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Numerical and Symbolic Scientific Computing

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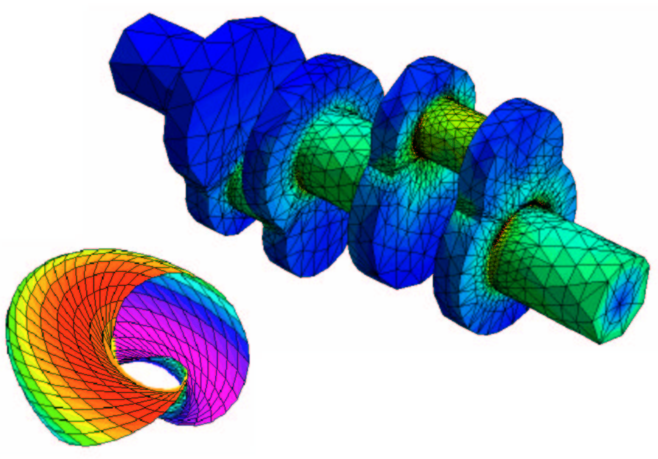
Johannes Kepler University Linz
A–4040 Linz, Austria



Supported by

Special Research Program SFB F013

"Numerical & Symbolic Scientific Computing"

Speaker: Prof.Dr. U. Langer
Vice Speaker: Prof.Dr. F. Winkler
Office: A. Krennbauer

The long-term scientific goal of the SFB is the design, verification, implementation, and analysis of

- numerical,
- symbolic,
- geometrical and graphical

methods for solving **large-scale direct and inverse problems with constraints** and their **synergetical** use in scientific computing for real-life problems of high complexity. We have in mind so-called field problems (usually described by partial differential equations) and algebraic problems (e.g. involving constraints in algebraic formulation). The particular emphasis of this SFB is put on the *integration* of numerical and symbolic methods on different levels:

Numerical and symbolic methods have been developed so far by two fairly disjoint research communities. The University of Linz is one of the few places with strong groups both in numerical and symbolic computing. Thus, the joint work on numerical and symbolic methods is one of the main focuses of the SFB.

The methodological coherence of the SFB can be summarized as follows: In the Subprojects F1302 - F1305, new symbolic proving and solving algorithms for various domains of mathematics (integers, real number, complex numbers, general domains defined by functors) have been developed that can be used in connection with numerical methods for treating a benchmark class of direct and inverse problems described by partial differential equations with constraints, which is the subject of a second group of subprojects (F1306, F1308, F1309, F1311, F1317). Refined graphical tools are used for the visualization and presentation of the results, which is one of the subjects of Subproject F1301. Another point of Subproject F1301 consists in the coordination of the development of scientific computing tools such as solver and parallelization tools. The Subproject F1315 entered the SFB in its second period (April 2001 - March 2004) as one of the central projects aiming at the combination of numerical and symbolic methods in geometrical scientific computing.

The integration of symbolic and numerical methods described in the comprehensive view above must be seen as a long-term goal. In the first period of the SFB project (April 1998 - March 2001), we have concentrated on

- the interaction of those methods where this integration is relatively immediate (e.g. in the pre- and postprocessing phases of numerical methods),
- joint training of project co-workers with either symbolic or numerical background to build up a common language and expertise for a closer interdisziplinary cooperation,
- preparing the methods from symbolic computation (e.g. computer-support in formal proofs and algebraic constraint solving) that should later be seamlessly integrated with the numerical analysis.

A more precise discussion of this topic is given later in the section on the coherence within the SFB.

The scientific results obtained in the SFB enable the participating institutes to rise their activities in the knowledge and technology transfer to the industry, especially, in Upper Austria. The highlights are the foundation of the Software Competence Center Hagenberg and the Industrial Mathematics Competence Center in 1999. A more detailed report about these and other transfer activities is given in the section "Transfer of Knowledge and Technologies".

The following institutes of the Johannes Kepler University of Linz are currently involved:

- Institute of Analysis,
- Institute of Computational Mathematics,
- Institute of Industrial Mathematics,
- Institute of Mechanics and Machine Design,
- Institute of Symbolic Computation.

For more information about our SFB please visit our internet home page

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or contact our office.

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Linz, March 2002 Ulrich Langer

F 1301: Service and Coordination Project

Prof. Dr. U. Langer

Dr. M. Kuhn, Dr. G. Haase, Dr. S. Reitzinger

A. Krennbauer, F. Tischler

The scientific part of Project F1301 is concerned with the coordination of scientific software and the development of scientific computing tools including graphical pre- and postprocessing tools. In 2001, we finished our work on the visualization tool VIPP, we have been working on the mesh generator NETGEN and the numerical software package FEPP, and we have developed the algebraic multigrid package PEBBLES. The detailed description of these packages can be found on the SFB home page.

1 Scientific Computing Tools

The applications considered within the SFB cover a wide range including problems from elasticity, plasticity, piezoelectricity, electromagnetics, and magnetomechanics. Most of these applications are based on common principles which can be implemented very efficiently using the advantages of C++. The aim of the development of scientific software consists in providing modular tools which allow the fast implementation of new problem classes and new algorithms. The close interaction of these modules is essential for the efficient processing of extremely large data sets. Thus the hierarchical data structures provided by the numerical schemes are used for real-time interactive visualization. The problem solving environment has been applied successfully to the simulation of magnetic valves and electro-mechanic-acoustic-transducers. The simulation of these problems is based on the numerical solution of the underlying transient, nonlinear, 3D coupled magneto-mechanical field problems by advanced adaptive multigrid techniques developed in the SFB. Figure 1 shows the finite element model of a magnetic valve generated by NETGEN and the B-field (magnetic induction) computed by FEPP [9]. This picture steams from a movie made by VIPP and shows the interaction of the mechanical (displacements) and the magnetical (magnetic induction) field in time. Moreover, VIPP allows us to visualize the simulation results in a virtual reality environment such as the CAVE.

