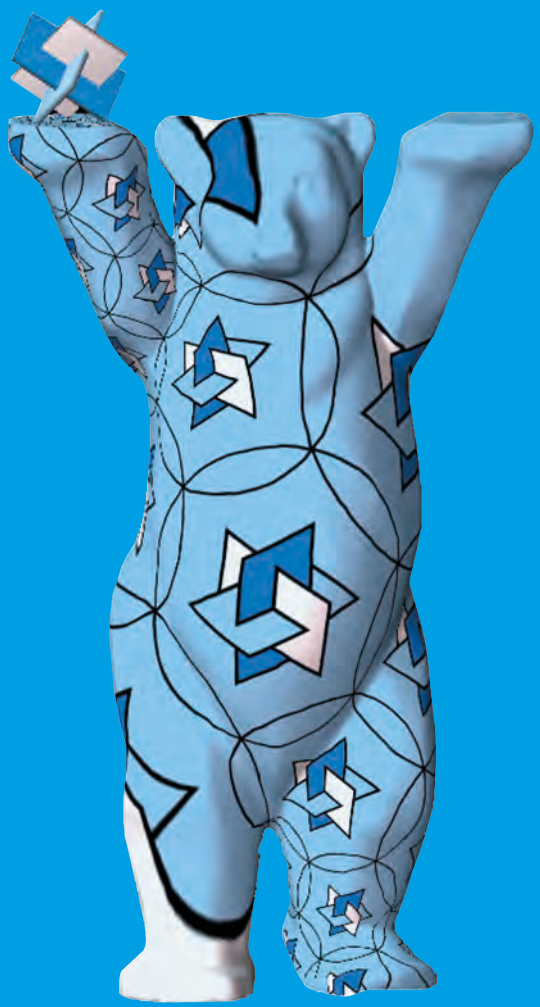
DFG Research Center

MATHEON

Mathematics for Key Technologies

Showcases



Showcases

Introduction

Martin Grötschel and Volker Mehrmann

Making ourselves understood is a challenge for us mathematicians. Since its foundation the DFG Research Center MATHEON has been trying hard to provide insight into its research activities, to illuminate the mathematical theories and techniques that are developed, to highlight where this methodology is employed outside of mathematics and how MATHEON mathematics affects industry, commerce, society, other sciences, and even our daily life.

This booklet presents twenty six showcases illustrating some of the achievements of the DFG Research Center MATHEON during the years 2002–2014. The examples concentrate on applications, mention the mathematics involved only briefly, and are written in a language that is (we hope) easily understandable by non-mathematicians.

At its establishment in 2002 MATHEON started with the following mission:

Key technologies become more complex, innovation cycles get shorter. Flexible mathematical models open new possibilities to master complexity, to react quickly, and to explore new smart options. Such models can only be obtained via abstraction. This line of thought provides our global vision: Innovation needs flexibility, flexibility needs abstraction, the language of abstraction is mathematics. But mathematics is not only a language, it adds value: theoretical insight, efficient algorithms, optimal solutions. Thus, key technologies and mathematics interact in a joint innovation process.

The mission of the Center is to give a strong push to the role of mathematics in this interactive process. The Center's research program is application-driven. Its implementation will have a strong impact on the development of mathematics itself and will define a new stage of inter- and transdisciplinary cooperation.

The showcases demonstrate that these goals have been achieved and indicate the transversal role that mathematics plays a in the solution of a wide variety of application problems. The presentation of the success stories is organized along the MATHEON *Application Areas: Life Sciences, Networks, Production, Electronic and Photonic Devices, Finance, Visualization*, and *Education*. These examples show that mathematical research in current key technologies requires a strong interdisciplinary effort performed in teams from applications and several different mathematical disciplines.

We hope that these showcases find a wide public readership, in particular, in schools, universities, and in the media and that they lead to a better understanding of the great impact that application driven mathematical research has on our quality of life.

November 30, 2007: Matheon wins "'Germany Land of Ideas"' award – applause from the next generation (Photo: Kay Herschelmann/MATHEON)

Mathematics without pain

Marcus Weber and Peter Deuflhard

In 1803/04, the 20 year old German apothecary Friedrich Sertürner (1783–1841) extracted morphine from opium poppy as a potential pain relief drug. In his later life he used it to cure his depressive moods, which got him addicted and thus made him the victim of his own invention. Chemically speaking, the morphine molecule binds to the μ-opioid receptor. These receptors occur both as central and as peripheral ones. The central receptors located in the brain are responsible for the undesirable side effects such as drowsiness, respiratory depression, or addiction. The aim of the project has been to construct potential drugs that activate the peripheral receptors, thus relieving the pain at the location where it originates, while leaving the central receptors unaffected. The approach taken here is rather different from other approaches pursued in recent years. It relies heavily on the efficiency of algorithms developed within MATHEON. The main consideration is as follows: Pain is predominantly connected to inflammation, which, in turn, is accompanied with tissue acidosis. This means that the pH-value of inflamed tissue is lower than the one of healthy tissue. The idea is to find a morphine-like molecule active at low pH-value, but inactive at normal pH-value. Such a molecule would react only with the peripheral μ-opioid receptors in inflamed tissue, but not with central ones in healthy tissue (such as in the brain).

The project has been carried out in close cooperation with C. Stein and C. Zöllner at Charité. Data about the three-dimensional structure of the receptor protein were not available before 2012. In a first step, upon using chemical modeling tools (based on molecular homologies) as well as mathematical molecular simulation, we were able to propose a possible binding pocket for the morphine molecule. On this basis, we identified important amino-acids of the receptor that actually interact with the morphine molecule in a pH-dependent manner. Subsequently, these basic model assumptions were confirmed by chemical experiments at Charité.

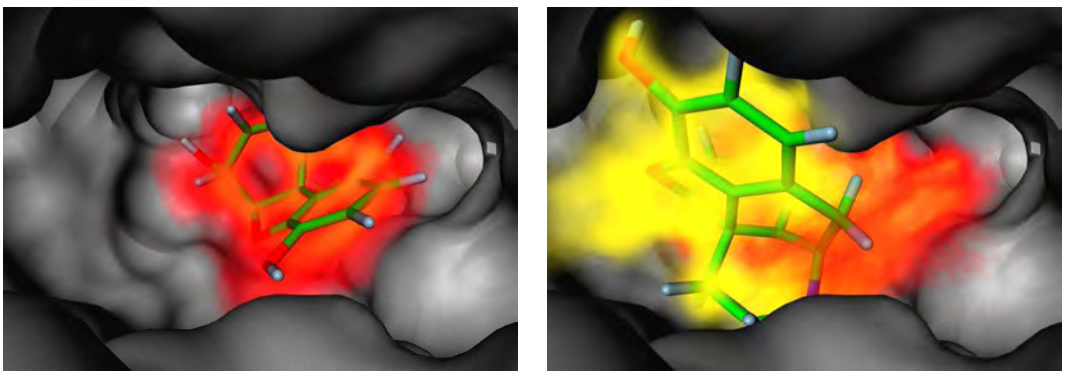


Figure 1. *Different conformations of the new morphine-like molecule in the binding pocket.*
Left *(inflamed tissue, low pH): The new substance remains inside the molecular pocket (red conformation), thus activating the receptor.* Right *(healthy tissue, normal pH): The new substance predominantly escapes from the receptor pocket (yellow rather than red conformation is now dominant).*

The next step was to figure out, which kind of chemical manipulation of "morphine-like" molecules would lead to a pH-dependent change of their electrostatic properties in the proximity of the identified amino acids. Upon using conformation dynamics analysis as well as quantum chemical calculations, a shortlist of five potential drug candidates was created. In order to find out, which of the possible candidates would exhibit the desired selective binding affinity to the receptor, a fully flexible receptor-drug binding process needed to be simulated numerically. This task was based on our mesh-free approximations of metastable conformations as membership functions in high-dimensional spaces. For each drug candidate, binding modes inside the receptor pocket were carefully identified. The binding modes were computed as metastable subsets [1] of the full receptor-drug system. Figure 1, left, shows that, at low pH values, there is only one metastable conformation locally confined to the inflamed tissue. In contrast, Figure 1, right, reveals that, at normal pH value (healthy tissue, e.g., brain), there are two metastable conformations, with the "escape" mode (yellow) being the dominant one. However, careful inspection of the thus identified molecule revealed that its synthesis seemed to be too expensive (if at all possible). After several interdisciplinary loops between organic chemists and MATHEON numerical analysts, we found a fentanyl-like candidate expected to have the same desired properties. This molecule was then synthesized. Meanwhile, the substance was tested in animal experiments: After injection of the fentanyl-like molecule, the laboratory mice showed a clear analgetic effect only in the inflamed paw. Moreover, first tests on side effects were successful: While already small amounts of "normal" fentanyl kill the mice, our fentanyl-derivate did not kill them, even after an administration of 400 times the lethal dosis for the "normal" fentanyl. This is not yet a fully creditable proof, but definitely a clear hint that healthy central μ-receptors (in the brain) are not activated. The whole design process was significantly speeded up by our fast algorithms, saving a lot of money and time of development and animal testings. On this basis, we submitted two patents, one for the drug candidate and one for the computational design method [2].

The fentanyl-like molecule was synthesized by a chemical company in Berlin (NDA). The tests and computations were partially supported by the BMBF-initiative VIP. In order to be able to commercialize the two patents, the spin-off company mathPharm GmbH was started. In the near future, we aim at developing more selective drug molecules for different types of diseases. The mathematical part of the design process will always be the same: detailed modeling and simulation of the binding process on an atomistic level, made possible by our new efficient algorithms.

Further reading

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[2] C. Stein, C. Zöllner, M. Weber, and O. Scharkoi. Fentanyl derivatives as pH-dependent opioid receptor agonists. Published patent, PCT/EP2012/066071.

Mathematical secrets of the female cycle

Susanna Röblitz and Peter Deuflhard

A detailed understanding of the human menstrual cycle is both medically and economically important. In close funded cooperation over years with the pharmaceutical company Pfizer the mathematical model GynCycle [1] has been developed as a basis to study the administration of drugs. Three main steps had to be taken: (I) from a physiological model to a compartment model, (II) from the compartment model to a differential equation model, (III) identification of unknown parameters from comparison with measurements.

Step (I) means the establishment of the governing regulatory circuit. Figure 1 shows the compartments hypothalamus, pituitary gland, and ovaries, connected by the bloodstream. In the hypothalamus, the hormone GnRH (gonadotropin-releasing hormone) is formed, which reaches the pituitary gland through a portal system in the form of pulses and stimulates the release of the gonadotropins LH (luteinizing hormone) and FSH (follicle-stimulating hormone) into the bloodstream. The gonadotropins regulate the processes in the ovaries, i.e., the multi-stage maturation process of the follicles, the ovulation and the development of the corpus luteum, which control the synthesis of the steroids progesterone and estradiol and of the hormone inhibin. Through the blood, these hormones reach the hypothalamus and pituitary gland, where, in turn, they influence the formation of GnRH, LH and FSH.

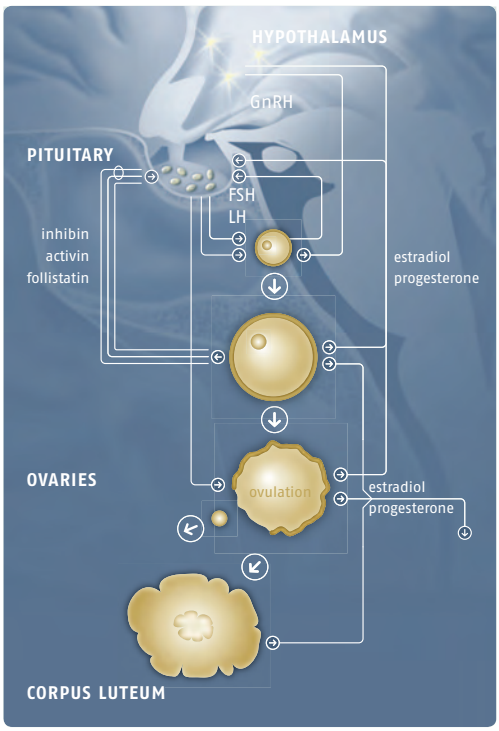

Figure 1. *Physiological compartments of the human menstrual cycle*

Step (II) comprises the mathematical description of the physiological processes by means of ordinary differential equations (ODEs) that describe the time dependent behavior of the species concentrations involved. In order to be able to formulate the ODEs, the occurring physiological and biological processes must be known quite accurately. In reality, however, the exact chemical reaction mechanisms are often not understood in sufficient detail; rather one only knows whether certain hormones exert either a stimulating or an inhibiting effect on other hormones – here modeled by Hill functions. If the reaction mechanisms are known more specifically, e.g., from a database, more detailed equations can be formulated. Once all processes are included in the model, a large system of ODEs arises.

Step (III), the identification of unknown parameters occurring in the models, is still mathematically challenging. Only few of them can be measured or associated with approximate ranges of values. The aim is to identify interpretable parameter values, so that not only the modeled concentration curves match measured data, but also predictions can be made beyond the domain covered by given measurements. Subtle mathematical techniques are needed to measure the quality of these approximations; we used sophisticated affine covariant Gauss-Newton methods. For other researchers in systems biology, we

developed the public domain software package BioPARKIN.

Our model GynCycle [1] describes the idealized cycle of an idealized woman. The model consists of 33 ODEs and generates periodic solutions with a mean period of 28 days. From the 114 unknown parameters, 24 could be determined from blood measurement values of LH, FSH, E2, and P4 for healthy women (Pfizer study). In addition, data from the additional administration of GnRH analogues were used, increasing the number of identifiable parameters to 63. There exist two types of analogues: GnRH "agonists" act like natural GnRH, whereas GnRH "antagonists" block the action of natural GnRH. Both are used to either delay or enhance the cycle, thereby regulating the time-point of ovulation. GnRH analogues are applied in reproductive medicine as well as in the treatment of diseases that go along with endocrine disorders like cancer, endometriosis, or PCOS (polycyclic ovarian syndrome).

Crucial for the drug efficiency are time-point, dosage, and duration of medication. Figure 2 shows the long-time administration of a GnRH agonist suppressing ovulation for three months. This simulation result agrees with clinical observations. Such dosage recommendations, however, apply to "average" patients. In order to determine a therapy for real patients, individual models would be necessary. For such models, data over at least two cycles would need to be collected, a setting that can only be realized within hospital care. Together with medical doctors, biologists, and computer scientists from different European countries, we will continue our work within an EU funded project on patient-specific models and treatment strategies for infertility-related endocrinological diseases.

