systems the general system descriptions can be classified at the three different levels:

- behaviour level,
- state level and
- structure level.

Simultaneously the engineering and control aspects of such systems have to be considered with the preceding epistomolgy to give some guidance as to approach this problem, in which aspects of control and optimization will go together very closely.

If complex systems are considered at some detail with mathematical tools and languages at the behavioural and state level, these methods have to be transformed to allow a mathematical approach from the structure level. This point of view is in view of this conference the major challenge to the areas combined from mathematics, physics, chemistry biology, engineering, and informatics.

The question of setting up layer systems and devices is closely relating mathematical sciences, lifesciences and technical sciences, as for instance can be seen in the principle of selforganization of processes in chemistry, physics, biochemistry, genetics as well as in traffic control and growth processes of the combinatorial type. Combinatorial optimization techniques go closely together with molecular modelling and energy minimization. Large networks such as Internet or telephone are examples of large discrete systems they grow according to laws which are not inherent in the design principles and programming at structure and state level. However, such systems are working

rather well. We hope that this conference has contributed to the understanding, why?!

H. Meinhardt

Models of biological pattern formation during the development of higher order organisms

A fascinating aspect of biological systems is the generation of complex structures of an organism during its embryonic development. This process can be separated into relatively independent elementary processes that are accessible to modelling. Molecular feasible interactions are able to describe the observed developmental regulation after an experimental interference. The following processes are proposed to play a decisive rôle. (i) By local self-enhancement and long ranging inhibition, local concentration maxima are generated, that, for instance, generate the main embryonic axes. (ii) Non-linear autocatalytic activation of genes cause region-specific gene activations with sharp borders. These borders become the organizing regions for the next structures to be formed; for instance legs and wings are initiated this way. By computer simulation we have shown that such sets of coupled differential equations describing production, decay, and diffusion of substances account for experimental observations in fine details

H. Jürgensen

Molecular Switching

In the early 80's F. L. Carter proposed to use the fact that soliton waves travelling through molecules change the bonds as a switching mechanism - "soliton valves". Abstracting from the physical and chemical situation, we consider automata the state sets of which are weighted graphs - "soliton automata". We describe their computational power in terms of their transition monoids. One finds that comparatively simple soliton graphs give rise to quite large primitive groups of permutations, thus promising to be highly efficient switching elements in computers of the (distant) future.

Th. Lengauer

Prediction of Receptor - Ligand Interaction

We report on the results of a cooperation with pharmaceutical industry

(BASF, Merck) and molecular biologists (EMBL). The Task is to develop algorithms for predicting the three-dimensional structure of the molecular complex of a protein with a ligand molecule with low molecular weight. Input to the problem is the 3d-structure of the protein and the structure formula of of the ligand molecule. In order to find low-energy structures for the molecular complex we have to (i) model chemical interactions such as H-bonds, salt bridges, and lipophilic interactions explicitly, (ii) take the flexibility of the ligand molecule into account and use it in order to structure the configuration space. We formulate a discrete version of the problem and use modifications of methods from computer vision, data clustering, and tree traversal to construct low energy solutions. Our algorithm has been tested on 10 resolved molecular complexes. It computes realistic samples of low-energy complexes, among them solutions with satisfactory accuracy - i. e., accuracy within the limits of experimental resolution, in a few minutes on a common workstation. Joint work with: M. Rarey, S. Wefing , B. Kramer.