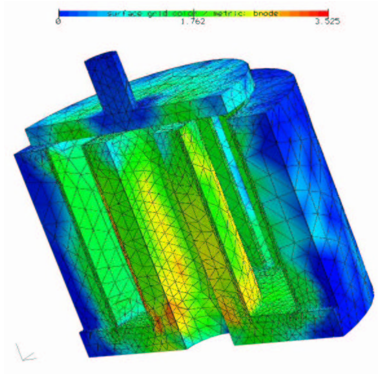

Figure 1: B-field of the Magnetic Valve.

2 Algebraic Multigrid

The Algebraic MultiGrid (AMG) method is a very powerful tool in the area of numerical simulation if standard discretizations are used, e.g. Finite Element (FE), Boundary Element (BE), Finite Integration Technique (FIT). We use AMG especially as preconditioner in a Krylov subspace method as the CG-, QMR-, or the BiCGCRbi-method. For the considered problem class of elliptic second order partial differential equations, the resulting linear (nonlinear) system of equations can be solved very efficiently by means of AMG preconditioning.

For the construction of an AMG method, we use the general approach proposed in the PhD theses by S. Reitzinger [7]. The proposed algorithms therein are implemented in the AMG software package PEBBLES. Some recently developed methods:

1. BE-matrices from the single layer potential and the hypersingular integral operator: The resulting matrices are dense and ill conditioned. Therefore we require fast preconditioners. A preparatory work is given in [5].

2. Complex symmetric matrices from the FIT discretization: This is a joint work with the group of Prof. U. van Rienen, University of Rostock, Germany [8]. The AMG method was developed in order to solve complex symmetric equations arising from the simulation of high voltage insulators.

3. Symbolic methods for the element preconditioning technique: Such methods are required for the efficient construction of an M-matrix. A promising approach consists in the symbolic solution of the arising (small) restricted optimization problems [6]. This is a joint work with J. Schicho, F1303.

3 Parallelization

A parallel version is needed if additional speed up is required. In addition to the very efficient parallelization of FEPP based on domain decomposition ideas we had to apply theoretical parallelization results from [2] to get a parallel AMG method [3]. Finally AMG achieved the same excellent parallel performance as much simpler solution algorithms.

4 Applications in Life Sciences

Computational methods are widely used in the human brain research for the diagnosis- and pre-surgical phase. Such non-invasive tools are clearly preferred in comparison to invasive methods, e.g., surgery having high risks for the patient. Very often there is no other choice besides computational methods. However, the acceptance of tools depends highly on their speed, reliability and robustness.

The joint work with C. Wolters et.àl, Max-Planck-Institute, Leipzig, Germany [1] applies our AMG-solver in the software package NeuroFEM-Pebbles as a part of the inverse source reconstruction. The principle is shown in Figure 2, i.e., we have to detect the sources (yellow arrows) of given measurements (green dots). Therein we have to solve

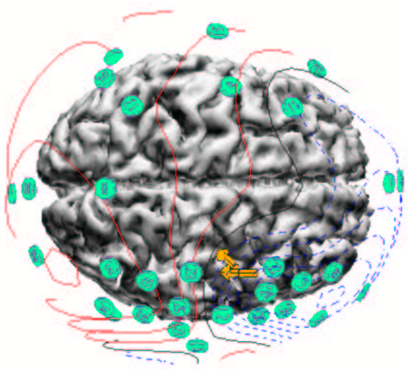

Figure 2: Inverse Source Reconstruction - Principle.

a huge linear system with approximately 10000 different right-hand sides within 6 hours. A naive approach on a single processor computer hardly reaches these requirements. Consequently that part consuming most CPU-time has to be done in parallel. The acceleration by parallelization is given in Figure 3. The solver part is of special interest and we get a CPU-time reduction of 10 on 12 processors, i.e., the speed up is almost optimal. Additional acceleration of the solver part can be obtained by a special treatment of the right-hand sides. Further studies consist in the efficient solution of several right-hand sides simultaneously [4], which accelerates the code by an additional factor 3.

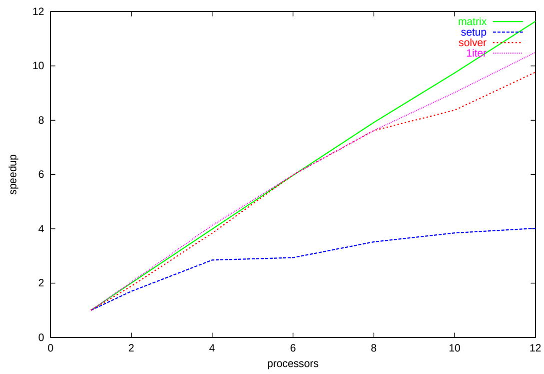

Figure 3: Acceleration by parallelization.

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F 1302: Solving and Proving in General Domains

Prof. Dr. B. Buchberger

Prof. Dr. T. Jebelean, Dr. W. Windsteiger

D.I. F. Piroi, A. Craciun, D.I. K. Nakagawa, D.I. Judit Robu

1 "Solving and Proving in General Domains"

The goal of Subproject F1302 is to provide computer support for all phases of the mathematical development cycle: to prove theorems, use them for computations and experiments, conjecture new theorems, prove those, extract solution methods from them, apply them in other proofs, etc. The *Theorema* system, which is being developed in the frame of this SFB, offers these features in one coherent software system which is currently based on the rewrite engine of the computer algebra system *Mathematica*.

In the year 2001, various strong components have been built on the foundations laid in the previous years of this SFB. One of them is the *set-theory prover* of Theorema [12], an implementation of special inference rules for set theory, corresponding to various reasoning steps used by the working mathematician in a typical informal proof. Since set theory is at the heart of mathematics (e.g. all the volumes of the monumental Bourbaki oeuvre are based on a version of Zermelo-Fraenkel set theory), this gives the user a powerful tool for proving many important theorems occurring in all branches of mathematics, see for example [11].

Another important component developed intensively in 2001 is the *geometry prover* of Theorema. Geometric theorem proving is a very traditional—maybe even an original—branch of mathematics, going back to the ancient school of Euclid. It is a marvellous fact that all of these classical theorems (and many more) can nowadays be proved by purely algebraic methods like Gröbner bases or the area method. This is in complete accordance with the overall philosophy of Theorema, which emphasizes the importance of combining provers and solvers for obtaining more powerful proving methods. The geometry prover of Theorema provides various such combined methods for deriving a lot of substantial results like Pappus's Theorem [9, 10].