Further reading

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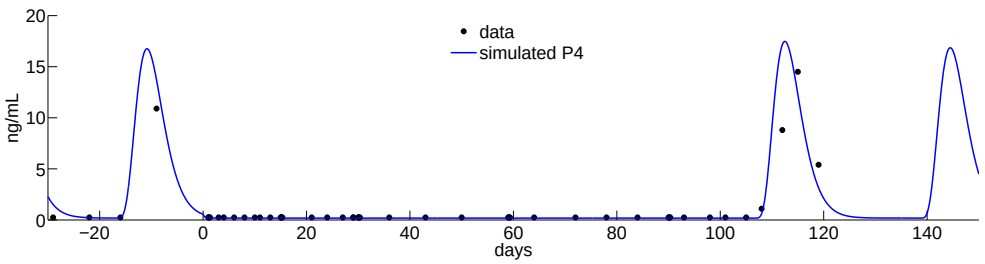

Figure 2. *Long-time administration of the GnRH agonist Nafarelin suppresses ovulation for several months, indicated here by the absence of corpus luteum producing progesterone (P4)*

Information-based medicine

Christof Schütte and Tim Conrad

Tumor diseases rank among the most frequent causes of death in western countries coinciding with an incomplete understanding of the underlying pathogenic mechanisms and a lack of individual treatment options. Hence, early diagnosis of the disease and early relapse monitoring are currently the best available options to improve patient survival. In addition, it seems imperative to develop biological markers that can identify patients who are likely to benefit from a specific form of treatment. The progress in understanding molecular mechanisms underlying pathologies has started to revolutionize diagnostics. Most of these mechanisms are controlled by proteins (e.g., hormones) which can be detected in the blood stream using mass spectrometry technology. The entire set of all expressed proteins at a certain time is called the proteome. Monitoring and understanding changes in the proteome is going to bring the next wave of progress in diagnostics, since many changes can be linked directly to disease onset and progression. We call these disease-induced changes *disease fingerprints* since they represent a trace that a particular disease left in the proteome.

A mass spectrometer can be used to uncover the proteome from just a drop of blood. It produces a signal where every protein is represented by some peaks whose intensities are proportional to the protein concentration profile. Proteomics-based diagnostics means to find the fingerprint of a disease in this signal. Every increase in sensitivity and robustness of the fingerprint identification yields earlier and more robust disease detection and results in an increase in therapy success rates for most serious diseases, such as cancer.

Mathematical and algorithmic problems and their solutions. Our approach to fingerprint detection is via signal classification based on mass spectrometry data of large patient cohorts. These signals are extremely high-dimensional (typically 100.000 dimensions for a low-resolution spectrum and more than 150 million dimensions for high-resolution spectrum) and often show a bad signal to noise ratio. In close cooperation with physicians we developed a specific Standard Operating Procedure (SOP) under which the blood sample has to be processed in order to reduce the signal to noise level to below 25 %. Even for such high-

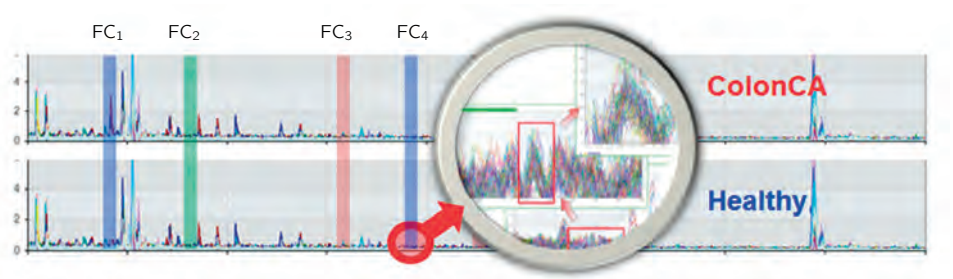

Figure 1. *This figure shows an illustrative example of mass spectra data and a fingerprint for Colon cancer with the exceptionally small number of four components ($FC_1 \ldots FC_4$). Note that only a very small fraction of the actual data set is shown. This data was acquired from two groups of individuals (after adequate preprocessing). The spectra in the top panel were created from blood serum of colon cancer patients. The lower spectra were created from healthy controls. The area inside the gray circle shows the magnified part of the red circled area to illustrate that our method allows detection of very small signals.*

quality mass spectrometry signals the high dimension renders standard signal classification infeasible. Therefore we invented a novel signal preprocessing technique that exploits knowledge about the physical processes underlying mass spectrometry, allows for peak detection across all available signals and results in peak detection with unprecedented accuracy. Based on the thus preprocessed signals we have designed novel sparse classification schemes. The idea behind these schemes is the following: the statistically significant differences between the classes ("healthy" and "different states of disease") results from a relatively small number of peaks that somehow reflect the proteins being characteristic for the disease in focus. This means that the fingerprint/classifier is sparse in comparison to the signal dimension even if the signals themselves are not sparse. Last but not least these preprocessing and classification techniques were implemented in a software environment able to handle this mass data (about 2.5 GB per patient, summing up to several TB for a typical patient population).

Impact and collaborations. The mathematical algorithms developed in this project were further improved towards real-world applicability in a subsequent BMBF-funded project within the ForMaT framework. In particular, components for handling very large medical data-sets from our clinical partners were added. This was done in very fruitful collaborations with our industrial partners IBM Germany and SAP Innovation. The pipeline has been applied to several data-sets and allowed to identify fingerprints for four different cancer types: lung, pancreas, colorectal, testicular (see, e.g., [1]). This was done together with our clinical partners from Helios Clinics, Charité – Berlin University Hospital, Leipzig University Hospital and Inselspital – Bern University Hospital. The resulting intellectual property has been patented [2] and is now been transferred into a spin-off company which will bring this to market. For their business plan for market entry the company won the second place in the *Berlin-Brandenburg business plan competition 2013*.

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Overcoming the curse of dimension in quantum chemistry

Harry Yserentant

The discovery of quantum mechanics in the first decades of the last century changed our view of the world fundamentally and had tremendous consequences for the development of modern technology. The basic equation underlying nonrelativistic quantum mechanics is the Schrödinger equation

$$\mathrm{i}\,\frac{\partial\psi}{\partial t} \;=\; -\sum_{i=1}^{N}\frac{1}{2m_i}\,\Delta_i\psi \;+\; \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\frac{Q_iQ_j}{|\mathrm{r}_i-\mathrm{r}_j|}\,\psi,$$

the equation on which our understanding of matter is based and which links chemistry to physics. It describes a group of N atoms or subatomic particles like electrons and nuclei that interact by electrostatic attraction and repulsion forces. The m_i and Q_i are the masses and charges of the particles under consideration and the r_i associated with their positions in space. The complex-valued solutions

$$\psi(\mathrm{r}_1,\ldots,\mathrm{r}_N,t)$$

of this equation are called wavefunctions. They depend on the positions of the particles, that is, on $3N$ spatial variables, three for each of the N particles, and on time, and in fact also on an internal property of the particles suppressed here, their spin. They know everything about the system under consideration. Their square $|\psi|^2$ describes the probability that the particles are located at the positions r_i at time t. The Schrödinger equation is usually split into an equation in which the positions of the nuclei are kept fixed (the electronic Schrödinger equation) and a separate equation for the motion of the nuclei. This is a mathematically very subtle process but can be explained by the fact that the nuclei are much heavier than the electrons and the electrons thus follow their motion almost instantly. The admissible solutions of the electronic Schrödinger change their sign under the exchange of the positions of two electrons with same spin $\pm1/2$, the Pauli principle.

Neglecting time, a naive discretization of an N-particle wavefunction requires

$$n^{3N}$$

data points to reach the same resolution as with n data points for a function of only one variable, or with n^2 data points for a function depending on two coordinates, like a picture taken by a digital camera. The number N of particles enters exponentially, the curse of dimension. The symmetry properties following from the Pauli principle at first do not change this significantly. It is impossible to approximate such high-dimensional functions without a rather detailed knowledge of their structure. Dirac, one of the fathers of modern quantum theory, commented on this with the often quoted words,

> the underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.

Dirac continued,

> it therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.

Physicists and chemists followed Dirac's advice and invented, during the previous decades, a whole raft of such methods of steadily increasing sophistication. Modern quantum-chemical approximation methods are based on deep insights into the nature of atoms and molecules. They are used with much success and form the basis of a steadily expanding branch of chemistry. Their power and efficiency are impressive. There is, however, no real mathematical explanation for their often amazing accuracy. From the perspective of a mathematician, all these methods have a decisive drawback. They either simplify the basic equation

and suffer from a priori modeling errors, or it is unclear how the accuracy can be systematically improved without that the effort truly explodes with the number of particles.

MATHEON scientists tried to understand the mathematical effects and the properties of electronic wavefunctions from which the success of such methods originates. An astonishing and surprising result is based on a careful study of the mixed regularity of electronic wavefunctions in exponentially weighted L_2-spaces, roughly speaking on their behavior at the points where two or more particles meet and their decay and localization properties. It turned out that asymptotically only

$$n^3$$

degrees of freedom are needed to reduce the approximation error (more precisely, its H^1-norm) to $\sim 1/n^{1-\delta}$, δ arbitrarily small; see [2] and subsequent papers. The construction uses modified sparse grid or hyperbolic cross approximation spaces and the symmetry properties of the wavefunctions enforced by the Pauli principle. The approximation order for the energies doubles correspondingly. The convergence rate no longer deteriorates with the number of particles and behaves almost like that for the one-particle Schrödinger equation. That means the curse of dimension is broken, at least as concerns the convergence rate. Such complexity results raise hope for true numerical methods for the Schrödinger equation with a well-understood convergence behavior, methods as they are known from continuum mechanics or computational fluid dynamics. Potential building blocks of such methods are coupled cluster methods [1] and tensor product approximation schemes, approaches that are size consistent in the language of quantum chemistry and thus able to break the dependence of the constants in the error estimates on the number of electrons.

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Automated radio network optimization

Andreas Eisenblätter and Hans-Florian Geerdes

The surge in mass-market mobile speech and data communication since the early nineties is stunning. At the start were second generation (2G) GSM networks with data extensions GPRS and EDGE. Next, 3G UMTS and its enhancement HSPA introduced data rates up to 42.2 Mbps. Nowadays, commercial 4G LTE networks offer data rates beyond 100 Mbps.

Instead of short periods of overlap between one generation and the next, all of these are operated in parallel nowadays – with little indication that this will change soon. Hence, radio network operators have to maintain large, complex multi-technology networks. Stiff competition calls for highly optimized networks as well as efficient operations.

Network operators thus insisted that LTE includes features simplifying and accelerating the planning, configuration, optimization, management, and healing of networks. Such features are called self-organizing network (SON) functionalities. A SON function can be pictured as open- or closed-loop control (depending on how strong the feedback is). This is where mathematics offers strong theory and tools.

The EU FP7 SOCRATES project developed a SON approach for the *Automatic Generation of Initial Parameters* for base stations [2]. The goal is to seamlessly integrate a new LTE base station into the network. This is achieved by means of, first, *pre-deployment optimization* of transmit power and antenna tilts based on planning data and measurements from the already active base stations and, second, *post-deployment optimization* of tilts at the new base station and in its surrounding also taking into

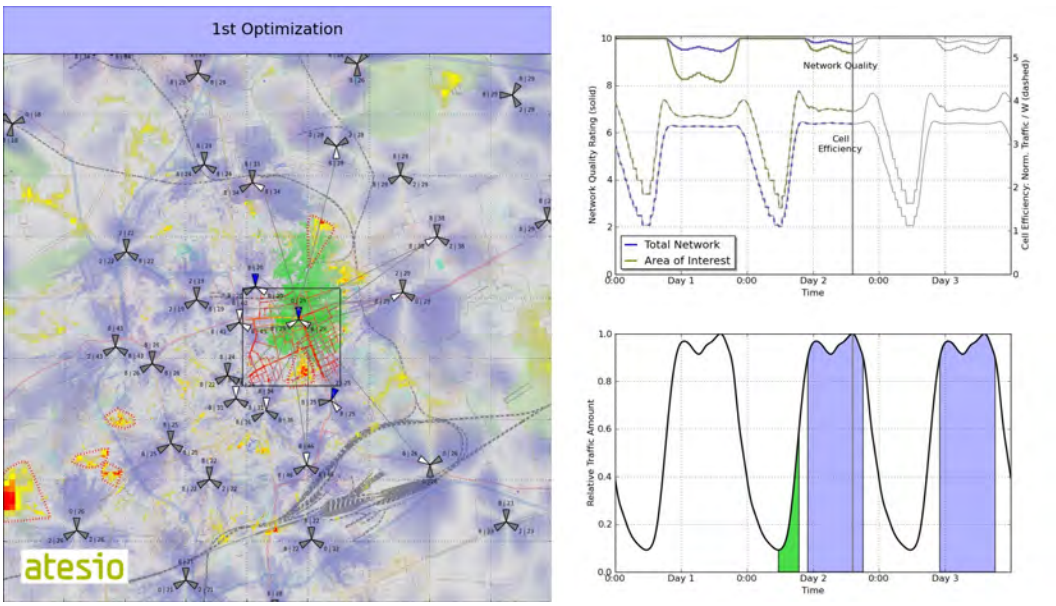

Figure 1. *Seamlessly integrating a new LTE base station with its surrounding by automatic pre- and post-deployment optimization of transmit power and antenna tilts*

account measurements from the new base station.

Figure 1 illustrates the approach. The base station to be integrated is the one depicted fully within the box on left-hand side. It is configured, activated, and optimized together with its surrounding in the course of three days. The diagram on the lower right-hand side illustrates how the users' demand varies with time. During the first day – the new base station is still inactive – the network is analyzed and areas of lacking coverage or high interference are recorded. These are the yellow to red patches, the most severe ones are enclosed by red dashed polygons. Based on this analysis, transmit powers and antenna tilts for the new base station are automatically derived. During the second night, at low traffic, the base station is activated and slowly powered up to the target power (giving SON functions at other base stations time to adapt to the changes). During the peak traffic times of that second day, the antenna tilts of the new base station as well as those of the directly surrounding ones (colored white or blue) are fine-tuned for reducing interference (blue ones are changed). During the third day, an extended surrounding is considered for optimization. The chart on the upper left-hand side shows the impact on network performance.

Once several SON functions are active within a network, the impact of individual functions, changes in their parameter settings, and potential interactions among the functions are hard to predict. Experts still argue whether coordination among SON functions is required and if so, how. Some of these questions can be addressed by means of simulating the behavior of SON functions in realistic networks [1].

The borders of SON have blurred in recent years. In one direction, SON functions operating very close to the hardware are being developed mostly by equipment vendors with the objective of improving network performance by constantly fine-tuning the network's working point. Such SON functions operate in a domain that was previously allocated to radio resource management functions. In another direction, network operators also show interest in decision support functionalities (*Decision Support Systems*). Such functions can support network design before equipment is about to become operational. Examples range from qualified proposals for short-term network capacity upgrades over medium-term network extensions to long-term radio spectrum and technology management. In each of these examples, mathematical network planning and optimization techniques can be employed.

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Routing AGVs in a container terminal

Elisabeth Lübbecke and Rolf H. Möhring

Automated Guided Vehicles (AGVs) are state-of-the-art technology for optimizing large scale production systems and are used in a wide range of application areas. The productivity of the AGVs is highly dependent on the used routing scheme, i.e., on algorithms that route them efficiently through their environment.

In a cooperation with the Hamburger Hafen und Logistik AG (HHLA), we studied this problem for the Container Terminal Altenwerder (CTA), see Figure 1. About 70 AGVs transport containers between the quay and the storage in the routing area shown at the top of the layout in Figure 1. They know their position, report them back repeatedly by radio to a host computer (the router), and get back instructions for their driving behavior. AGVs are symmetric, i.e., they can travel in both of the two driving directions equally well and can also change directions during a route. They do not have any sensors and depend completely on the driving instructions from the router.

HHLA used a static algorithm which computes quickest paths in an underlying routing graph G, see Figure 1. This required an additional collision avoidance mechanism at execution time of the routes. However, this mechanism was quite complex and led to deadlocks and other performance degrading effects.