U. Oberst

The optimal Fast Gelfand, Fourier and Hartley Transforms

The *Discrete Gelfand Transform* (DGT) is defined on the complexification $\mathbf{C} \otimes_{\mathbf{Q}} A$ of an abelian $\mathbf{Q}$-algebra A and specializes to the *Discrete Fourier Transform* (DFT) on the complex group algebra $\mathbf{C}[G] = \mathbf{C} \otimes_{\mathbf{Q}} \mathbf{Q}[G]$ of a finite abelian group. The *Discrete Hartley Transform* (DHT) is defined on the *real* algebra $\mathbf{R} \otimes_{\mathbf{Q}} A$ and specializes to the Hartley Transform on the *real* group algebra $\mathbf{R}[G]$ ("real signals"). Algorithms which compute these transforms "fast", i. e. with low complexity, are called *Fast Transforms of the given type*, abbreviated as FGT, FHT or FFT. The complexity measure used here is the *relative multiplicative complexity* introduced by S. Winograd. In colloquial terms it counts the number of proper complex resp. real multiplications of the algorithm whereas $\mathbf{Q}$-linear combinations are considered costless or of complexity zero. A FGT, FHT or FFT is *optimal* if it has minimal complexity among all applicable fast transforms, and this complexity is then called the complexity of the transform. The main result of the work presented in this talk is the determination of the complexities of the DGT, DHT and DFT and the construction of the associated optimal FGT, FHT, and FFT algorithms.

The original idea for the optimal fast transforms presented here is due to C. M. Rader (1968) who used a fast convolution for the FFT on a cyclic group of prime order. This idea was taken up and extended by S. Winograd,

L. Auslander and E. Feig from 1978 to 1984 and others. An important and for the field new ingredient of the theory and the algorithms is the Galois Theory of abelian number fields.

The usefulness of the FFT for *Large Discrete Systems*, for instance in signal processing and in particular image processing, is well established. The general FGT and FHT can be applied to the Fourier transform of complex or real signals with additional symmetry properties where the FFT does not nearly yield the best results.

T. Minkwitz
Spectral Analysis of Non-Continous Systems

Classical signal transforms define a spectrum for a signal over $\mathbf{R}^n$. They are used to observe invariant features of some sort (e. g. the power spectrum of the Fourier transform) or to manipulate a signal(e. g. through a filter). To do the needed computation for the transform on a digital computer, the $\mathbf{R}^n$ is sampled and thus the signal becomes discrete. It is now possible to generalize this concept. Many systems in engineering can be viewed as coupled subsystems of some sort. An example is a parallel computer or the telephone system. The subsystems are the processors or switches resp. and the physical connections link these subsystems. This architecture (structure) can be viewed as a graph with subsystems, being vertices and connections being edges. To analyse a feature (observable variable or state) of the subsystems, one can often use the automorphism group of the graph and define a spectral transform for that group. This way features of the systems can be found that are invariant under the system structure's automorphism group. It is also possible to use the group to derive fast algorithms for the spectral transform. A difficult and still not understood problem is the construction of spectral transforms that use a "nice" basis of the spectral space. The nice properties one would like are usually defined in terms of analysis (such as smoothness) which is difficult to incorporate into algebraic considerations.

F. Vogt, R. Wille
Conceptual data and knowledge systems

Conceptual data and knowledge systems are recent developments of the research group on concept analysis at the TH Darmstadt. They are based on notions and results of formal concept analysis which is a formal theory of

concepts and concept systems. Conceptual data systems can be realized by the program system TOSCANA and applied for analysing and exploring data. Examples of applications are discussed in a wide range. Conceptual data systems can be extended to conceptual knowledge systems by adding components of knowledge inference and acquisition. Several mathematical and computer science problems are mentioned in this context.

A. Ekert
Quantum Computation

As computers become faster they must become smaller because of the finiteness of the speed of light. The history of computer science has involved a sequence of changes from one type of physical realisation to another - from gears to relays to valves to transistors to integrated circuits and so on. Quantum mechanics is already important in the design of microelectronic components. Soon it will be necessary to harness quantum mechanics rather then simply take it into account, and at that point it will be possible to give data processing devices new functionality. Quantum entanglement and quantum interference will make quantum computation so powerful that many problems which are believed to be intractable on any classical computer, will become efficiently solvable. In order to illustrate the power of quantum data processing a brief discussion of Shor's quantum factoring algorithm has been provided and possibilities of its practical implementation have been discussed

D. DiVincenzo
Physical Realisation of Quantum Computers

There are severe constraints on the physical implementation of computation in quantum mechanical systems. Some of the best possible systems today, nuclear spin systems and cold ion traps, have been identified. A protocol for executing computations in these systems, borrowed directly from the physics of magnetic resonance, has been worked out. A minimal repertoire of such operations has been identified.