The *general provers* of predicate logic have also been enhanced in various ways: First, there is a new meta-strategy called "S-decomposition" for obtaining very natural proofs of theorems such as the ones typically encountered in elementary analysis [3]; see also the SFB report 01-40. The main idea is to introduce Skolem constants and meta-variables in goal and assumptions in various parallel waves. Second, a new natural-style predicate prover has been developed for a sound treatment of meta-variables and deferred proof obligations [4]; see also SFB report 01-36. Third, the PCS proving strategy (basically a predicate-logic prover that is skilfully enhanced by a special solver over the reals, see the previous SFB report) has been improved [2].

The rewrite prover, an essential building block for many proof problems, has been rewritten completely. Among other features, it provides a Knuth-Bendix completion procedure and a *unification algorithm for sequence variables*. The theory of sequence unification is a very young research topic which is also advanced by the Theorema project [5]. It has a powerful impact on formalizing and proving theorems e.g. about arithmetic operators in a natural way. The main advantage compared with the traditional fixed-arity approach is that one can dispense with the parentheses in terms like $a + b + c$ where the operator is associative, since the term is understood as $plus[a, b, c]$ instead of $plus[plus[a, b], c]$ or $plus[a, plus[b, c]]$. Hence one does not have to struggle with shifting parentheses, which is of great help both for generating and reading proofs.

Besides these prover modules, the system environment has been extended in several directions. The so-called focus windows are a novel method for *advanced proof presentation* [8]; see also SFB report 01-38: The user sees the whole proof like a movie in a series of snapshots, each of them specifying one proof situation, where the relevant assumptions are filtered out from the knowledge base and the current inference step is described. The advantage of this presentation style is that a reader is not distracted by dozens of irrelevant assumptions, and the mind becomes free to concentrate on the essential parts; this is of great help especially for understanding complicated proofs.

Another new feature is the *interactive interface to provers*. In the community of automated-theorem proving, there are two main interest groups: one for proof search, the other for proof verification. All the provers described up to now (including everything that was described in the previous SFB report) are fully automated, thus giving the user maximum computer support by doing the whole proof search. On the other hand, it is often desirable to interact in certain critical moments, e.g. by providing witness terms in an existential subgoal; this is now possible for Theorema provers. Since one can still delegate the "routine parts" of a proof to the machine, this seems to be an optimal compromise between full proof search and mere proof verification.

A novel approach to advanced logical syntax is realized by so-called *logico-graphical* symbols [1, 7], see also SFB reports 01-35, 01-37. They combine the indispensible quality of mathematical rigor with the intuitive power of well-chosen graphical symbols. In Theorema, it is now possible to use any self-created symbol or even arbitrary Postscript images for denoting function symbols, predicate symbols, object constants or special quantifiers. This opens new possibilities for displaying proofs that are as easy to read as possible, while still having the full logical precision of traditional proofs.

Besides all these internal components of Theorema, there are also numerous *interfaces to external proof engines* [6]; the current list runs as follows: Otter, Gandalf, Waldmeister, Spass, Bliksem, Vampire, E, Setheo, Scott, EQP, Mace. Hence one can formulate a complicated theorem once in Theorema and then call the various proof engines on them without leaving Theorema. Since each of these engines has its own strengths and weaknesses, it can be very benificial to go over this interface. They can also be combined with other Theorema provers or amongst themselves for gaining special efficiency. An example described in the above paper is the combination of the first-order prover Otter with the counter-model searcher Mace: started on some formula (and we do not know whether it is true or false), Otter will attempt to prove it; if this fails, Mace is started for searching a couter-example.

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F 1303: Proving and Solving over the Domain of the Reals

Josef Schicho
Gábor Bodnár, Stefan Ratschan

1 Parametrization

In many cases, the problem of finding real parametrizations for real algebraic surfaces can be reduced to the problem of finding real parametrizations of tubular surfaces (see [13]). As a continuation of the joint resarch with co-investigators in subproject 1304 (see [10]), numerical and symbolic techniques for the parametrization of pipe and canal surfaces – which are an important special case – have been developed in [9]. We investigated the relation of the problem to the problem of representing a positive polynomial as a sum of two squares. This does not only lead to faster numerical algorithms, it also gives a negative result stating that for the generic case, symbolic solutions have exponential complexity.

An interesting spring-off result was the classification of all multiple conical surfaces [14]. This are the surfaces that can be generated as the union of a one-parameter-family of conics in more than one way. For instance, the surface in Fig. 4 is generated by two families of circles passing through a fixed point. The horizontal sections form a third generating family, consisting of hyperbolas. One of the results is that

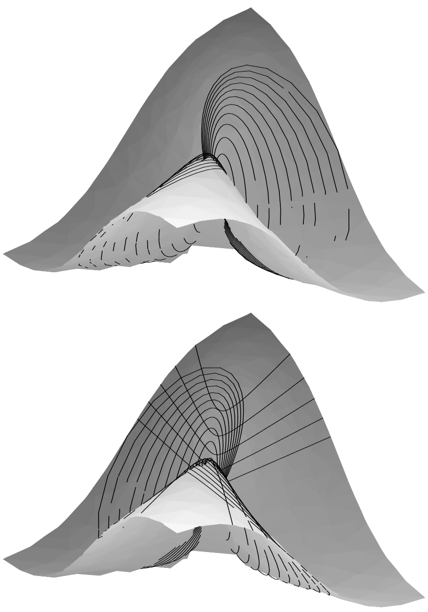

Figure 4: A multiple conical surface.

the number of generating families is either less than or equal to 12, 15, 16, 21, 27, or ∞.