We developed a dynamic algorithm that uses the paradigm of discrete flows over time [2]. It routes AGVs sequentially and keeps track of previously computed routes in an implicit time-expanded graph, which blocks times on edges of the graph when an AGV is driving through or waiting on them, see Figure 2. We showed that computing a quickest path respecting the blockings can be done very efficiently by a generalization of Dijkstra's algorithm if waiting along a route is permitted. We also could incorporate the change of the driving direction, the driving dynamics, and other practical conditions into the algorithm. Sequential routing, i.e., one AGV at a time, and allowing waiting on the route was essential, as the problem becomes NP-hard otherwise.

To use a router in daily operation, it must be robust under small disturbances. We therefore also developed rerouting techniques that react to unforeseen events in real time and compute changes to routes or even new routes. To this end, it was essential that the router was so fast and needed only 20–50 milliseconds for computing a quickest route and updating the blockings. These rerouting techniques required much experimental work and tests on specially designed scenarios with an asynchronous message management between the router and an AGV control unit that triggered the

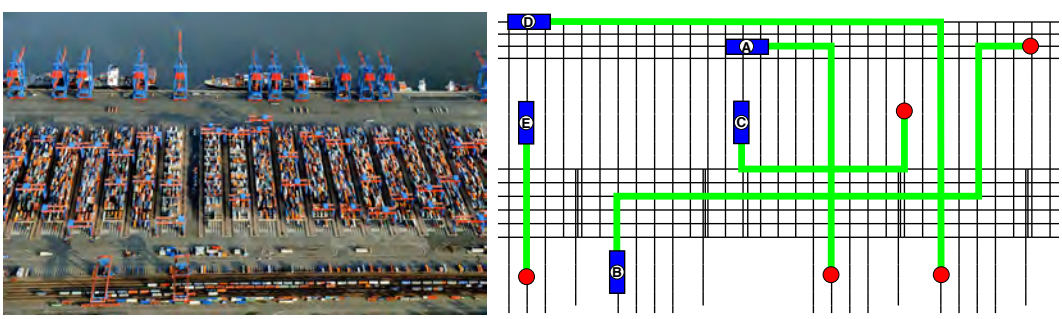

Figure 1. *Layout of CTA (left, ©HHLA) and part of the routing graph*

disturbances. HHLA acquired the source code and the copyright for its use in 2009.

This project has stimulated several research questions that were not part of the project with HHLA, but are typical examples of how industrial applications trigger new research. One type of questions concerns the sequential approach. Why route AGVs sequentially one after the other? Might it not be better to first gather some routing requests and then compute routes for them simultaneously? What is the optimality gap between these two approaches? Another type of questions deals with the difference between the static router and the dynamic router developed in the project. Is it possible to improve the static router by better deadlock avoidance? Is it then competitive with the dynamic router?

In both cases, these questions were answered in [1] with a combination of new theoretical results and again experiments. The optimality gap is below 2 % if the underlying grid graph has at least six parallel routing lanes, which is the case at CTA. A better deadlock avoidance wins by narrow margins against the dynamic router in scenarios with low traffic, but, due to its large runtime (checking for deadlocks is NP-hard), the dynamic router has a clear advantage in scenarios with high traffic density.

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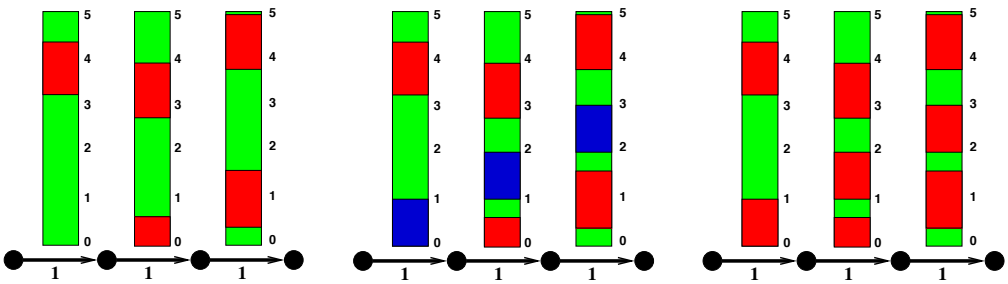

Figure 2. *Steps in the route construction: Graph with blockings (in red,* left*), new path (blue) compatible with the blockings (*middle*), updated blockings (*right*). Numbers on edges denote travel times.*

Routing ships through the Kiel Canal

Elisabeth Lübbecke and Rolf H. Möhring

The Kiel Canal connects the North Sea and the Baltic Sea. It is about 100 km long, and ships using it save 460 km compared with the route around Skaw. It is the canal with the highest traffic worldwide and has become too narrow for future and even today's traffic. The problem is caused by ships in opposing directions that together are too large to pass each other, see Figure 2. One of them must then wait in a siding to let others pass. This can happen several times for the same ship along its route, but must in total not be too long so that the passage through the canal is still attractive. Currently, there are 12 sidings of different capacity along the canal, which correspond to the green columns at the top of Figure 3.

This situation bears some similarities with opposing trains on a single track with sidings, but is more difficult since some ships may pass each other, whereas opposing trains cannot.

In a billion Euro project, the German Federal Waterways and Shipping Administration WSV had decided to enlarge the canal in the coming years. They came to MATHEON because of our expertise in routing automated guided vehicles (AGVs, see previous Showcase), and wanted an algorithm to improve current and simulate future traffic such as to recommend suitable measures (new sidings, widening of narrow segments, etc.) for the canal enlargement. The movie [2] illustrates this cooperation.

We started with the AGV routing algorithm and enhanced it to take care of the scheduling decisions, i.e., which ship should wait in which siding for which other ships. In addition, we had to observe the limited capacity of the sidings

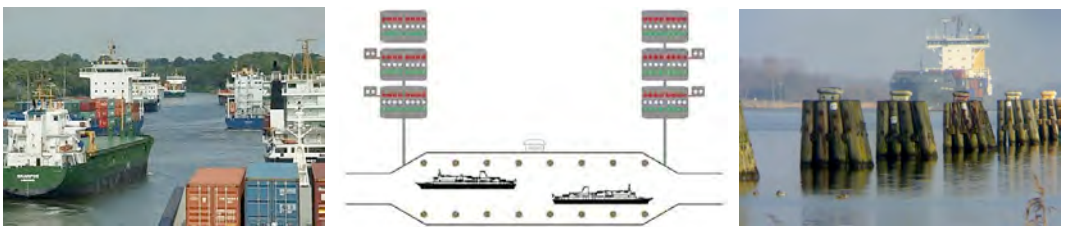

Figure 1. *Glimpses of the canal and a siding with traffic lights (*middle*)*

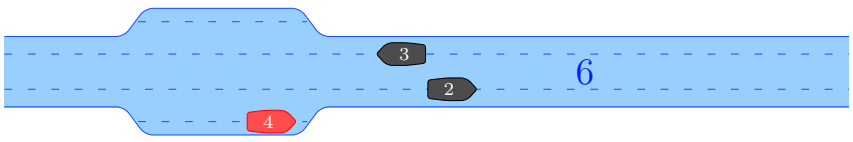

Figure 2. *Ships cannot pass each other when the sum of their sizes (here 3 and 4) exceeds the width of the canal (here 6). The red ship waits in a siding.*

and the lock scheduling at both ends of the canal.

To this end, we enhanced the AGV routing algorithm considerably, see [1]. The problem really is a combination of scheduling (deciding the waiting) and routing (does the scheduling permit a feasible routing). We could show that if we find "good" scheduling decisions, then the routing can be done quickly with the AGV routing algorithm. Other complications occurred with the limited capacity of the sidings, and determining the places for mooring in the sidings. Altogether, we combined the AGV routing algorithm with a rolling time horizon, local search for the scheduling decisions, a suitable modeling of the sidings, and lock scheduling at both ends of the canal.

We calibrated our algorithm on data from 365 days, for which we could show an average daily improvement of 25 % in waiting time for current traffic, and ran it for future traffic scenarios to make our recommendations. These were combined with a cost-benefit analysis done by a different group and have led to the final plan for enlargement, which is currently being prepared by WSV.

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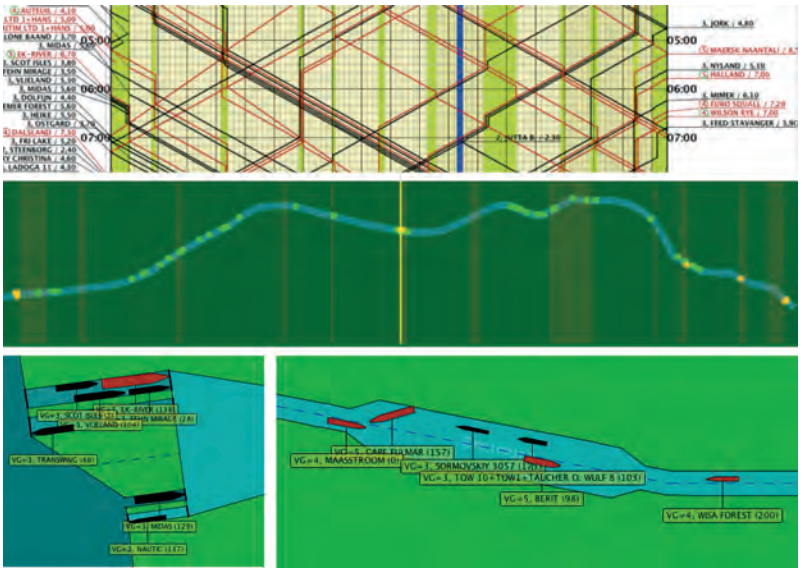

Figure 3. *Glimpses of the algorithm. Space-time diagram (*top*), overview of the current traffic situation (middle), lock scheduling in Brunsbüttel (*bottom left*), scheduling in siding Breiholz (*bottom right*).*

Line planning in Potsdam

Ralf Borndörfer and Marika Karbstein

A reorganization of the line plan in Potsdam became necessary when the public transport company of Potsdam, ViP Verkehrsbetriebe Potsdam GmbH, took over six additional bus lines that were formerly operated by Havelbus Verkehrsgesellschaft mbH. The new line plan should minimize the travel time at a same cost level, and ViP emphasized the importance of a minimal number of transfers.

Line planning can be interpreted as a mathematical optimization problem by considering the public transport network as a graph and all possible lines as paths in this graph. The task is then to find a subset of lines with frequencies of operation such that a given travel demand can be routed. There are usually a set of practical requirements that has to be considered as well, e. g., a minimum cycle time for certain transportation modes or a minimum frequency requirements for each station. The main objectives are the minimization of operating costs and the minimization of travel and transfer times. Both aims are usually in conflict with each other which can be handled by a weighing parameter. Great challenges in line optimization are the integration of line planning and passenger routing and the treatment of transfers. Existing models in the literature that integrate a passenger routing in line planning either treat transfers in a rudimentary way and, hence, neglect an important aspect for the choice of the passenger routes, or they treat transfers in a too comprehensive way and cannot be solved for large scale real world problems. We developed a novel direct connection approach that allows an integrated optimization of line planning and passenger routing including accurate estimates of the number of direct travelers. The attractiveness of transfer free connections is increased by introducing a transfer penalty for each non-direct connection. In this way, a passenger routing is computed that favors direct connections. Further details can be found in [2].

Our mathematically optimized solution for the Potsdam line plan 2010 minimizes the total number of transfers by around 5 % in comparison to a "hand made" plan on the basis of experience, compare with Table 1, see also [1]. It further reduces the cost by around 4 % and the perceived travel time by around 6 %. The bottom of Figure 1 shows that the optimized solution yields more districts with a higher number of direct travelers than the "hand made" plan. ViP finally established a slightly modified version of our optimized solution, see top of Figure 1.

Table 1. *Statistics (generated with* Visum*) for the optimized line plan and the "hand-made" plan*

	Optimized solution	ViP-solution
average total travel time	36min 3s	36min 39s
average time in vehicle	13min 8s	14min 36s
average transfer waiting time	1min 30s	1min 29s
average start waiting time	13min 23s	12min 32s
average walking time	1min 38s	1min 37s
average perceived travel time	26min	27min 37s
total number of transfers	10595	11141
passengers with 0 transfer	37338	36851
passengers with 1 transfer	10088	10503
passengers with 2 transfers	243	306
passengers with more than 2 transfers	7	9

Further reading

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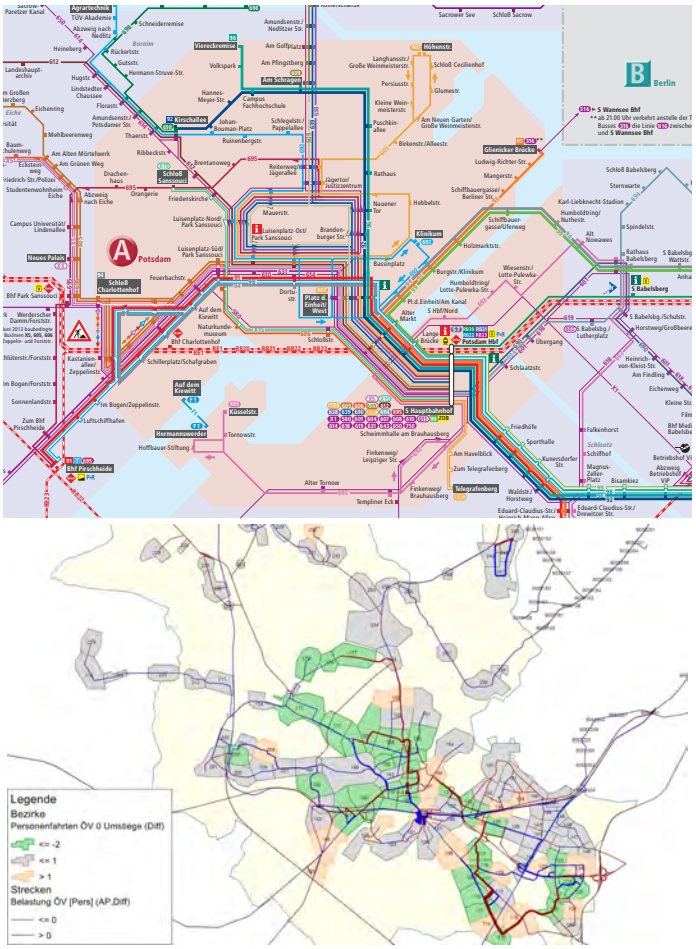

Figure 1. Top: *Line plan of the inner city of Potsdam.* Bottom: *Potsdam and its districts. A green (red) district symbolizes more direct travelers in the optimized line plan ("hand made" plan).*

Optimizing periodic timetables in public transport

Christian Liebchen and Rolf H. Möhring

Designing a periodic timetable is even nowadays largely performed manually. Software tools only support the planners in evaluating a periodic timetable, or by letting them comfortably shift sets of trips by some minutes, but they rarely use optimization methods. Planners argue that there is no clear objective and that optimization cannot meet different criteria such as amount of rolling stock, average passenger changing time, average speed of the trains, or the number of cross-wise correspondences.

We have demonstrated on the Berlin subway (BVG) that all these goals can be met if carefully modeled, and that optimization can lead to considerable improvements. We have investigated the weak traffic time of the Berlin subway network and were able to model all the – stepwisely identified – requirements from practice. Our final timetable improved all criteria significantly.