G. Mahler
At Home in a Quantum World

Quantum properties come in mutually exclusive subsets: Those being "compatible" (their operators commute) and those being incompatible (then formally appearing as superpositions). For a composite system this may lead to a situation in which local subsystem - and non-local cluster - properties are incompatible. The destruction of this web of correlations (in a local measurement) can give rise to observable effects like "spooky" action at a distance (entanglement) and even "time-travels" (non-locality in time).

Our limited experience with those strange features is now rapidly being enlarged via novel experiments and numerical simulations alike. On a very large scale, quantum computation (factoring problem) tries to exploit these fragile effects for exponential speed-up. The physical requirements for this to work in a controllable fashion are extremely demanding, though.

P. Hammerling
Lasers: Principles, Propagation and Interactions

This talk will discuss the physical principles and some practical issues underlying high-energy glass laser design. Also to be discussed is the propagation of the laser beam in the atmosphere and its interaction with a target in the context of laser induced fusion.The laser may be viewed as an example of the design of a large discrete system whose output beam can be used in a variety of applications. As will be seen, the nuclear fusion problem involves many complex physics issues and is described by equations that are solved numerically. The laser design in itself is not too numerically intensive, however, the fusion application requires the numerical solution of the hydrodynamic equations coupled to radiation transport, laser absorption, and nuclear particle transport to mention but a few features. This will be illustrated and discussed in the talk.

In its propagation within the laser glass, the beam can, due to a non-linear interaction with the glass, self-focus and cause damage. This can be controlled by limiting the propagation length as well as in the glass production process. Another non-linear process is used to double or triple the laser frequency. The plasma physics experience indicates that higher frequencies couple better to matter. However, the large glass lasers operate in the infra-red part of the

spectrum. Hence the necessity of frequency conversion.

Propagation of an intense laser beam in the atmosphere can suffer distortion due not only to turbulence but to a self-interaction wherein the beam heats the atmosphere it travels in thereby altering the refractive index. This effect, called thermal blooming, can increase the beams divergence. If one imagines an intense beam propagating downwards from above the atmosphere, there can be the possibility of stimulated Raman scattering by the atmospheric nitrogen, leading to generation of lower frequency beams and degrading the energy of the main beam.

The interaction of laser light with matter and its later comportment also can involve non-linear processes. Consider the laser fusion scheme wherein one illuminates a spherical target filled with a mixture of deuterium and tritium, eventually leading to an implosion which compresses and heats the fuel to ignition conditions.The incident laser beam first heats and vaporizes part of the target creating a low density corona. This region is susceptible to various plasma instabilities, stimulated Brillouin scattering which can lead to enhanced reflection of the beam and stimulated Raman scattering which can lead to acceleration of some of the electrons in the coronal region, these can penetrate and pre-heat the interior of the target and thus degrade its performance. While these two effects can be minimized by using higher frequency light, there are various hydrodynamic instabilities, such as the Rayleigh-Taylor instability, which can lead either to target breakup or degradation of the implosion conditions. This can be controlled by reducing the surface finish imperfections to a minimum as well as the laser intensity fluctuations around the target. The difficulty of achieving a sufficiently smooth incident laser beam, has led to the further conversion of the incident beam into incoherent soft X-rays. This latter takes place within a high Z capsule surrounding the original target. The laser beams impinge on and heat the inside walls of this cavity so that it acts like a black-body with radiation temperature in the range of millions of degrees. This can create a much smoother driving pressure around the target than direct illumination by a laser. These experiments take place in the temporal range of nanoseconds and the energy range of tens of kilojoules with megajoule facilities now being designed and developed. This combination of numerical modeling, experimental checks, materials research, etc. is typical of a modern, complex scientific project.

A recent development, still very much in the research phase is the advent of very intense laser light sources in the range of 100 femtoseconds. When focused the incident intensity can exceed $10^{19} W/cm^2$. Such intensities lead

to new effects, for example the electrons in the plasma created or interacting with such a beam can be accelerated to relativistic velocities. This leads to the intriguing idea that by suitably timing the arrival of such an intense beam on an imploding target, a part of the fuel could be heated to ignition conditions and thus ignite the rest.