2 Box Approximation

Box approximation is a method for computing approximate solution sets for first-order constraints over the reals, containing existential and universal quantifiers (see Fig. 5). The existing algorithm for

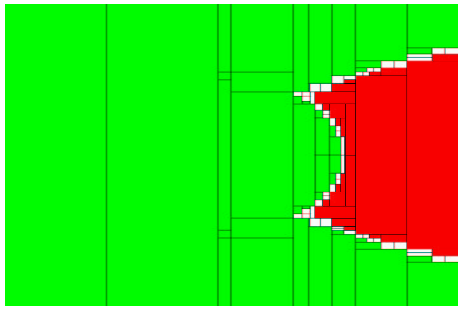

Figure 5: A multiple conical surface.

box approximation has been applied and adapted to problems arising in discrete time robust control. The problem is clearly out of reach for current symbolic solvers.

We formulated (together with L. Jaulin, university of Angers) the problem as a program in a (fictituous) constraint programming language with explicit quantifier notation. This allows to clarify the special structure of the problem and the necessary extensions of the existing algorithm [12] for computing approximate solution sets of first-order constraints over the reals. The solution was presented in [8], and is electronically available in the conference proceedings under `http://arXiv.org/html/cs/0110012`.

The new method performed also quite promising in many benchmark examples arising in the stability analysis of difference schemes for partial differential equations (see [7]). A report is in progress.

3 Singularity Analysis

We improved our program [3] for the resolution of singularities, using some new computational techniques described in [4]. The resolving parameter space of the given singularity is usually represented by an atlas of charts. This chart representation also carries significant redundancy, which originates in the presence of isomorphic subsets (chart overlaps). Let the charts of the atlas of a nonsingular quasi-projective variety be indexed by natural numbers. A relevant point of a chart with a given index is one that lies in no chart with smaller index. Now it is easy to see that a chart with no relevant point is redundant, while to detect such a chart efficiently (without examining chart change maps explicitly) is not at all trivial.

In the resolution algorithm, multiple treatment of singularities that lie in overlaps of several charts causes computational redundancy. Obviously, such redundant resolutions should be avoided for the sake of efficiency. However, the charts that contain isomorphic singularities might also carry unique information, thus a careful separation of relevant and redundant subsets has to be done in each chart.

Using our technique, we can cope with both kind of problems, on the relatively low cost of some additional bookkeeping.

4 Exact Real Computation and Regularization

Exact real computation allows many of the advantages of numerical computation (e.g. high performance) to be accessed also in symbolic computation, providing validated results. We implemented a Maple package representing a transparent and easy to use connection between the two worlds, using the exact real paradigm. Exact real numbers are represented as a class of objects that can provide arbitrarily close floating point approximations. The basic operations (field arithmetic, polynomial substitution, aso.) on these real numbers have been programmed in an object-oriented way, depending only on the methods that are available for this class. This makes it possible to change the internal representation of the objects without a complete re-implementation of the basic operations.

The package also includes some higher-level operations (root computation, greatest common divisor of polynomials, solution of linear equations). Some of these operations turn out to be ill-posed. For the problem of solving over-determined linear systems of equations, we used the scheme of Tikhonov regularization [1]. For the GCD computation, we used a regularization scheme developed in [5]. The package was presented in [2].

5 Symbolic Methods in Numerical Algorithms

In the element preconditioning technique developed in [6], the problem arises to construct an M-matrix that is as close as possible to a given symmetric positive definite matrix. The problem has to be solved for a large number of instances (the number of elements). The solution of this subproblem could be considerably accelerated in [11], using symbolic methods.

Together with B. Kaltenbacher, we use symbolic methods to make an optimal choice of the regularization parameter in a multigrid method for solving nonlinear ill-posed problems (ongoing research). solved in an interactive Maple session.

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F 1304: Symbolic-Numerical Computation on Algebraic Curves and Surfaces

Prof. Dr. F. Winkler
R. Hemmecke, E. Hillgarter
G. Landsmann

1 Results of the Project

We report on the achievements of the project from September 2000 (date of the last report) to December 2001. During this time results have been achieved in reliable visualization of algebraic curves, in analyzing the covering (i.e. the tracing index) of rational parametrizations, in rational parametrization of pipe and canal surfaces, and in application of Gröbner basis transformations to problems in coding theory. In addition to these new research results, we have been active in scientific editing and in the organization of workshops and conferences. In several invited lectures we have presented our ideas on symbolic and numerical computation in algebraic geometry. A new version of our program package CASA has been released.

1.1 Reliable visualization of algebraic curves

Continuing the work started in the year 2000, we have further investigated the problem of reliable or faithful visualization of algebraic curves. Such algebraic curves are reasonably defined in the projective complex plane $\mathbb{P}^2(\mathbb{C})$, but of course we can only visualize a curve $\mathcal{C}$ in an affine real plane $\mathbb{A}^2(\mathbb{R})$. This leads to the problem of locating the area of the plane in which we can find real components of $\mathcal{C}$. Such components might be rather small, in degenerate cases even isolated points (i.e. singularities of $\mathcal{C}$ in which complex branches meet). Our approach can find all these interesting regions of the plane and give faithful plottings in these regions.

In particular, in [6] we have considered a cluster architecture for approaching this visualization problem and we have presented our approach to an audience in symbolic and numerical scientific computing.

1.2 Parametrization of curves and surfaces

In this central topic we have achieved several new results (we refer to the 1999 report for a specification of the parametrization problem). One of the central problems is the analysis of the singularities. In his phd thesis [10] P. Stadelmeyer has investigated this problem for the case of curves. He gives a detailled analysis of the field extensions necessary in the resolution of singularities and computation of adjoints. The complexity bound could be lowered from $\mathcal{O}(d^8)$ to $\mathcal{O}(d^5)$, where d is the degree of the curve.

In [32] we have continued our work on rational parametrization of pipe and canal surfaces, and the relation of this problem to the quadratic forms over various fields. See a picture of a canal surface around Viviani's temple in Figure 6.