The construction of periodic timetables is a special step in the entire planning process of a traffic company which usually takes place between the line planning and the vehicle scheduling. The routes of the lines have then been fixed and now one must fix the times at which the trains enter a station, how long they stop or are cleaned at their endpoints etc., and all these times must repeat periodically with the given period length T, which was 10 minutes in our case. These times determine the comfort and the cost of a schedule. The comfort depends on the waiting times when passengers change lines, while the cost results from long stopping times at stations or cleaning times, which result in more trains and staff and thus higher operational cost for the traffic company.

We model this task as a periodic event scheduling problem, PESP for short, which is a mathematical model for periodically repeating events. It represents the driving conditions as a graph (see Figure 1). Its nodes v represent events π_v such as arrivals and departures in stations or at important switches. Arcs $a = (v, w)$ between nodes v and w model the time difference $\pi_w - \pi_v$ between v and w. These differences are restricted by lower and upper bounds ℓ_a and u_a expressing, e.g., bounds for stopping times. One then wants to calculate periodically repeating event times π_v that respect the bounds and optimize an objective such as the sum of the passenger waiting times at the transfers (the passenger comfort version), or the total stopping time to keep the number of trains small (the company friendly version). There is a trade-off between these two goals, and therefore one of

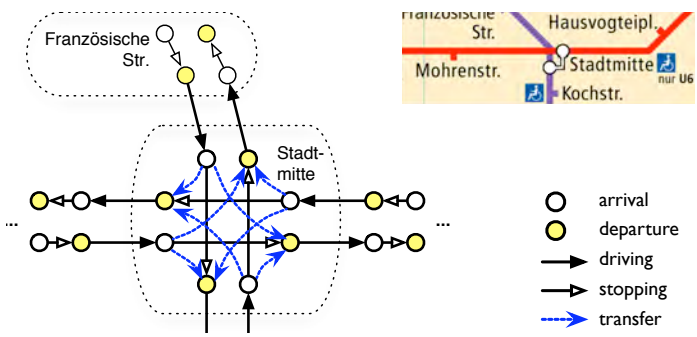

Figure 1. *From the line plan (upper right) to the PESP graph*

them is usually expressed as a constraint, e.g., a maximum number of trains.

This problem is a special mixed integer linear program (a MIP) that could only be solved by transforming it into a different space of variables that are related to cycles in the PESP graph. This transformation leads deeply into graph theory and has resulted in a considerable speedup with standard MIP solvers.

At the time of our calculation in 2005, the Berlin subway transported 1.3 million passengers per day on a network of 144 km length, 170 stations, and 168 transfer arcs at 19 stations. The optimization included all transfer times. In addition, the top 50 transfers were upper bounded by 5 minutes of waiting time, compared to 5.5 minutes in the previous timetable. Our best timetable achieved a maximum transfer time of five minutes at 55 of the 86 next important transfers, compared with 44 transfers before (+25 %). The maximum stopping time at stations was reduced by 29 % from 3.5 to 2.5 minutes. Moreover, the new timetable required one train less [1]. We even developed a new diagram for visualizing the transfer quality of a timetable, see Figure 2.

The Berlin subway company BVG was highly satisfied with this, for them unexpected, result of the optimization and has put our timetable into practice with only minor modifications. The 4-minute movie [2] gives an illustration of our model, the methods, and the results.

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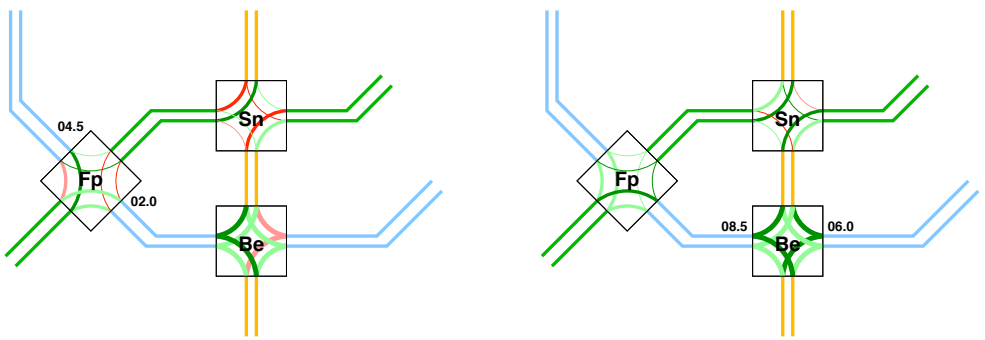

Figure 2. *Visualizing progress at important transfer stations*

SCIP Optimization Suite

Timo Berthold and Stefan Heinz

Modern applications of mathematical programming must take into account a multitude of technical details, business demands, and legal requirements. Today, companies are forced to rethink their planning methods due to the high innovation pressure. Knowledge in the practical application of mathematical modeling is becoming a key skill in industry, since the solution of mixed-integer nonlinear programs (MINLPs) is one of the very few areas which can provide globally optimal answers to discrete questions (yes/no, choose an option).

Problem solving requires the execution of three basic steps: modeling, running the solver, and analyzing the solution. Often, these three steps have to be iterated until all important side constraints of the application are adequately modeled, maybe some irrelevant side conditions are neglected, and the solution appears to be satisfactory. In complex cases, the solution software may have to be modified as well, so that the production code runs in an acceptable time frame.

The SCIP optimization suite (http://scip.zib.de) is a toolbox for modeling, solving, and – to a certain extend – analyzing MINLPs. For the mathematically involved step of solving an optimization problem, a so-called branch-and-bound algorithm is performed. In the following we sketch four important components for this approach. For more details we refer to the tutorial [1].

Relaxation. Computing a tight linear outer approximation plays a central role for solving MINLPs. This relaxation provides a solution candidate as well as a dual bound for the original problem, which can be used to measure the solution quality. Figure 1a shows such a relaxation.

Cutting planes. To strengthen the relaxation, cutting planes are generated. These are hyperplanes separating the current relaxation solution from the set of feasible solutions, see illustration in Figure 1b.

Branching. If the relaxation does not yield a feasible solution for the original problem, branching is performed. Thereby, the problem is gradually divided into smaller sub-problems for which the process is repeated. Figure 1c shows a branching which generates two disjoint sub-problems.

Primal heuristics. During the process of solving MINLPs, primal heuristics are called as supplementary procedures to construct feasible solutions as early as possible. An example is given in Figure 1d.

The SCIP Optimization Suite has become a standard for research in various areas of discrete optimization, it has been downloaded more than 25 000 times, and is nowadays used at more than

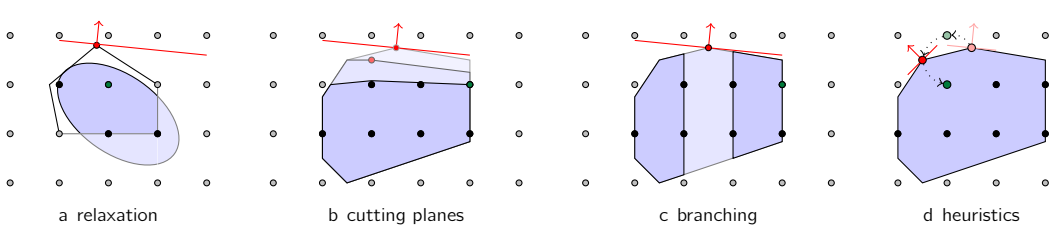

Figure 1. *Visualization of important solving techniques for MINLPs*

100 universities around the world, see Figure 2. SCIP is one of the fastest academic solvers for MIP and competitive to commercial solvers, see Figure 3. For MINLP, SCIP is one of the fastest solvers on publically available benchmark sets.

Further reading

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Figure 2. *Optimization software from MATHEON is used at more than 100 universities and research institutions on all continents (except Antarctica – yet) (Image source: Google Maps)*

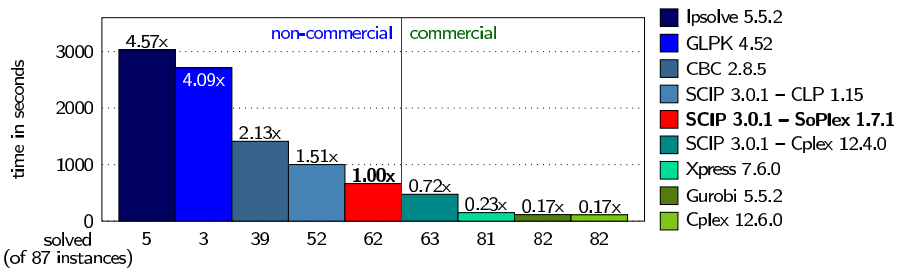

Figure 3. *Benchmark results for MIP solvers, data by H. Mittelmann (http://plato.asu.edu), as of November 18, 2013*

Wafer production and energy storage – Two technologies, same mathematics

Wolfgang Dreyer

Background. The production and subsequent applications of new advanced materials often involve phase transitions denoting drastic changes of the material properties on the nanometer scale. However, usually only macroscopic data of the phenomena are available, therefore their mathematical modelling poses a real challenge because the microscopic model is not known in advance. Therefore a hierarchy of microscopic models must be established and at first tested before predictions about the subject can be made. In industrial productions, experiments are usually too expensive and consume too much time. This is the context where the two corresponding MATHEON projects gave rise to two success stories.

How a MATHEON project explains the appearance of unwanted droplets during the production of gallium arsenide wafer. During the production process of semi-insulating gallium arsenide wafer an extremely unwanted solid-liquid phase transition with large differences of the arsenic concentration appears. While the mean arsenic concentration must be exactly 0.500082, the liquid phase appears within crystalline gallium arsenide as small liquid droplets with 0.9 mass fraction of the arsenic. Clearly the droplets represent unwanted heterogeneities damaging the functionality of the semi-insulator. However, the induced decline of the arsenic in the external surrounding of the droplets is even much more worse.

In collaboration with the wafer manufacturer Freiberg Compound Materials, a MATHEON project could identify the crucial parameter of the phenomenon and established a hierarchy of mathematical models for the various involved time and length scales. The complex phase diagram of gallium arsenide was calculated for the first time, which infact is a tremendous success.

How a further MATHEON project has lead to a breakthrough in the interpretation of the voltage charge diagram. A different phase transition of high industrial importance concerns the charging process of modern lithium-ion batteries and the storage of hydrogen in metals. During the charging process of a battery, lithium atoms are reversibly stored in electrodes consisting of a large ensemble of nanosized storage particles which undergo a phase transition. However, the kind of phase transition was unclear until 2010 when the MATHEON project achieved to a breakthrough in the mathematical modelling of lithium-ion batteries.

The worldwide strongly disputed nature of the storage process was definitely clarified. Before its treatment within MATHEON, the electrochemical community assumed that the phase transition happens in the individual storage particles of the ensemble. Moreover, it was assumed the lithium is simultaneously stored in the particles. However, these ideas were not successful to predict the volt-

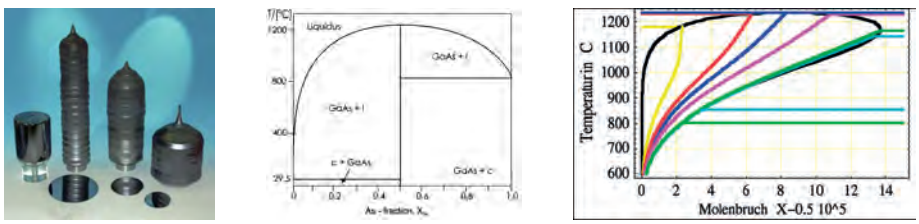

Figure 1. *Wafer and phase diagrams.* Middle: *Textbook.* Right: *Resolution of the phase structure right to X = 0.5 due to consideration of the microstructure.*

age charge-plot. Therefore we proposed a different scenario. The phase transition happens in the ensemble, and the lithium is stored according to the rule *one after the other*.

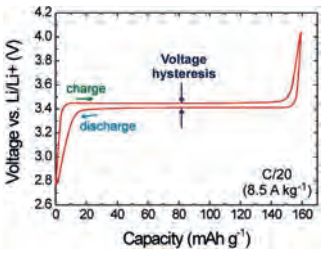

Figure 2. *Voltage-charge plot for the slow charging-discharging cycle. It shows a broad plateau indicating a phase transition and hysteresis notifying a non-optimal charging process. Within MATHEON the confusion about the two phenomena was removed, from* [1].

The hypothesis is mathematically described by a new nonlinear and nonlocal Fokker Planck equation whose analysis is quite intricate. However, a PhD thesis could solve the mathematical problems. An analog storage process where air is stored in a system of interconnected rubber balloons serves to visualize the phenomena. The experiment is an impressive demonstration of the rule *one after the other*. The common supply of air is not equally distributed over the balloons. At the same time there are large balloons and small balloons, constituting the phase transition within the ensemble.

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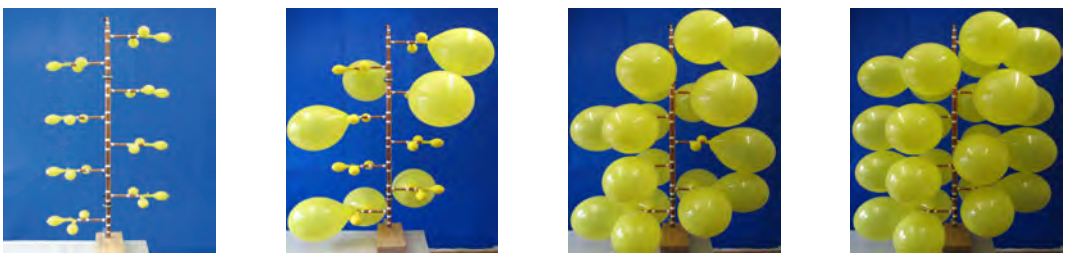

Figure 3. *Evolution of interconnected balloons*

The mathematics of nanostructuring free surfaces

Barbara Wagner

Nanostructuring is fundamental in order to functionalize and optimize modern materials. Developing structuring techniques enables, for example, the design of next generation thin-film solar cells or new concepts for high resolution printing via deposition of nanoparticles. Topics of this kind were addressed during the MATHEON interdisciplinary workshops *Mathematics in Industry: Process Engineering of Thin Liquid Films* and *Mathematics in Industry: Technologies of Thin Films Solar Cells* that were initiated by the project heads Barbara Wagner and Andreas Münch (now at the University of Oxford) of the MATHEON project *Modeling, Asymptotic Analysis and Numerical Simulation of Interface Dynamics on the Nanoscale* together with Volker Mehrmann and partners from the applied fields.