D. Lazic

The Channel Coding Problem considered as Optimisation and Control of Large Discrete Systems

Using the channel-determined topology for bounding the error exponent of specific encoding spaces, it is shown that either binary codes with minimum distances that exceed the Gilbert-Varshamov bound do not exist, or if they exist they cannot reach the capacity of the binary symmetric channel. The solution to the still open famous problem in coding theory, of finding binary codes that exceed the Gilbert-Varshamov bound, does not yield codes that perform better according to the error probability criterion than almost all linear and nonlinear binary codes if these are optimally decoded and if the code rate is in the permissible range.

Th. Liebling

Polycrystal Growth Models in 3D

Polycrystals are structures found in various kinds of materials in particular ceramics. They can be modeled as Partitions of a region in $\mathbf{R}^3$ into convex polyhedra. From a theorem by Chandler Davis we know that any (simple) partition of $\mathbf{R}^d$ ($d \geq 3$)into convex regions can be viewed as a power or Laguerre diagram generated by a corresponding set of spheres or weighted sites. Such diagrams are therefore well suited to model polycrystalline structures. Analogous structures can be constructed in the unit flat torus T^d allowing for periodical boundary conditions. The construction of Laguerre diagrams (viz. their duals, Delaunay partitions) is accomplished using an incremental flip algorithm that is demonstrably finite and experimentally efficient. Dynamics are introduced into the model by minimizing an energy function, which is essentially measured as the total grain interface area. This function, i. e. its gradient is reported on the generating site parameters thereby defining motion equations. These are integrated until the first elementary topological transformations becomes necessary to keep the structure coherent. The

corresponding generalized Whitney move is then executed and the process is continued. Identifying such events is efficiently carried out via Sturm polynomials. Numerical simulation on large scale examples (with up to 10000 3D cells) shows good agreement with empirical data from plane cuts of real alumina polycrystals. This is based on work joint with A. Mocellin from Ecole des Mines de Nancy and H. Telley, F. Righetti and X. Xue from EPFL.

R. Burkard

Assignment problems and asymptotic properties of combinatorial optimization problems

After a survey of linear and quadratic assignment problems and their applications we discuss the recently introduced biquadratic assignment problems which arose in connection with circuit design.

We show the bad performance of branch and bound codes on this problem class and the favourable behaviour of simulated annealing. this might be connected with the asymptotic behaviour of this problem class. We can show that all objective values tend a. s. with increasing size to the expectation value of the cost coefficients. This finds a nice setting by applying Boltzman statistics.

A. Bachem

High-speed microsimulations of traffic flow

In this talk we report on the usefulness of very fast hardware-oriented microscopic models for traffic simulation. For this purpose the methodology of cellular automata is adopted to the needs of traffic simulations. It correctly reproduces start-stop-waves and fundamental diagrams. Two limits of the model are investigated in detail - the deterministic limit, where all randomness is taken out of the model; and the "cruise control limit" when only the randomness at full speed is set to zero.

In the second part of the talk we report on experiments with traffic in networks. We show that traffic management (ATMS) will push traffic near maximum flow and thus prediction and control will become harder and harder. Finally we discuss the effect of road and congestion pricing on the maximum throughput

A. Schrijver
Discrete Systems at the Dutch Railways

We discuss two combinatorial problems of the Dutch Railways. The first considers minimizing the amount of rolling stock to be purchased in order to provide enough seats on each scheduled train. This would be an ordinary minimum cost circulation problem if only one type of stock is involved, but when two types should be routed (mutually couplable) we get a multicommunity flow problem. We show how this problem can be solved with the method of combinatorics.

The second problem concerns the design of the hourly pattern of the railway schedule. This reduces to solving a system of linear equation over the cyclic group of 60 elements. We describe a method to find a solution with the help of identifying a short cycle basis for the underlying graph.