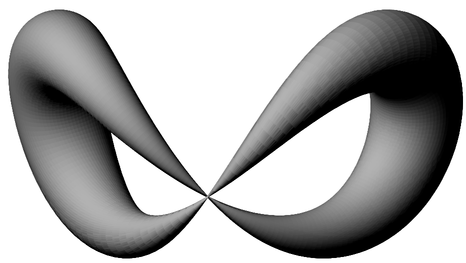

Figure 6: Viviani's temple

Finally, in a series of publications, e.g.,in [42, 43], we have investigated the degree of a rational map between varieties, in particular curves. This leads to the notion of the tracing index of a rational parametrization, i.e. the number of times such a parametrization "traces" the given curve. We have reduced the problem of determining the tracing index to a few GCD (greatest common divisor) computations on polynomials derived from the parametrization.

1.3 Gröbner basis theory

In 1998 at the IMACS-ACA conference in Prague there was a session on *Applications of the Gröbner Basis Method*. Paper presented at this session and also some additional papers have been edited by Q.-N. Tran and F. Winkler and appeared in [11].

During his year at RISC-Linz, M. Borges Quintana has worked with F. Winkler on ideas for using basis transformation techniques from the theory of Gröbner bases for designing new approaches to linear codes. The results have been reported in [14].

R. Hemmecke has given talks at the IMACS-ACA conference in Albuquerque, New Mexico, and at the SFB conference SNSC'01 in Hagenberg on his new dynamical division algorithm in the theory of involutive bases. His sliced division improves the complexity behavior in many interesting examples.

F. Winkler was invited to give a minicourse on *Computer Algebra in Geometric Computing* at the workshop of the European project ECG (Effective Computation Geometry) [53]. The workshop took place at the Lorentz Center at the University of Leiden.

1.4 The software system CASA

Our software system CASA (Computer Algebra Software for Algebraic geometry) has been released in a new version, CASA 2.5 [4]. This new version was presented by R. Hemmecke in [18]. Novel techniques in parallel and distributed computing for CASA and similar software have been investigated in [41].

1.5 Miscellaneous

F. Winkler has written on computer algebra, computational geometry, and constructive ring theory in [12], [47], [46].

H. Gu has continued his research on approximation algorithms for constructing minimal surfaces [2].

2 Workshop SNSC'01

In 1999 we have organized the workshop *Symbolic and Numerical Scientific Computing (SNSC'99)*, which was considered a great success by the SFB and the participants. In September 2001 F. Winkler has again organized a similar event, the conference *Symbolic and Numerical Scientific Computing (SNSC'01)*, [13]. Due to the wish of many participants, we are now in the process of editing the proceedings of SNSC'01, which will be published by Springer-Verlag Heidelberg. A more detailled report on SNSC'01 is given separately.

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F 1305: "Symbolic Summation and Combinatorial Identities"

A.Univ.-Prof. Dr. Peter Paule

DI Dr. Axel Riese

DI Fabrizio Caruso, DI Dr. Carsten Schneider, Mag. Burkhard Zimmermann

1 Symbolic Summation and Combinatorial Identities

The scientific output achieved in 2001 by the project group F1305 is documented in the form of 14 publications: 7 refereed articles in journals, 4 refereed articles in proceedings, and 3 technical reports which have been accepted by journals. Additionally, one PhD thesis and one Diploma thesis have been completed, both closely related to the project work.

1.1 Indefinite and definite summation

The WZ method, in particular Zeilberger's algorithm, has become an indispensable tool for solving problems in connection with hypergeometric summation. Nevertheless, as described by Zeilberger [13] there remain still some classes which resist a convenient automatic treatment. A. Riese [38] was able to "cure the Andrews syndrome" by introducing suitable parameter substitutions to resolve this problem for an important subclass of identities.

Another achievement of A. Riese [15] was the development of `qMultiSum`, a computer algebra package for proving q-hypergeometric multiple summation identities. This development is based on another achievement made in the F1305 group, namely K. Wegschaider's refinement of the Sister Celine/WZ method. Identities from statistical mechanics or from partition theory are natural application domains for `qMultiSum`. For example, in cooperation with A. Berkovich and using his package, Riese [11] succeeded to give the first proof of an identity which has been conjectured (by humans).

Around 1980, M. Karr developed an algorithmic summation analogue (in the setting of suitable difference field extensions) to Risch-integration. Despite the fact that its domain of application potentially is very general (e.g., including harmonic numbers that arise in the analysis of algorithms), Karr's method has not achieved the attention it deserves. Now, within the SFB, C. Schneider [5] developed the first computer algebra package that implements Karr's machinery in full generality and extends its functionality significantly. For instance, Schneider succeeded to adapt Karr's approach also to *definite* summation problems. To this end, he needed to extend linear difference equation solvers to very general domains. Consequently, Schneider's package provides a new and sufficiently general algorithmic tool for attacking problems that have lain beyond the scope of the methods available so far. A series of papers describing his new theory together with new applications is in preparation.

1.2 MacMahon's Partition Analysis

In his famous book "Combinatory Analysis" (1916) MacMahon introduced partition analysis as a computational method for solving problems in connection with linear homogeneous diophantine inequalities and equations. For several decades this method has remained dormant. In SFB work, carried out jointly with G.E. Andrews (PennState, USA), it has been demonstrated, in the form of the Mathematica package `Omega` [3], that partition analysis is ideally suited for being supplemented by modern computer algebra methods. Based on a new decomposition of multivariate rational functions of a certain kind, the underlying algorithmic method has been significantly improved [7].

Applications of `Omega` range from the preprocessing for automatic theorem proving to enumeration problems in statistical physics. In [7] it has been used for finding bijections between sets of partitions; in [5] certain types of compositions have been enumerated. The papers [6, 4] describe applications where `Omega` has been used to compute the generating functions of combinatorial objects that are natural generalizations of classical configurations.

1.3 Additive number theory

The Rogers-Ramanujan identities belong to the most outstanding identities in additive numbers theory. Recently several algorithmic approaches have been developed in order to assist the treatment of such identities by computer algebra packages. With Zeilberger's algorithm polynomial versions can be proved automatically. However, informally spoken, all these methods start out with the sum side and try to derive the corresponding expression in product form.