The aim of these four-day workshops was to give the invited industrial partners the possibility to aim for innovative solutions and new perspectives for problems of their interest consulted by an interdisciplinary team of expert scientists from universities and research institutes. They resulted in a number of successful industry funded projects. One of them addressed the development of new concepts for high accuracy printing technologies without the health risks posed by conventional laser printers and copying systems. The

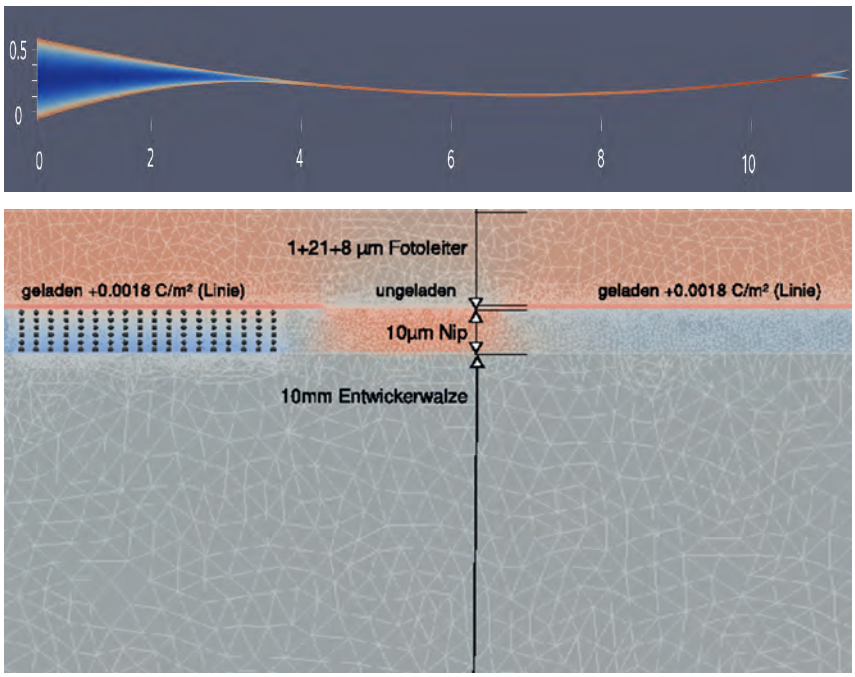

Figure 1. Top: *Flow profile between a hard roller and a deformed elastic roller, moving from the entrance region into the thin nip and merging onto the small meniscus region on the right.*
Bottom: *Typical computational domain, where the coupled system of Navier–Stokes equations, generalized Poisson equation, Nernst-Planck equation and equations governing the discrete particle dynamics is solved.*

central problem of a promising alternative concept is the control of particle transport in a colloidal liquid suspension through a narrow channel, the so-called nip region, between a photoconductor and an elastic developer roller. Here, the precise deposition pattern of the charged nanoparticles needs to be achieved before the resulting suspension enters the meniscus region. The challenge in the whole process lies in the control of the unwanted destabilisation of the free surface of the liquid film that emerges out of the meniscus that may distort or even completely destroy the pattern of the particle clusters.

At first sight it seems almost impossible to theoretically describe all of the electro-chemical and fluid-dynamical transport processes for a geometry with very disparate length scales, see Figure 1. It meant to establish a model of a system of nonlinear partial differential equations, coupling the hydrodynamic equations to the transport equation for the discrete particles and electromagnetic equations with equation for the dynamics of the ion density distribution.

For a company to succeed in this effort it was necessary to invest in a team of researchers that combines the expertise of several fields: The expertise of the project heads in deriving appropriate mathematical models together with their numerical and analytical solution to understand the interplay of the various physico-chemical and fluid dynamical properties; the expertise of chemical engineers (IFG, Friedrich-Alexander-University Erlangen-Nuremberg) to bridge the gap between the molecular understanding of the particle interactions to a continuum description of the electrorheological liquid; the expertise in numerical methods to achieve large scale numerical simulations for comparison with experiments.

The initial research team of the MATHEON project heads that expanded to this new collaborative research group, supported by three industry funded doctoral researchers, eventually laid the fundamental theoretical work that was necessary to enable the company to make the next step into this new technology.

On the other hand, the research carried out during this project also pointed to a number of fundamental research problems that now, as a collaborative research effort, were possible to investigate. One of these problems is discussed in the reference [1].

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Growth of semiconductor bulk single crystals

Olaf Klein and Jürgen Sprekels

Semiconductor materials like silicon or gallium arsenide constitute the heart of modern technology. Without them, achievements such as iPods, LED screens, digital cameras, solar energy, or electronic parking assistants would not be possible. However, it would not be sufficient to have the semiconductor materials to hand in just any form: they are needed as high-purity single crystals, a form that is hardly to be found in nature and has to be manufactured.

In industrial practice, the most important class of production techniques runs under the name of *Czochralski type* growth. In such a process, the semiconductor material (silicon, say) is first melted in a rotating crucible; then, a small silicon seed crystal is dipped from above into the melt and very slowly pulled upwards. In this way, a liquid silicon film is lifted upwards – just as if you dipped a spoon into a glass of honey and pulled it up slowly. The liquid silicon film is cooled by the surrounding gas and solidifies – and a single crystal comes into being. With this technique, silicon single crystals of enormous size can be grown; they may reach diameters of forty centimeters and a length of more than one meter.

A typical growth apparatus for gallium arsenide is depicted in Figure 1; here, on the left side the overall furnance is presented, and on the right side its center is shown in more detail. Therein, the geometry (left-hand side) and the temperature distribution (right-hand side) during a growth run calculated with the software package `WIAS-HiTNIHS` are presented.

In many growth processes of Czochralski type, the melt flow is turbulent, which creates the problem that impurities can find their way into the crystal, lowering its quality. However, if the melt is electrically conducting then time-dependent elec-

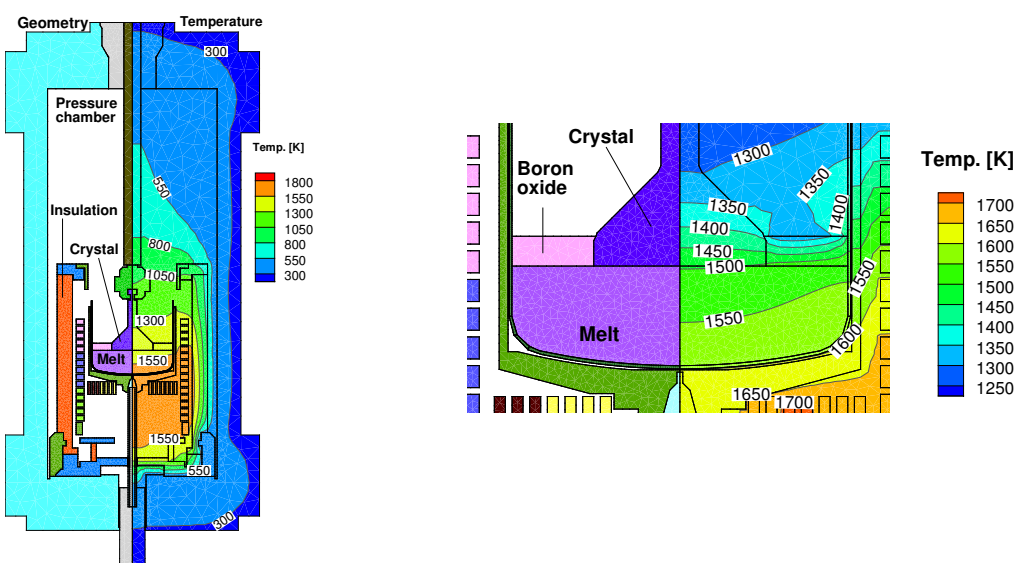

Figure 1. *A cut through the overall cylindrical furnance (left-hand side) and a zoom to its central part (right-hand side). In both cuts the left side shows the configuration and the right side shows the computed temperature field.*

tromagnetic fields can be applied to control the melt flow. In the past, various kinds of magnetic fields have been employed for this task with some success, until in the project KRISTMAG® a consortium led by the Leibniz Institute of Crystal Growth (IKZ) achieved a major technological breakthrough: a so-called *internal heater-magnet module* was developed, which operates as a resistance heater while simultaneously generating a *traveling magnetic field*. Such traveling magnetic fields turned out to be very effective tools for controlling the melt flow, which resulted in high-quality single crystals. Within the project, several patents were granted, and all over the world crystal growth machines have been equipped with the new technology. As a recognition of this success story, the KRISTMAG® consortium was awarded the Innovation Prize Berlin-Brandenburg 2008.

What did all this have to do with mathematics and MATHEON? As a matter of fact, mathematical modeling and simulation played a crucial role for the success of the KRISTMAG® project, to which the WIAS project heads of the MATHEON project *Simulation and Optimization of Semiconductor Crystal Growth from the Melt Controlled by Traveling Magnetic Fields* belonged. To avoid expensive time- and energy-consuming experiments, the entire growth process was modeled and eventually cast into a complicated system of highly nonlinear partial differential equations. To solve this system, the software package WIAS-HiTNIHS, originally developed in the MATHEON project for other crystal growth processes, was adapted. In this way, a *virtual* crystal growth furnace was created in which different growth configurations could be simulated very efficiently. Using this virtual growth furnace, promising scenarios could be identified and proposed to the crystal growers, which contributed a lot to the eventual success of the project.

Within MATHEON, the project permanently dealt with crystal growth technology. Besides developing the simulation software WIAS-HiTNIHS, many important mathematical questions were addressed over the years (cf. [1]). In particular, systems of partial differential equations governing the growth process were studied analytically. The outstanding theoretical work was the PhD thesis of the project coworker P.-É. Druet, which was honored with the Young Scientists Award 2010 of the Leibniz Association. And, last not least, a whole hierarchy of optimization problems of ever increasing complexity was studied in order to optimize various aspects of the growth process.

Further reading

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How math reduces noise

Jörg Liesen, Christian Mehl, Volker Mehrmann and Reinhard Nabben

Noise emissions by vehicles such as cars, trains or airplanes are not just annoying, their negative impact on health is one of the key factors restricting the quality of life in urban areas. The World Health Organization (WHO) calls traffic noise "a pervasive and underestimated ambient stressor".

Acoustic waves transporting noise emit from many different sources. In traffic vehicles these include the engines and brakes, and the vibrations of the structure due to external excitations like road contact or head wind. Reducing such noise emissions is on the agenda of EU legislation, and also an important factor for the economic success of new products.

Today, all vehicle manufacturers use *virtual prototyping*. The performance of a product is predicted using engineering simulation software, and the production of physical prototypes is avoided as much as possible. This reduces environmental hazards, production cost, and development times.

Figure 1. *Illustration of the acoustic wave propagation inside a car emitting from the windshield*

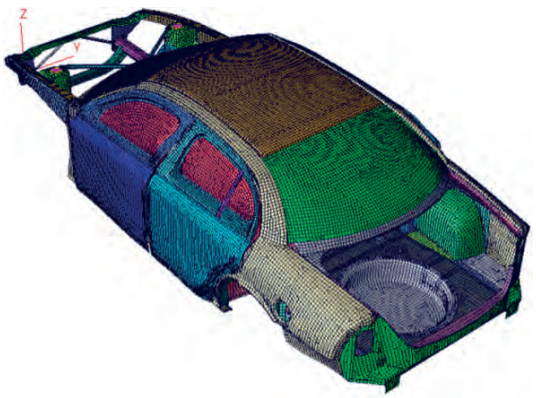

Figure 2. *Computer model of a car (courtesy of SFE GmbH, Berlin). The simulation requires solving systems of equations with millions of unknowns.*

In addition, it can lead to significantly better results because in a software simulation a much wider range of options can be explored and optimized upon.

In the context of noise reduction, the acoustic fields are mathematically modeled using systems of partial differential equations. These equations model, e.g., the vehicle's geometry, its interaction with the environment, and material parameters. Once such models have been derived they can be used for numerical simulation and optimization.

A typical task is to solve the *frequency response problem* which involves simulating the behavior of the acoustic field under excitations of the vehicle structure, caused for example by an uneven road surface or by wind. Based on the frequency response analysis it is then possible to detect places where excitation leads to large noise emissions (so-called hot spots). This approach subsequently can be used to improve the frequency response behavior within an optimization loop.

In the MATHEON project *Numerical methods for large-scale parameter-dependent systems* we successfully collaborated with the software company SFE GmbH, Berlin, one of the competitors in the vehicle acoustic software market. We developed and implemented, on current high-performance computers, problem-adapted mathematical techniques for the frequency response problem that became part of SFE's software tools.

Since the methods that are used in industrial practice cannot be constructed using textbook approaches, the collaboration with SFE raised a number of challenging mathematical questions. Consequently, the collaboration became a two-way-street involving transfer to industry on the one hand, and producing ideas for new developments in fundamental mathematical research on the other.

Although much research is carried out in academic and industrial research and development departments, the model-based minimization of noise emissions of a complete car or train (not to mention an airplane) is still a vision for the future.

Further details about this project and the mathematical methods applied in car acoustics are described in [1] and in the film *Noise Reduction through Numerical Linear Algebra* available at www.youtube.com/watch?v=iHqeZSOgpbs.

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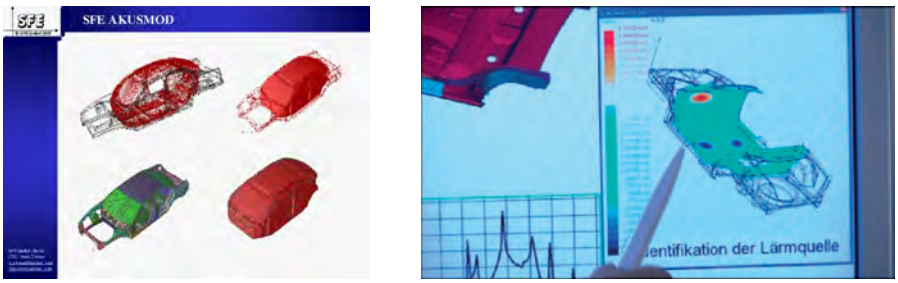

Figure 3. *The SFE Akusmod software allows to analyze the acoustical behavior and interior noise of road and rail vehicles. In particular, car parts with large noise emission (hot spots) can be identified (pictures courtesy of SFE GmbH, Berlin).*

Semiconductor lasers for information processing

Mindaugas Radziunas

The rapid growth of internet traffic pushes the interest in high speed all-optical signal processing. A variety of important functionalities of the optical data transmission such as pulse generation, clock recovery, signal regeneration, or fast switching can be realized by specially designed and differently interconnected multi-section semiconductor lasers. Especially interesting for the optical communications are lasers operating at dynamical regimes characterized by a large variation of the emission intensity on the scale of several tenths or hundreds of GHz. A deep understanding of nonlinear dynamics in semiconductor lasers obtained during the simulations and analysis of models on different levels of complexity is crucial for designing new devices with a specific dynamical behavior.

For simulation and analysis of dynamics in multi-section edge-emitting semiconductor lasers we have developed the software package LDSL (Longitudinal Dynamics of Semiconductor Lasers, see Figure 1). It is based on the traveling wave model (a hyperbolic system of first-order one-dimensional PDEs nonlinearly coupled with several ODEs) describing spatial-temporal evolution of the optical fields and the carrier density. Besides of numerical integration of model equations, LDSL-tool performs various post-processing procedures, solves spectral problems defining longitudinal optical modes, and analyzes the dynamics of these modes. For certain classes of problems, LDSL-tool generates reduced models, which can be further investigated by means of software tools for numerical continuation and bifurcation analysis. All together, this makes our software a powerful tool perfectly suited for simulations and analysis of dynamics in semiconductor lasers. It is used in the framework of academic and industrial cooperation projects aiming for a deeper understanding and an optimized performance of dynamically operating semiconductor lasers. The project diMOLA supported by Investitionsbank Berlin is a nice example of such cooperation between the WIAS and the Fraunhofer Heinrich Hertz Institute (HHI) in Berlin.