D. Welsh
Problems about Knots

This surveys some combinatorial questions about knot recognition and enumeration. Deciding whether two knots are isotopic is still not known even to be in double exponential time (or space). The knot polynomials excluding the Alexander have all been shown to be ♯P-hard to evaluate at all but a few special points. Thus these offer little hope of success. The enumeration problem :- I have shown (1991) that the number of prime links lies between $O(4^n)$ and $O(27/2)^n$ where n is the crossing number. However the limit of $n^{-1} \log l(n)$ is not known to exist. I conjecture it does and that the inequalities $l(m+n) \geq l(m)\, l(n)$ are true $(n, m \geq 3)$. A similar inequality for $a(n)$ is also conjectured. Proving either of these would settle the limit question above.

A. Kerber
Constructive Theory of Discrete Structures and Applications

(Joint work with R. Laue et al.). It was reported on some methods used in the construction of discrete structures like

graphs and multigraphs,

molecular graphs,

linear codes,

designs.

Emphasize lay on molecular graphs and our software package MOLGEN, as well as on the recent discovery of 7-designs with small parameters ($\lambda = 10, 16$).

R. Weismantel, G. Ziegler
Test sets in Integer Programming

In this talk we study an integer programming problem of the type:

$$\max cx,$$

$$Ax \leq b,$$

$$0 \leq x \leq u,$$

x integral and $A \in \mathbb{Z}^{n \times m}$, $b \in \mathbb{Z}^m$, $u \in \mathbb{N}^n$, $c \in \mathbb{Z}^n$.

A test set is a subset of vectors in $\mathbb{Z}^n$ such that from any feasible, non-optimal point, one can move to a better point by applying an element of the test set. We show in particular, how to compute a test set for integer programs when the matrix has non-negative entries. This algorithm has a connection to the Buchberger algorithm for computing the reduced Gröbner basis of an ideal.

If the integer programming problem is a 0/1 program, we establish the equivalence of the following three problems in terms of complexity:

1. The optimization problem.
2. The augmentation problem, i. e., given an objective function c and a feasible point x^{old}, find v such that $cv > 0$, $x^{old} + v$ is feasible, or assert that no such v exists.
3. The problem of finding an augmentation vector that is irreducible.

A. Martin

A polyhedral approach to the routing problem in VLSI

One of the major tasks in VLSI-design is the routing problem. Here, given sets of points (so-called nets) have to be connected by wires where many technical side constraints have to be taken into account and an objective function like the total wiring length must be minimized. Usually the routing problem is to complex to be solved in one step. Depending on the users choice of decomposing the problem, depending on the underlying fabrication technology and depending on the given design rules many subproblems arise that can be formulated as follows: Given a graph $G = (V, E)$ with edge weights ω_e, edge capacities c_e, $e \in E$, and node sets $T_1, \ldots, T_N$, find edge sets $S_1, \ldots, S_N$ such that each S_k connects T_k, at most c_e of these edge sets use edge e for each $e \in E$, and the weighted sum of the edge sets is minimal. We call this problem the Steiner tree packing problem and every feasible solution a Steiner tree packing. We consider the Steiner tree packing problem from a polyhedral point of view. We define an appropriate polyhedron P whose vertices are in one-to-one correspondence to the Steiner tree packings in the graph and look for a good inequality description of P. We use this inequality description to develop a branch and cut algorithm. We will sketch some of the implementation details of this algorithm including separation and primal heuristics. Finally, we present some results for a special routing problem in VLSI design, the so called switchbox routing problem. (This is joint work with M. Grötschel and R. Weismantel.)

A. Ekert

Quantum Cryptography

The purpose of cryptography is to transmit information in such a way that access to it is restricted to the intended recipients. While classical cryptography employs various mathematical techniques to restrict eavesdroppers from learning the content of encrypted messages, in quantum mechanics the information is protected by the laws of physics. In classical cryptography an absolute security of information cannot be guaranteed. The Heisenberg uncertainty principle and quantum entanglement can be exploited in a system of secure communication, often referred to as "quantum cryptography".

Quantum cryptography provides a means for two parties to exchange an encyphering key over a private channel with absolute security of communication. I have discussed one particular quantum cryptosystem in which the key encoding is based on quantum entanglement and the Bell theorem

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