In recent years, A. and J. Knopfmacher derived an algorithm, the Extended Engel Expansion, that leads to unique series expansions of Rogers-Ramanujan type if starting from the product side. In joint SFB work with G.E. Andrews and A. Knopfmacher it has been shown that the new and elegant Rogers-Ramanujan generalization found by Garrett, Ismail, and Stanton also fits into this framework. This not only reveals the existence of an infinite, parameterized family of extended Engel expansions, but also provides an alternative proof of the Garrett, Ismail, and Stanton result.

In a previous report we already indicated that this achievement can be viewed as the starting point for further investigations. Such work has been carried out in the articles [1, 2].

Related work, but using different methods, are the papers [11, 12].

1.4 Symbolic methods for wavelet construction

Wavelets are widely used in many practical applications such as data compression, or for the solution of partial differential equations. They are special functions which often have a fractal character. This makes it relatively difficult to work with them explicitly. However, to work with wavelets one can use the nice feature that they are defined by a small number of parameters, the so-called filter coefficients. In general, any algorithm relying on wavelets only uses the filter coefficients and not the wavelet function itself.

In cooperation with O. Scherzer and A. Schoisswohl, the project group F1305 carried out a detailed study of the basic equations for the filter equations [12]. In particular, it turned out that Gröbner bases methods enable to compute closed form representations of the wavelet coefficients. To this end a more economic description of the underlying algebraic variety has been found. Remarkably, various combinatorial identities play an important role in this process. A new study, again with O. Scherzer and A. Schoisswohl, on the extension of this approach towards the construction of new wavelets with scale dependent properties is in preparation.

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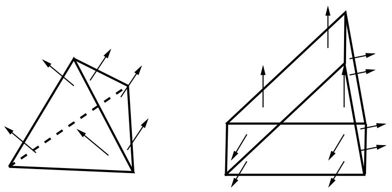
F 1306: Adaptive Multilevel Methods for Nonlinear 3D Mechanical Problems

Prof. Dr. U. Langer,
DI. J. Kienesberger, Dr. M. Schinnerl,
Dr. J. Schöberl

This project is concerned with the developement of finite element technology for mechanical and related coupled field problems. This period we focused on the improvement of central components as described below.

1 Mixed Finite Elements

The standard finite element approach for elasticity is to approximate the displacement field by continuous finite elements, and then compute the stresses in the postprocessing step. An alternative is to approximate both fields simultaneously by mixed finite element methods. Here, a better accuracy in the practically more important stresses is possible. Since the 80s several such elements have been proposed. A new family of stabilized equilibrium elements has been achieved by J. Schöberl. These elements use optimal order shape functions for all components and do not need additional bubble functions. The reduction to non-conforming displacement elements is possible such that the implementation is simple. We also have developed prismatic elements which are robust for the thin plate limit. The stress components are approximated by BDM - $H(\text{div})$ elements, which are drawn below:



A related result by J. Schöberl are local and stable quasi-interpolation operators satisfying the de Rham commuting diagram [5]:

$$\begin{array}{ccccccc} H^1 & \xrightarrow{\nabla} & H(\text{curl}) & \xrightarrow{\text{curl}} & H(\text{div}) & \xrightarrow{\text{div}} & L^2 \\ \downarrow \Pi^W & & \downarrow \Pi^Q & & \downarrow \Pi^V & & \downarrow \Pi^W \\ W_h & \xrightarrow{\nabla} & Q_h & \xrightarrow{\text{curl}} & V_h & \xrightarrow{\text{div}} & S_h \end{array}$$

These operators enable improved multigrid analysis and a posteriori error estimates. Similar operators were also used in the construction of algebraic multigrid methods in $H(\text{curl})$ and $H(\text{div})$, [3]. The work on anisotropic error estimates and multigrid methods continued [1].

2 Elasto-plastic Simulation

Elasticity and elasto-plasticity are interesting subjects in solid mechanics. The governing equations describing this phenomenon are the equilibrium of forces, the non-linear relationship between strain and stress, the linear dependence of the strain on the displacements and the Prandtl-Reuß normality law describing the time evaluation of plastic materials.

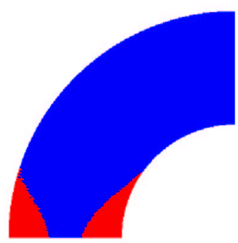
By discretizing the time derivatives occurring in the normality law and calculating the weak dual formulation, the problem can be considered as a variational inequality, which is equivalent to the minimum problem in the displacement u and the plastic part of the strain p

$$f(u,p) = \min_{v,q} f(v,q)$$

under incompressibility constraints.

An algorithm solving this problem using the finite element method was developed by J. Kienesberger in her Master's thesis [2]. The strategy is alternating minimization in the two variables: p can be minimized locally, whereas u is determined by solving a system containing a Schur complement matrix with a multigrid preconditioned conjugate gradient method.

The algorithm was tested on a two dimensional quarter of a ring, with its lower edge fixed and an upward acting force on the right edge. The domain with plastic behavior is drawn below: In the two lower corners the material plastifies.



3 Multi-Body Systems

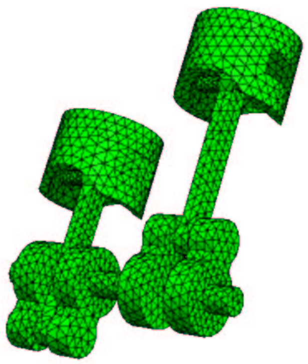
J. Schöberl and J. Gerstmayr developed finite element algorithms for multi-body systems. The governing principle is the Jacobi-Hamilton system

$$\frac{d}{dt}\left(T(\dot{u}) + V(u)\right) = 0,$$

where T is the kinetic energy and $V(u)$ is *some* inner energy expression. We used a hyperelastic material law applied to a partially non-linear strain tensor. More precisely, we split the displacement u as

$$u = u_0 + u_f,$$

where $u_0 = \Pi u$ is a linear approximation in each subdomain and thus contains the rigid body motions. Then, the postulate is that quadratic terms in u_f are small and thus neglected in the strain tensor. The outcome is that the resulting stiffness matrix can be obtained by simply rotating the stiffness matrix in the reference domain, and thus expensive re-assembling is avoided. Different versions of time integration schemes for differential algebraic equations were applied. One of the simulated examples is a slider crank mechanism as drawn below:



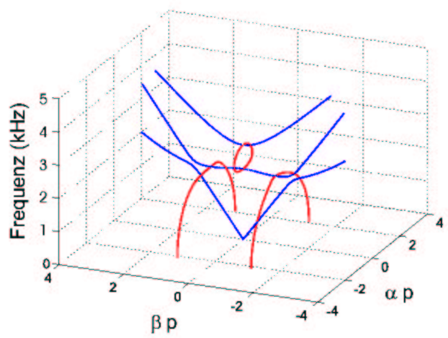
4 Piezo-electric device simulation

S. Zaglmayr finishes her Master's thesis on multigrid methods for piezo-electric device simulation [6]. She works together with Prof. U. Langer and J. Schöberl, and Prof. Lerch from Institute for Sensor Technology, University Erlangen.