In modern telecommunication systems electronically generated signals should be transmitted through optical fibers. Thus, devices for conversion of electronic signals into optical ones at high speed are key components in modern data communication networks. The main goal of the project diMOLA was to create a multi-section laser which would exploit a fast photon-photon (PP) interaction and would guarantee an electri-

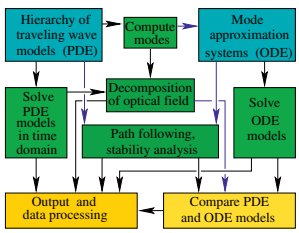

Figure 1. *Structure of the software LDSL-tool.*

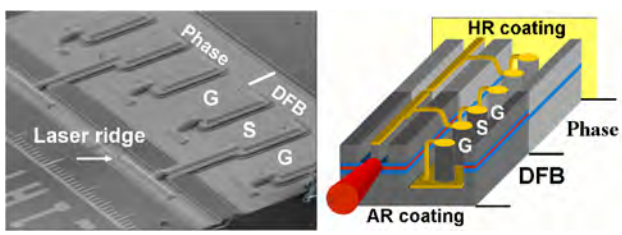

Figure 2. *Scanning electron microscope picture* (left) *and scheme* (right) *of the passive feedback laser (HHI Berlin)*

cal signal conversion at 40 GBit/s rate. We note that the data conversion rate in standard single-section directly modulated lasers usually does not exceed 10 Gbit/s, and is mainly limited by the frequency of relaxation oscillations determined by a carrier-photon (CP) interaction. In this project the possibilities for a new device concept were first explored theoretically at WIAS, and then, after a suitable device performance was found, realized experimentally at HHI [1].

Different laser configurations proposed by engineers from HHI as well as suggested by ourselves at WIAS were simulated with LDSL-tool. The best required performance could be achieved in a relatively simple two-section passive feedback laser (PFL). It consists of an active DFB (distributed-feedback) section and a passive section, which provides an optical feedback and admits a control of the feedback phase (see Figure 2). Under certain operation conditions this device could provide an appropriate electrical signal conversion (Figure 3a). The bifurcation analysis has explained the physical mechanism behind this particular behavior. We have found that provided the feedback strength is large, tuning the feedback phase in the PFL implies the oscillatory regime defined by two adjacent optical modes. Shortly before this regime the frequency of well damped relaxation oscillations is still determined by the fast PP interaction, which significantly increases the modulation bandwidth. All this knowledge has allowed us to optimize other laser parameters, such as section lengths, strength of the field coupling in the DFB section, etc. The performance of the PFL laser made at HHI according to our recommendations (Figure 3b) was even better than expected, and was easily satisfying all necessary requirements.

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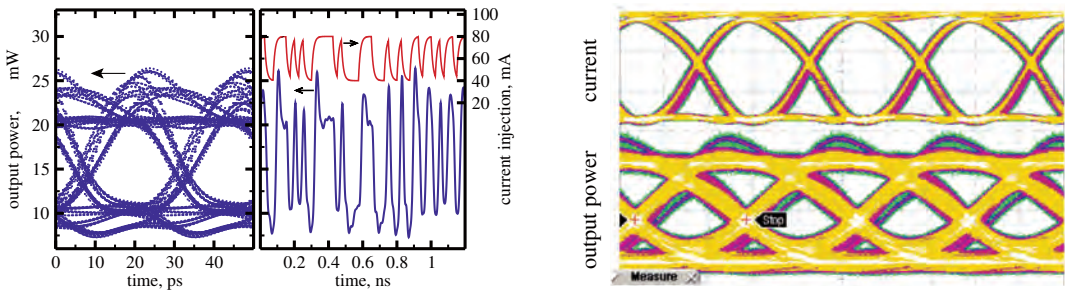


a Theory (WIAS Berlin)

b Experiment (HHI Berlin)

Figure 3. *Conversion of the electrical signal to the optical one in theory* (a) *and experiments* (b). *Open "eyes" in sampling diagrams (left theoretical and lower experimental pictures) indicate an error-free signal conversion at 40 Gbit/s rate.*

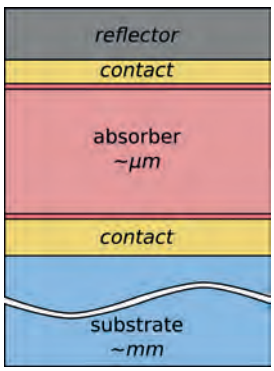
Optics of thin film solar cells

Daniel Lockau, Martin Hammerschmidt, Mark Blome and Frank Schmidt

Sustainable energy. A technology of high prospect on the road to a clean and sustainable world energy supply is photovoltaic (PV) energy conversion. The technology roadmap of the *International Energy Agency* predicts an annual market of 105 GW for photovoltaic systems in 2030 and a total installed capacity of 900 GW that contributes 5 % to the total electricity generation. To maintain the current annual growth rate in photovoltaics of over 20 %, inexpensive solar cell technologies with a potential for high throughput production need to be established. In view of a sustainable energy supply these technologies should also not be limited by the abundance of the required materials. Silicon thin film technology has the potential to meet all these requirements if efficiencies of solar cells incorporating silicon thin films (today $\sim$ 12 %) can be brought into the range of silicon wafer devices (20–25 %).

Improving efficiency by light management. A promising way in increasing the efficiency of thin film solar cells is the use of so-called light management structures. These structures should keep the light as long as possible inside the active region of the solar cell enhancing the conversion of photons into electrons this way. Figure 1b shows the possible impact of such a light management structure, here a complex, periodic texture, to the overall efficiency. The graph displays the absorption, which is an indicator for a successful conversion, versus the wavelength of the sunlight. The absorption of a flat cell is indicated by the blue area. The addition of the light management structure yields the additional red area, hence the cell exhibits a much better light absorption.

Analysis of light management structures: A challenge for numerics. Figure 2 depicts some of the structures we analyzed. From left to right these are a tandem cell combining two solar cells active in different spectral regions, a cell with a pyramidal silver back reflector exploiting plasmonics and



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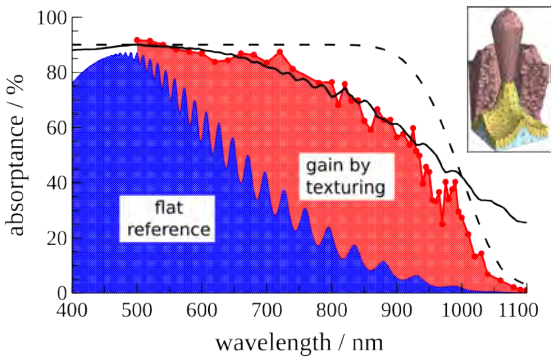

b

Figure 1. *(a): Solar cell schematic with approximate height scales. (b): Simulated absorption efficiency for a flat cell (blue) as in (a) and for a textured cell (red). The inset shows the cell geometry. Experimental reference (black) for the textured cell and Yablonovitch limit (dashed) are shown as well.*

a cell based on a micro hole arrays with tailored light trapping. A sound prediction of the optical device performance is possible only if all optical elements are present in the simulated system. This is challenging, as it combines micrometer sized cell optics and millimeter sized elements like the glass encapsulation.

Geometric modeling. The integration of very thin layers and geometric interfaces with strong curvatures makes the generation of computationally efficient grids for thin film solar cell devices a demanding task. We developed a CAD-based geometric modeling system well suited for complicated multiscale geometries with complex interfaces that allows to generate mixed meshes by combining surface and volume meshing techniques.

*Optical field computation.*The optimization requires the rigorous and efficient solution of Maxwell's equations. Using adaptive finite elements of high order and domain decomposition strategies the scattering and absorption efficiencies of different textures can be estimated with high accuracy.

Projects and impact. Progress in optimization of thin film silicon solar cell concepts was achieved in several joint projects with different academic and industry partners. Projects were realized in cooperation with Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) [1], Competence Centre Thin-Film- and Nanotechnology for Photovoltaics Berlin (PVcomB), the Optical Materials Engineering Laboratory at the ETH Zürich, and the companies Schott and Masdar PV.

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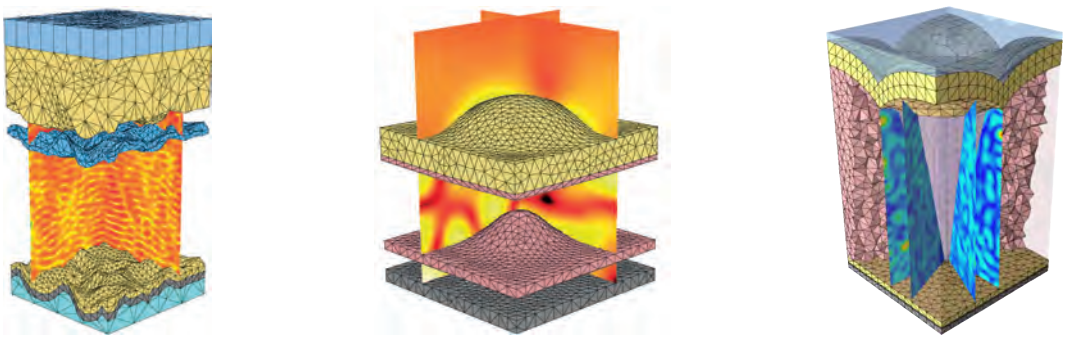

a b c

Figure 2. *Solar cell models for three different types of light scattering elements.* a: *Random texture in a micromorph tandem solar cell.* b: *Amorphous silicon thin film cell on silver pyramid back reflector.* c: *Periodic, conically shaped scatterer in etched polycrystalline material*

Expiry-wise Heston LIBOR model

John Schoenmakers

The Libor interest rate modeling framework, developed almost two decades ago, is still considered to be the universal tool for pricing and hedging of interest rate products. On the one hand, the Libor framework allows for great flexibility as it may include random sources of different types, such as Brownian motions, Lévy processes, or even more general semi-martingales, connected with different types of volatility specifications (factor loadings). On the other hand, however, in spite of this flexibility, the construction of a Libor model that can be calibrated to a full set of liquid market quotes (e.g., swaptions, and caps for different maturities and different strikes) in a fast, stable, and accurate way at the same time, has been a perennial problem to date. Early versions of the Libor model were typically driven by a set of Brownian motions and equipped with deterministic factor loadings. Such Libor models, called *market models*, gained much popularity since they allow for closed form cap(let) pricing and quasi-closed form pricing of swaptions based on Black 76 type formulas. As a main drawback, however, these market models cannot reflect implied volatility "smile/skew" behavior in cap and swap markets. This shortcoming became more and more serious when the smile/skew effects became more and more pronounced over the years. As first attempts for incorporating smile/skew behavior, the Constant Elasticity of Variance (CEV)-Libor model and the displaced diffusion Libor market model were proposed. These solutions turned out to be still unsatisfactory as their implied volatility patterns were of monotonic nature, that is only positive or negative skew effects could be generated. Inspired by the success of the Heston asset model that allows for modeling smile behavior for asset call options in a reasonable way (in contrast to the Black-Scholes model), a Heston version of the Libor market model was proposed a few years later. In this model the volatility of each forward Libor L_i (spanning over the interval $[T_i, T_{i+1}]$) contains a common stochastic volatility factor $\sqrt{v}$ where v is a Cox–Ingersoll–Ross type square-root process, correlated with Libor driving Brownian motions. It turned out that this Heston–Libor market has strong potential to produce smiles and skews, and moreover caps and swaptions can be computed quasi-analytically via Fourier based approximation methods. As such this new approach may be considered as an important but merely first step since there was still not enough flexibility for matching larger systems of market quotes, such as cap(let) volatility-strike

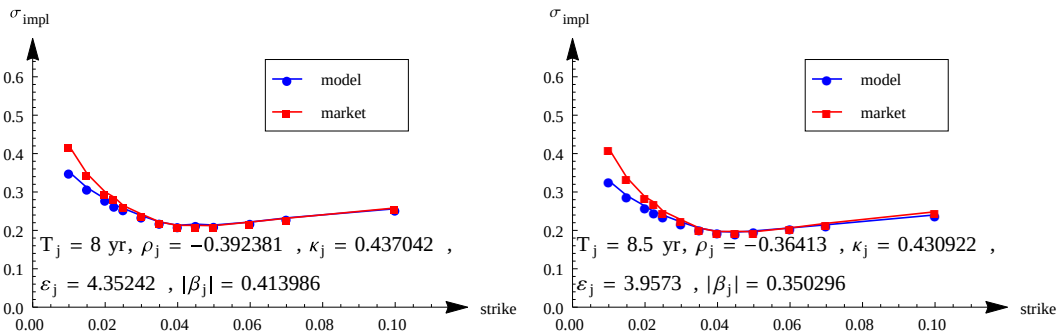

Figure 1. *Some caplet volatilities patterns due to market data vs. calibrated model values*

(short capvola-strike) panels for a whole system of maturities.

As a significant contribution in MATHEON, the too restrictive Heston–Libor model was extended in the following direction,

$$\frac{dL_i}{L_i} = \ldots dt + \sqrt{v_i}\beta_i^\top dW, \quad 1 \leq i < n, \quad (1)$$

where the β_i's are deterministic volatility loadings, W is a standard (multi-dimensional) Brownian motion, and the v_i's are Heston type volatility processes. By taking $v_i \equiv v$ the simple Heston–Libor model is retrieved. As a result, this extension turns out to possess the required flexibility, even in crisis times with structural breaks in the market data. Although (1) looks natural and easy to guess, several technical issues had to be resolved. As a main point, even after standard Libor freezing in the drift of the full stochastic differential equation (SDE) corresponding to (1), we do not have an affine Libor model allowing for quasi-analytical cap and swaption price approximation as in the simple Heston version anymore. As a solution, affine Libor approximations to (1) and affine swap rate approximations connected with (1) were nevertheless constructed. But, the price that had to be payed was that these approximations are typically (a bit) less accurate than in the Heston case. Careful tests revealed that the developed approximation procedures are still accurate enough for calibration purposes in the following "philiosophical" sense.

Any modeling framework that contains only medium accurate procedures for calibrating to quoted market prices, but, which is able to achieve a medium but acceptable fitting error in an efficient way, is highly preferable to a modeling framework that allows for very accurate pricing procedures, but, which is unable (not flexible enough) to match market quotes in an acceptable way.

For example, a medium accurate modeling method that has on average a model pricing error of 1.5 % but achieves a fitting error of about 3 % may be considered to match the market implicitly with an average accuracy of about 4.5 %. Put differently, a far more accurate modeling method that allows for a pricing accuracy of 0.01 % (say), only achieves a fitting error of about 10 % (say) due to lack of flexibility. For further flexibility, the structure (1) is finally extended with a standard Gaussian part and with so called displacement factors α_i, that is in (1) dL_i/L_i is replaced with $dL_i/(L_i + \alpha_i)$. The corresponding extensions for the pricing routines are straightforward and in no way problematic.

Cooperation with industry. The development of the *expiry-wise Heston Libor Model* has resulted in sustained cooperation contracts with a medium-sized bank, which adopted a suitably tailored version of the above sketched Libor model for its purposes.

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Active and passive order management

Peter Bank and Ulrich Horst

Today most trading in financial markets takes place on competing electronic platforms. In recent years, these platforms have seen a vast growth in both the number of orders handled and the speed at which orders can be placed or cancelled. In fact, trades are timed in milliseconds and the order volume posted at the New York Stock Exchange in four seconds exceeds the hourly order volumes from two decades earlier. Hence, the trading environment has evolved into a highly complex random system whose opportunities and pitfalls are subject to an ongoing debate in academia, praxis and politics.

Mathematics can contribute to this emerging challenge in a number of ways. For instance, the development of computer programs for order execution necessitates the thorough analysis of suitable mathematical models to, e.g., minimize the expected trading costs or to assess the risk of a given execution strategy. At the same time, mathematical research can contribute to our understanding of these systems and thus support the crafting of effective and efficient regulations.