One application of interest are surface accoustic wave filters as commonly used in cell phones. The device consists of several 100 equidistant electrodes. For computing, we may assume a periodic domain. One asks for the frequencies of waves which can pass the filter. These are exactly the Eigenfrequencies of the differential operator. Bloch theory reduces the problem from the inifinite, periodic domain to the shifted unit-cell problem. This means we seach for Eigenfunctions $u = (u_{mech}, u_{elec})$ such that

$$\begin{aligned} L\,u &= \omega^2 u \\ u_r &= e^{i\gamma} u_l \\ \frac{\partial u_r}{\partial n_r} &= -e^{i\gamma}\frac{\partial u_l}{\partial n_l}. \end{aligned}$$

Here, L is the pieco-electric differential operator coupling the mechanical and electrical field, u_l and u_r are the boundary values at the left and at the right boundary of the unit-cell, respectively, and ω is the frequency. The shift γ is also unknown, and one searches for solutions $(\omega, \gamma(\omega))$. S. Zaglmayr is mainly concerned with iterative solvers for the resulting quadratic eigen-value problem. A solution set, a so called dispersion diagram, is drawn below. Real solutions (drawn in blue) correspond to passing frequencies.



M. Schinnerl finished this PhD thesis [4] on coupled magneto-mechanical systems. He simulated challenging benchmark problems as an electro-magnetic-acoustic-transducers (EMAT).

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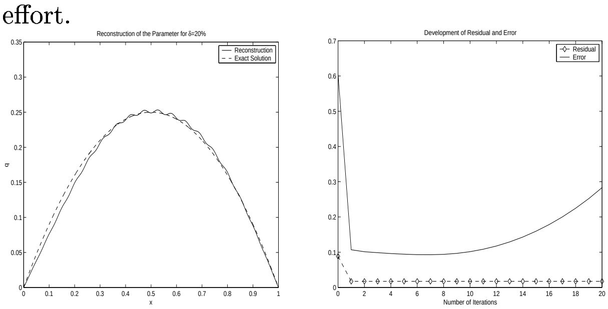
F 1308: Large Scale Inverse Problems

Prof. Dr. Heinz W. Engl

Dr. Hend Benameur, Dr. Martin Burger,
Dr. Barbara Kaltenbacher, Dr. Antonio Leitão,
DI. Markus Rosenkranz, DI. Herbert Egger

1 Iteratively Regularized SQP

A close cooperation within the SFB F 013 was started with Project F 1309 concerning the iterative regularization of parameter identification problems by SQP-type methods and their numerical realization, resulting in two joint papers by Martin Burger and Wolfram Mühlhuber (cf. [3, 4]). In the first paper [3] iterative regularization methods for parameter identification problems based on the idea of sequential quadratic programming where presented and analyzed with respect to their convergence and regularization properties. In the follow-up [4], the numerical approximation of these methods and their efficient implementation was discussed. Besides error estimates and a convergence analysis of the discretized methods, a simultaneous solution strategy (in the product space for state and parameter) has been discussed, which leads to a sequence of well-posed saddle-point problems. Employing preconditioned iterative solvers for parameter identification problems, a significant speed-up with respect to common approaches was achieved. Moreover, a multilevel implementation was presented and analyzed, which allowed a further reduction of the numerical effort.

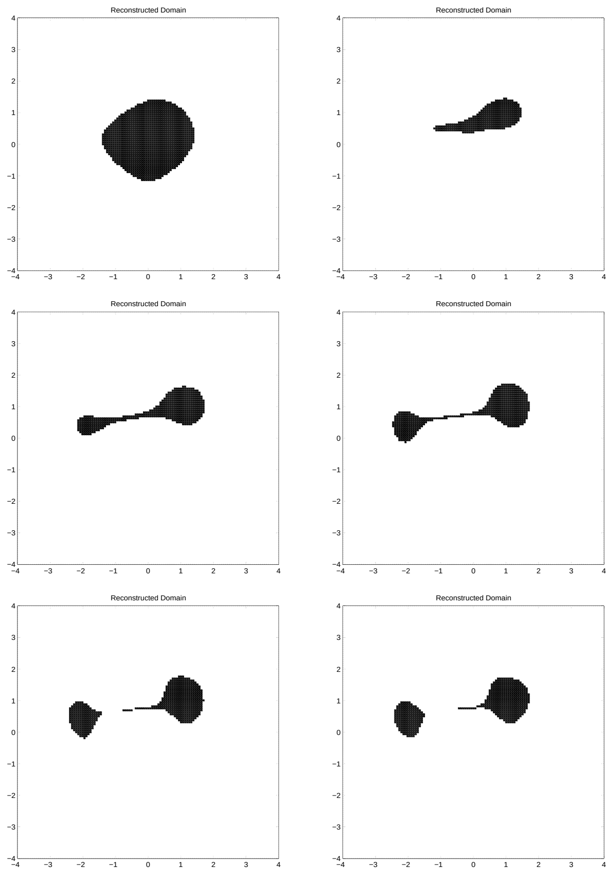


Left: reconstructed parameter (solid) versus exact parameter (dashed).
Right: development of error in parameter (solid) and error in target (dashed) during the iteration for noise level $\delta = 20\%$.