Limit order books give market participants access to buy or sell offers for varying prices. They can choose to add to this collection by a limit order of their own or they can take away from this collection by submitting a market order for immediate execution. Apart from these classical options, modern markets also include so-called dark pools of liquidity where orders are submitted but not openly displayed, triggering a trade only if a counterparty is found. The computer algorithms needed to operate in this environment of high-frequency trading have thus to be developed for a highly complex stochastic system which mathematical research has only just begun to address.

A benchmark problem in this context is that of a broker who has to execute a large order over, say, a few hours. The trading system being so fast evolving and intricate, many brokers resort to a multilevel scheduling approach to parcel out such an order. On the coarsest level, the broker may want to specify a rough schedule of how many shares to trade over the next hours, typically using her knowledge of long-term averages of market activity at different times of the trading day. On a finer level, a scheduling algorithm will seek to exploit trading opportunities such as mean-reversion effects for the depth of an order book.

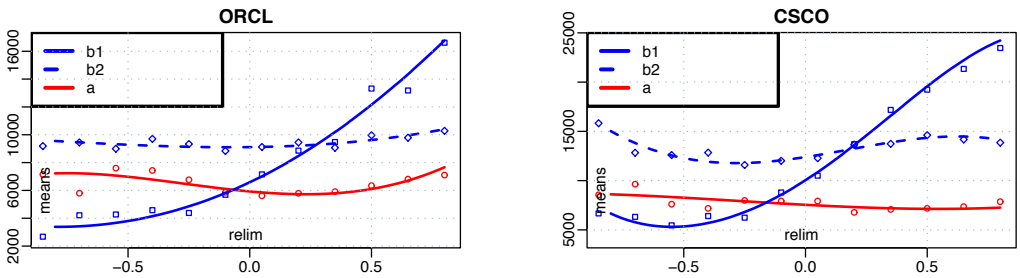

Figure 1. *Expected order flow volume as function of volume imbalances at submission price level (dotted blue line), one tick into the spread (solid blue line) and market order flow (red line) for Oracle (left) and Cisco (right)*

On the finest level, a smart order router will have to decide what kind of order to send to which exchange or whether to use some dark pool instead.

In cooperation with partners from the financial industry we developed, for instance, optimal order routing strategies for clients that liquidate large portfolios by trading simultaneously in dark pools and regular securities markets, or use both openly displayed and hidden orders in regular markets. We obtained explicit solutions for the benchmark case of linear market impact dynamics and characterized market environments where dark trading is not beneficial. We also computed optimal display strategies for investors using both hidden and displayed orders.

We found in [1] that optimal display strategies depend significantly on the impact of liquidity shocks on various market parameters, especially liquidity provision and cancellations at the submission and more competitive price levels. We have estimated the impact of openly displayed orders on order flows and market prices for selected high-tech stocks (Figure 1). Our analysis shows that for short liquidation periods it is usually beneficial to hide orders at least partially and that choosing display strategies optimally can significantly reduce trading costs (Figure 2). For longer periods and order sizes generating very significant volume imbalances in the order book, hiding orders may result in an inefficient coordination of demand and supply of liquidity and hence full display may be optimal.

Further reading

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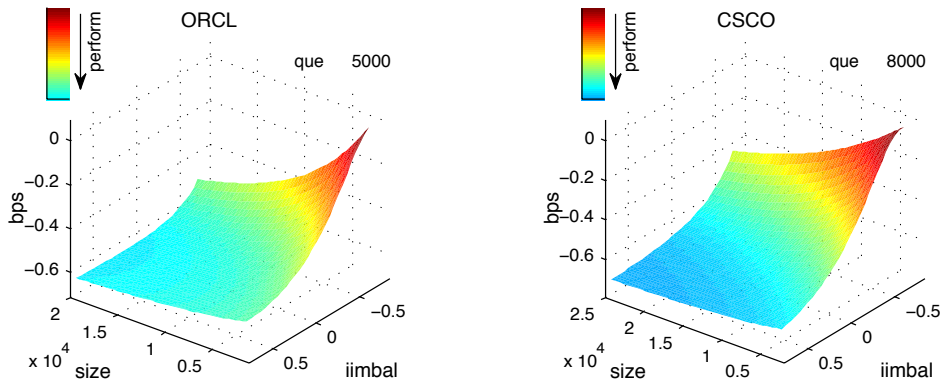

Figure 2. *Reduction in trading costs when displaying optimally is basis points (bps) as a function of the order book imbalance and order size for Oracle (left) and Cisco (right)*

MATHEON Buddy Bear – An application of discrete conformal mappings

Alexander I. Bobenko and Stefan Sechelmann

In computer graphics, digital geometry processing, and numerics, surfaces in space are usually represented by triangle or polyhedral meshes. A fundamental problem that appears in many applications is to parametrize such surface meshes, i.e., to map them to planar domains. For example, such mesh parametrizations are needed in computer graphics for texture mapping (the process of mapping a two-dimensional image, the texture, onto the surface of a three-dimensional object), and in geometry processing they are used for remeshing to improve the mesh quality or to turn a triangle mesh into a quad mesh.

A particular application often demands a certain type of parametrization due to its special geometric properties. For smooth surfaces conformal parameterizations are angle preserving. That means angles measured between intersecting curves on the surface stay the same at the intersection of the images of these curves. Conformal parameterizations are desirable for texture mapping, because infinitesimally they do not distort the form of the texture image.

For polyhedral surfaces, i.e., surfaces glued from planar polygons, there are various definitions of conformal maps. One definition deals with polygons inscribed in circles, and is formulated in terms of these circles. A conformal map then is a pair of circle patterns with equal intersection angles. A generalization of this definition (the angles are preserved as well as possible) was used to create conformal maps of triangulated surfaces in [1].

In 2005 such a discrete conformal map was used to create the design of the MATHEON Buddy Bear. This bear statue is one of many lifesize bear statues created for the city of Berlin. Every statue features a unique design associated with the spon-

Figure 1. *The MATHEON Buddy Bear*

sor. For the design of the MATHEON Buddy Bear a texture with the MATHEON logo and a circle pattern was used. The conformal map was calculated using methods developed in MATHEON and the California Institute of Technology [1] at that time based on the theory of circle patterns, in particular their variational description. The map is a discrete conformal map of a triangulated 3D model of the bear to the unit sphere followed by a Mercator projection, which in turn is a combination of a stereographic projection and the complex logarithm function. A digital model of the bear can be viewed online at http://www3.math.tu-berlin.de/geometrie/lab/misc.shtml#baer.

Recently these methods have been improved significantly using a new definition of conformal equivalence of triangle meshes which supersedes the previous approach using circle patterns both from the theoretical and from the practical point of view. It is formulated in terms of edge lengths of a discrete triangulated surface. In a conformal image of the surface, the lengths of edges are scaled by factors associated with the vertices of the mesh. Two meshes that are associated by scale factors at vertices are called conformally equivalent. This definition borrows the isotropic scaling behavior from smooth conformal mappings whereas the circle pattern definition emphasizes the angle-preserving property.

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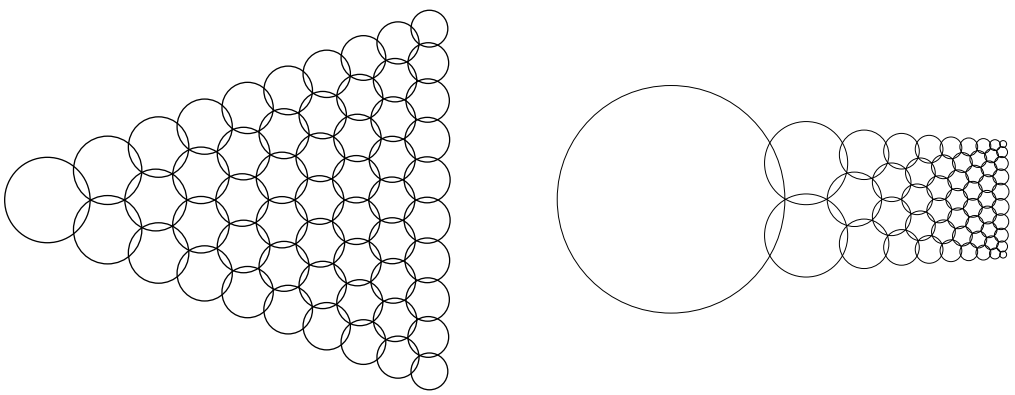


Figure 2. *Two discretly conformally equivalent circle patterns with equal intersection angles*

Towards in-vivo histology

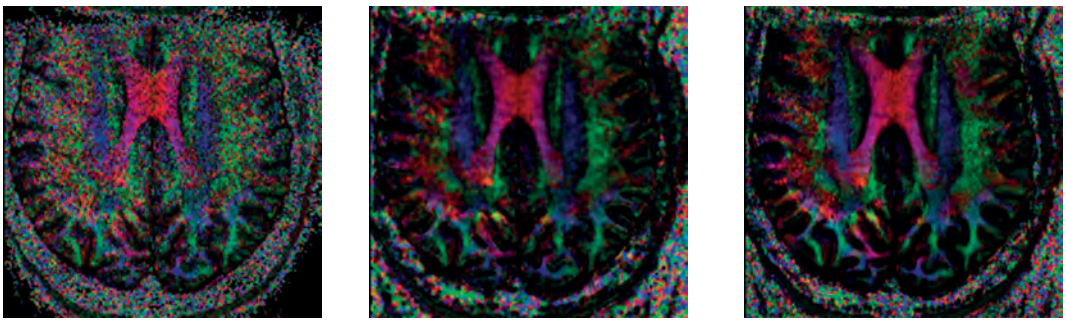
Karsten Tabelow and Jörg Polzehl

The development of imaging methods like CT and MRI enables an astonishing view inside the living human body, i.e., *in-vivo*. Still, the spatial resolution of CT or MRI is limited to a few hundred microns or even a millimeter. This is far above the resolution that can be achieved via post-mortem histology. Researchers at the Wellcome Trust Center for Neuroimaging at the University College London (UCL) are therefore working on improving the imaging techniques for structural imaging of the brain towards an in-vivo histology.

However, increasing the resolution comes with the price of a reduced signal-to-noise ratio. In MRI this can be compensated, e.g., by a higher field strength of the magnetic field, which requires a new scanner, or a much longer measurement time, which is not feasible for clinical use. Diffusion weighted MRI (dMRI) used to characterize the anisotropic structure in the brain is especially prone to this effect, as in principle the diffusion weighting itself leads to a very low signal-to-noise ratio compared to other MR sequences.

Within MATHEON we therefore developed a series of structural adaptive smoothing methods for dMRI data, that use the signal from neighboring voxel to reduce the noise. The methods automatically detect which signal values are similar enough to be used for this reduction. That is why they are called adaptive. In contrast to non-adaptive procedures they do not blur the image but preserve the edges and thus retain the spatial resolution at which the data is measured.

For dRMI it turns out that the geometry of the underlying measurement space for the data has a very useful structure. The measurements are not only performed in the three-dimensional (voxel) space, but also for a set of diffusion gradients applied for the diffusion weighting. The directions of these gradients are typically sampled uniformly from a sphere that forms an additional space of orientations. The resulting noise reduc-



a b c

Figure 1. *The effect of using POAS on color-coded fractional anisotropy maps for a dMRI dataset in comparison to the average of four repeated measurements.* a: *Original image;* b: *Reconstruction using POAS;* c: *Average of four measurements*

tion algorithm is called the position-orientation adaptive smoothing (POAS) method [1]. It draws its power from the additional relation of the signal in voxel and orientation space. As a result the post-processing of the data using POAS is able to reduce the noise in a dMRI measurement and achieves a comparable quality of the data, as if the measurement is repeated four times, see Figure 1 for a high resolution dataset acquired at a 7 Tesla scanner at the Max Planck Institute for Human Cognitive and Brain Sciences in Leipzig. However, while the repeated dRMI data took more than an hour to measure, the single dataset has been acquired within only 15 minutes.

Noise reduction is an intermediate step when modeling data from dMRI experiments. It enables significant improvements of parameter estimates. In Figure 1 this is illustrated for the case of fractional anisotropy (FA) and mean directions of diffusion (coded by colors). Streamline fiber tracking on the 3D vector field of mean diffusion directions reveals a much richer structure in case of the smoothed dMRI data, see Figure 2 for the result obtained.

For the colleagues at UCL our results are an important step towards the proclaimed goal of an in-vivo histology as the new mathematical tool will enable high quality dMRI datasets at the submillimeter level acquired at reasonable measurement times.

Further reading

[1] S. Becker, K. Tabelow, H. Voss, A. Anwander, R. Heidemann, and J. Polzehl. Position-orientation adaptive smoothing of diffusion weighted magnetic resonance data (POAS). *Med. Image Anal.*, 16(1668):1142–1155, 2012.

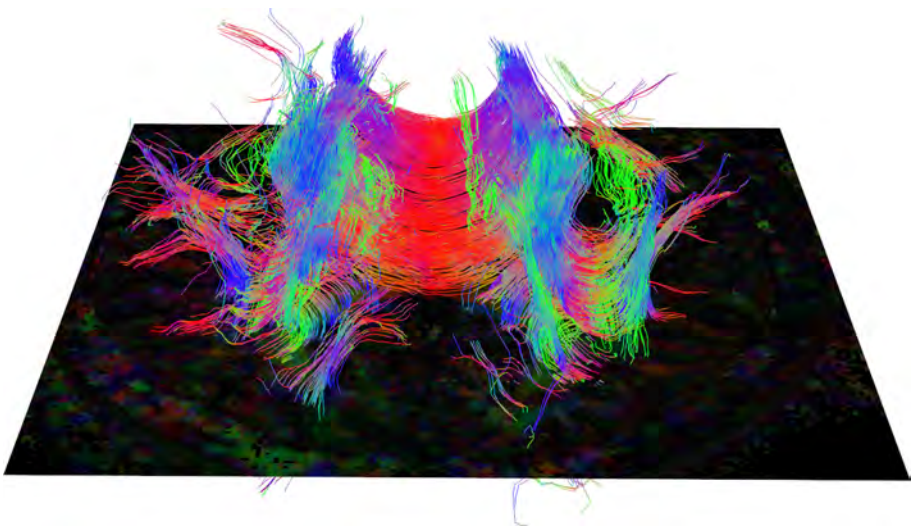


Figure 2. *Fiber tracks (longer than 4 cm) as obtained by streamline fiber tracking using the diffusion tensor model on the smoothed dMRI data*

Surgery planning for hearing implants

Hans Lamecker

Bone-anchored hearing implants directly submit sound to the inner ear by means of bone conduction. Those systems are indicated for mixed and conductive hearing loss. The Vibrant Bonebridge (MED-EL Elektromedizinische Geräte GmbH, Innsbruck, Austria) is an active bone conduction system, where the implant is completely positioned under the skin (Figure 1 left), and receives signals from an exterior audio processor. To allocate space for the implant the surgeon has to mill away bone, a procedure that requires a high degree of experience and precision. During surgery, a valid positioning of the implant is limited by a number of factors, e.g., good conduction properties, vulnerable structures, and a sufficient bone quality for a proper fixation within the cortical bone (dense outer bone layer).

We have developed a decision support system for an intuitive positioning of such implants (Figure 1 right) based on individual patients' anatomy derived from pre-operatively acquired 3-dimensional (3D) computerized tomography (CT) data. Our method performs a fully automatic geometric reconstruction of the anatomical structures that are relevant for the positioning of the implant, in 2 to 3 minutes. This reconstruction result is then used to automatically pre-position and interactively adjust the implant geometry on the bone with only a few mouse manipulations. During this interactive process, visual feedback is presented to the user that provides intuitive guidance for finding a suitable position. For further reading please refer to [1].

Further reading

[1] H. Ramm, O.-S. Morillo, I. Todt, A. Ernst, S. Zachow, and H. Lamecker. Visual support for the positioning of hearing implants. In *Proc. 12. Jahrestagung der Deutschen Gesellschaft für Computer-Roboterassistierte Chirurgie (CURAC)*, 2013.

Figure 1. *Surgery planning prototype for bone-conducting hearing implants.* Left: *Ear anatomy with implant.* Right: *Planning software for implant positioning*

Mathematics in Hollywood

Felix Kälberer, Matthias Nieser and Konrad Polthier

Triangle meshes are among the most commonly used data structures in computer animation for all kinds of shapes. Often meshed surfaces are created with a modeling software or alternatively obtained from digitizing physical shapes with a 3d scanner. Although meshes are very flexible data structures and allow easy processing, this flexibility sometimes appears to be a drawback when more structured grids are needed. For example, when two characters shall be morphed, that is, one character shall be deformed continuously into another character, then an identical structure of both of their meshes is needed in order to move one vertex to its corresponding vertex on the other mesh. If both meshes where obtained from a 3d scanner and have millions of triangles, then it is nearly impossible to automatically provide a pairing of the vertices from one mesh with the vertices of the other mesh.

The morphing of two characters is a key example where a structured grid, the same grid used for both characters, would be a tremendous help. The transition of one character to the other would just be a transition of the vertices of the first grid to the vertices of the second grid.

The algorithm QuadCover provides robust technique to convert a triangle mesh to a quadrilateral grid which is highly structured and adjusted to the underlying geometrical shapes. Generating such a coarse structure grid on one mesh and transferring this grid onto the second shape as well provides the basis for an effective morphing of two shapes.

Figure 1. *Automatic conversion of a triangle mesh* (left) *to a highly structured quadrilateral mesh* (right)

The educational chain in mathematics

Jürg Kramer and Elke Warmuth

Through our educational experiences in the Research Center MATHEON and the Berlin Mathematical School, we have been led to consider the education in mathematics from an early stage on in primary school until a possible postdoctoral phase followed by a position in academia or in industry. Even though this consideration primarily addresses mathematically talented and interested pupils and (high school) students, this approach is equally beneficial for the education in mathematics at large, in particular also for the teacher education.

Starting with grade 5, mathematically motivated and talented pupils are educated on the basis of specifically designed mathematics curricula in the five schools of the Berlin "Network of Schools Specializing in Mathematics and the Sciences", the so-called Berlin Network. The highly qualified teachers of these five schools support their fellow teachers, which has a positive impact for the education of the other pupils as well.

Continuing with grades 7 to 10, also in these classes the mathematically interested and talented high school students are taught according to specialized mathematics curricula elaborated by teachers of the Berlin Network and scientists of MATHEON. The mathematical and didactical expertise of the teachers involved has beneficial effects on the performance in mathematics of the high school students in the "normal" classes.

High school students, who graduated with grade A from the specialized mathematics classes of the schools of the Berlin Network, receive the required credits for the first semester at the university of their perspective studies in mathematics. For these high school students we thus created a fast-track option at the entrance to the university. Meanwhile, a total of about 160 students (i.e., ca. 50 %) achieved this goal.

In course of their studies in mathematics, we meet our former high school students from the Berlin Network among our students at the university. In general, these students prove to be among the top performers on the Bachelor's and Master's level.

After having completed the Bachelor's degree our very best students have the possibility to become Phase I students of the Berlin Mathematical

Figure 1. Left: *Pupil performing experiments (Photo: Heike Zappe);* right: *High-school students in the math laboratory (Photo: Kay Herschelmann)*

School (BMS), which opens them the option to enter the fast-track doctoral program of the BMS. After a successful completion of Phase I, the BMS students enter Phase II, the doctoral phase, which ends with the awarding of the Ph.D. degree. For students with an excellent Ph.D. from abroad, the BMS offers attractive postdoctoral researcher positions.

Further reading

[1] J. Kramer and E. Warmuth. Schnittstelle Schule–Hochschule: Berliner Aktivitäten zur mathematischen Bildung. *MDMV*, 15:228–237, 2007.

Figure 2. Left: *Work at Summer School "Fun with Mathematics" (Photo: Olav Bechmann);* right: *Network school student (Photo: Yiyang Huang)*

Figure 3. Left: *Lecture hall at a Berlin university (Photo: Ulrich Dahl);* right: *BMS students (Photo: Kay Herschelmann)*

The German Center for Mathematics Teacher Education (DZLM)

Jürg Kramer and Thomas Lange

The goal of the DZLM is to develop comprehensive training programs for mathematics educators in terms of a continuous professional development. The DZLM acts nationwide and cooperates with numerous partners in the federal states of Germany. Existing programs are supported and complemented by the DZLM. The work of the DZLM is research-based and all activities are based on the theoretical framework of the DZLM, which consists of a competency framework and mandatory design principles. The DZLM is an initiative of the Deutsche Telekom Stiftung and was launched in October 2011.

Implementation of certifiable teacher trainings. The DZLM develops and implements qualification and master degree programs for multipliers (training of trainers), qualification programs for out-of-field teachers and educators, as well as in-service teacher training for all teachers. The important mediator role of multipliers is illustrated in figure 1 on the left. In addition, professional learning communities for collegial hospitation or concept development are initiated and supported.

Networks and information. The DZLM connects school practice, educational administration, and research on a(n) (inter)national level (see figure 1 on the right) by conference and meeting organizations as well as institutional cooperations with ministries and teacher training institutes. In particular, networks of multipliers and teachers are moderated and supported. The DZLM has begun to build up an information and communication platform for mathematics teacher professionalization on www.dzlm.de.

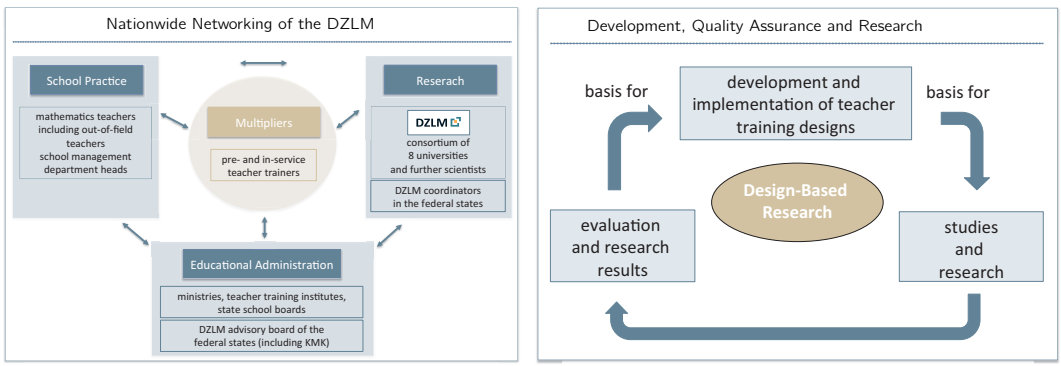


Figure 1. Left: *DZLM connects school practice, educational administration, and research on a(n) (inter)national level;* right: *DZLM teacher trainings are embedded in a cycle of research and practice to get effective designs for trainings*

Teacher education research. DZLM teacher trainings are embedded in a cycle of research and practice to get effective designs for trainings (design-based research). Innovative courses are developed on the basis of the above mentioned theoretical framework, scientifically accompanied, and evaluated. The evaluation and research data are then used for quality control to further improve the trainings, design innovations, and to get new research insights, in particular, on the effectiveness. The effectiveness chain is investigated starting from the multipliers via the teachers up to the high school students.

Material and concept development. The DZLM develops teacher training materials for the use of multipliers, for the use of teachers for self-studies and develops information material like movies and booklets. In addition, it develops training concepts in close cooperation with ministries and teacher training institutes.

Further reading

[1] J. Kramer and T. Lange. Mit Werkzeugen Mathematik und Stochastik lernen – Using Tools for Learning Mathematics and Statistics. In T. Wassong, D. Frischemeier, P. R. Fischer, R. Hochmuth, and P. Bender, editors, *Das Deutsche Zentrum für Lehrerbildung Mathematik (DZLM) – Ziele und Fortbildungsprogramme*, pages 487–497. Springer Spektrum, Springer Fachmedien, 2014.

Figure 2. *DZLM develops and implements qualification programs for multipliers, for out-of-field teachers and educators, as well as in-service teacher training for all teachers*

The mathematics Advent calendar

Katja Biermann, Martin Grötschel and Brigitte Lutz-Westphal

The by far biggest impact of all MATHEON outreach activities had and still has the "mathematischer Adventskalender", see www.mathekalender.de, that started in 2004 with about 7000 participants from Berlin and Brandenburg. Initially aiming at regional high-school students in the upper grades, it has evolved (joining forces with Deutsche Mathematiker-Vereinigung in 2008) into a three-tier competition with different problem sets for grades 4–6, 7–9, and above with students (and even quite a number of adults) from the world over. This competition became extremely popular, reaching a record number of more than 170 000 participants from more than 60 countries in December 2012.

The idea of challenging young people with mathematical problems is not new. Charged by Charles the Great with the task to reform the education system of the Frankish empire, Alcuin of York published (around 795 A.D.) the collection of mathematical problems *Propositiones ad acuendos iuvenes*. This book contains at least one problem everybody knows, the river crossing problem: "A man had to take a wolf, a goat and a bunch of cabbages across a river . . . ". The mathematischer Adventskalender intends to bring MATHEON's high-tech projects within the reach of high-school students as follows:

> Starting with a real application currently treated in MATHEON, single out an aspect that can be formulated as a mathematical problem solvable by the age group addressed, and describe the application background so that the

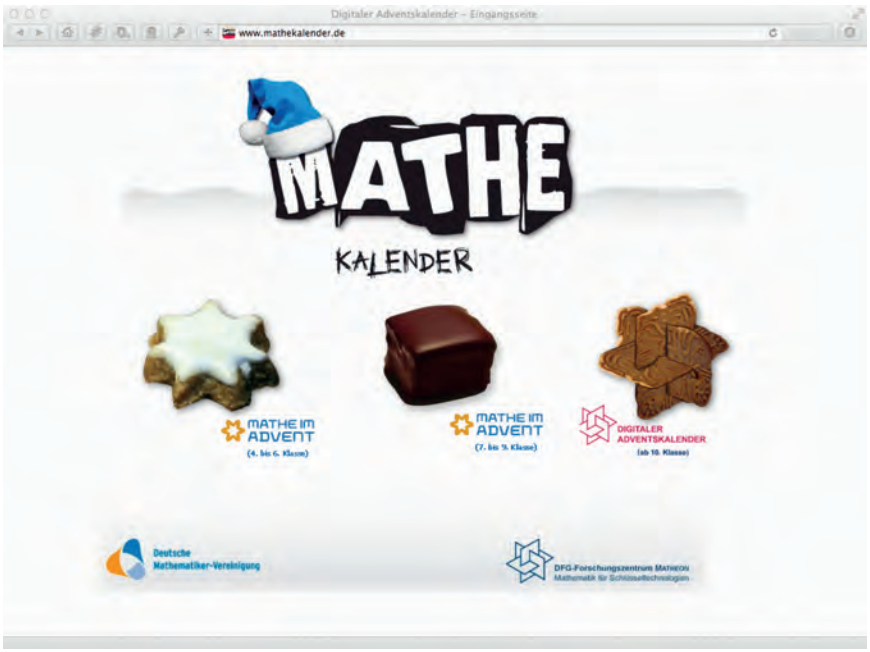


Figure 1. *www.mathekalender.de*

students can comprehend the real challenge.

Instead of revealing, when the daily window of a usual Advent calendar is opened, a small gift, every window of our Mathekalender Web page displays, from December 1 to 24, a mathematical problem as described above. The solution has to be electronically submitted within a certain time frame. The participants with the best solution record (details can be found on the Web page) receive significant prizes in various categories, sponsored by industry.

To our delight, some of the participants of the Adventskalender competition were best performers of the International Mathematics Olympiad, some are now studying mathematics, some are already employed as MATHEON research assistants, and one became in 2012 the youngest mathematics professor in Germany.

Further reading

[1] K. Biermann, M. Grötschel, and B. Lutz-Westphal, editors. *Besser als Mathe – Moderne angewandte Mathematik aus dem* Matheon *zum Mitmachen*. Springer Spektrum, Wiesbaden, 2. edition, 2013. Illustrated by Sonja Rörig. URL: http://link.springer.com/book/10.1007/978-3-658-01004-1.

Figure 2. *Marje Otten, winner 2014 in grade 4–6 (Photo: Kay Herschelmann/MATHEON)*

MATHEathlON: Fast minds – fast legs

Martin Grötschel and Rudolf Kellermann

The 12th IAAF World Championships in Athletics that took place in Berlin in August 2009 experienced the invention of a new discipline: MATHEathlON – created by MATHEON. Inspired by the highly popular biathlon, which combines cross-country skiing and rifle shooting, MATHEathlON is a combination of middle-distance track running and math problem solving. Of course, MATHEathlON was not a real championship event, but it was officially recognized as part of the supporting program.

MATHEathlON, designed for school children, is an event where – depending on age – a distance of 400 or 800 meters has to be run. At each of three stations on the way, one math problem has to be solved. Running distance and problem difficulty are age dependent. Each correct solution yields a bonus, an extra bonus is earned for the correct solution of all three problems. Runners who do not try to solve the math problems are disqualified. Bonuses are "paid" in seconds deducted from the running time.

The first MATHEathlON hit the news. Schools and sports clubs from all over Germany asked for the rules and "good MATHEathlON math problems". Since then, they have been provided by MATHEON via e-mail (free of charge). Lots of local MATHEathlON events have been staged since 2009 all over the country. They have become highlights, in particular, at school festivals.

Figure 1. *In 2010 the acting Berlin Senator for Science Prof. E. Jürgen Zöllner gave the starting signal for MATHEathlON (Photo: Kay Herschelmann/MATHEON)*

This positive public reaction encouraged MATHEON to organize the Berlin MATHEathlON as an annual event. Since 2009 every Berlin Senator of Education has agreed to act as the patron of this series. In 2010 Senator Zöllner even started the runs, as can be seen on the photo on the previous page. Top international track and field athletes also helped to cheer the young matheathletes.

The Berlin MATHEathlON, with its continuously increasing number of participants, takes place on a prime location: the field of the sports club IHW Alex close to Brandenburg Gate. IHW Alex as well as many other institutions, schools and companies support the whole event. Think Ing., e.g., provides particular financial support, there have been co-operative MATHEathlON events with UNICEF, Barmer GEK, ZDF, Bild-Zeitung, rbb Inforadio, "Deutsche Sportjugend" and with Klaus-Tschira-Stiftung.

Some versions of biathlon appeared as demonstration events in various Winter Olympics, the earliest one in the 1920ies. Biathlon made its official Olympic debut only in 1960. MATHEathlON had its first official appearance at an athletics world championship in 2009. Will MATHEathlON be an Olympic contest some day?

Figure 2. *Award ceremony for the first MATHEathlON within the official framework of the World Athletics Championships in 2009 in front of the Brandenburg Gate in Berlin (Photo: Kay Herschelmann/MATHEON)*

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