For 2D results see the report of project F1309.

2 Level-Sets and Regularization

In [16] a new level set method for a class of inverse problems, where the aim is to reconstruct some set with unknown number of connected components, was developed and analyzed with respect to convergence and regularizing properties.



Evolution of the Level-Set from one component (top left) to two components (bottom right).

To our knowledge, this paper is the first with a rigorous mathematical analysis of a level set method for inverse problems, which was also accomplished by the referees of the Journal Inverse Problems, who considered the results as very important and enabled a publication only 6 months after completion.

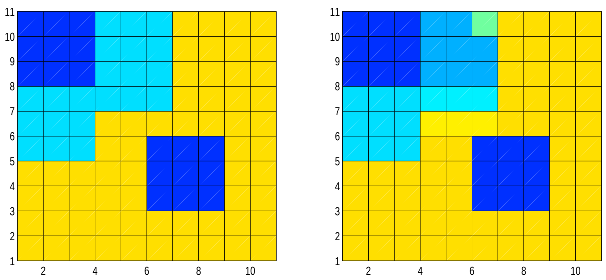
3 Neural Networks

In the field of neural networks and their connections with inverse problems, the application of Tikhonov-type regularization to function approximation by neural networks was investigated by Martin Burger and Andreas Neubauer [5]. Two different approaches to Tikhonov regularization, i.e., by regularizing either the network parameters or the approximating function, where analyzed and tested in numerical examples.

4 Regularization by Adaptive Discretization

Subsequent to our research on regularization by discretization methods, we continued our work by investigations on adaptive discretization in parameter identification [7].

For the reconstruction quality of parameters from measurements it is essential not only to choose the overall number of degrees of freedom in the representation of the parameter (i.e., how fine the discretization is in total) but also where they are positioned: In places where the parameter changes rapidly, the discretization should be refined locally, while in regions where the parameter only slightly differs from a constant a coarse resolution is sufficient. However, since it is just the parameter and its behavior that is to be determined and not known a priori, it is crucial to develop strategies that estimate this behavior from the data and therewith enable an adaptive discretization.



Exact solution (left), solution by adaptive refinement and coarsening (right).

Such a method, working with so-called refinement and coarsening indicators had been developed at the Institut National de Recherche en Informatique et Automatique (INRIA) with the collaboration of Dr. Ben Ameur, who worked in the SFB for two months this year. On that occasion, we did a convergence analysis and numerical tests for this method in [7].

5 Identification of Doping Profiles in Semiconductors

In cooperation with Prof. Peter Markowich (University Vienna) and Dr. Paola Pietra (IAN Pavia) we have investigated the identification of doping profiles in semiconductor devices (cf. [1, 2]), which is a challenging inverse problem due to several reasons. First of all, the underlying direct model, the *drift-diffusion equations*, are a rather complicated system of nonlinear differential equations with strong coupling with the parameter to be identified, the *doping profile*, being a function of location arising as a source term in one of the equations. In particular, the solution of this system may be non unique for high applied voltages, which means that the parameter-to-solution map is only well-defined close to equilibrium (i.e., for small applied voltages). Secondly, only few data for the inverse problems are accessible, namely the current on some contacts on the boundary. Exploiting similarities to impedance tomography we have shown identifiability of the doping profile in a special case, namely in the *stationary unipolar drift-diffusion model* close to equilibrium, under the assumption that we can apply a suitable large class of different voltages and measure the corresponding current. Moreover, we have investigated the interesting special case of the doping profile being piecewise constant, which lead to a class of severely ill-posed problems. While the first paper [1] was restricted to the stationary case, we investigated first properties of the corresponding transient problem in [2].

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F 1309: Multilevel Solvers for Large Scale Discretized Optimization Problems

Prof. Dr. Ulrich Langer, Prof. Dr. Heinz Engl, Dr. Ewald Lindner, Dr. Gundolf Haase, Wolfram Mühlhuber, Roman Stainko

1 General Frame

For the numerical treatment of optimal design problems as well as inverse problems a new common frame was developed. Starting with our experience of the last three years where we mainly worked on optimal sizing problems and shape optimization problems, we worked out the basic abstract structure which is behind these type of problems. We integrated also topology optimization into this frame. Later on, we began to analyze also inverse problems together with members of Project F1308. Inverse problems have a very similar structure to optimal design problems. This collaboration resulted in a generalized optimization framework which was implemented in FEPP, a finite element code written in C++. This environment can not only treat optimal design problems but can also be used to solve inverse problems. This abstract frame was the basis for our investigations of these two problem classes.

2 Optimal Design Problems

The main idea of optimal design is to modify the shape of an object in such a way that the resulting shape is optimal with respect to a certain criterion. During recent years, the importance of optimal design has been growing, especially in the commercial market. In most cases, the industrial design process shall be automatized in order to accelerate the whole design phase. Still nowadays, changes in the design are most often based on long lasting experience, rather than optimization methods. Engineers designing a product make parameter studies changing a few input quantities by hand and re-evaluate the resulting design. Unfortunately, due to lack of time this process is usually stopped after a few iterations – in most cases only two or three. Then, the best design obtained so far is taken because no more time is left for drafts that would possibly meet the requirements to a larger extent.

That is why, tools supporting such a design process have to fulfill mainly two goals:

- On the one hand, they have to be flexible enough to handle the various requirements. Nevertheless they also have to be robust to produce reliable results. Especially, it is desirable to spend only little work when the requirements change.
- On the other hand these tools have to be fast. Tools which automatize some parts of the design process strongly accelerate it and so more design drafts can be optimized.

During the last year, we continued our investigations on sizing problems. The method we used combines hand-coded derivative parts with automatic differentiation. For those parts of the function evaluation which change quite frequently, we use automatic differentiation, whereas for the most time consuming parts hand-coded derivatives were implemented. Luckily, these parts are not often changed, so that the additional effort for hand-coding these parts pays off. By accelerating the existing method we were able to solve also problems with about 1000 design parameters. Pictures of the optimal thickness distribution can be found in Figure 7 and Figure 8 (white indicates the thick part, violet the thin one). For details see [4, 30].

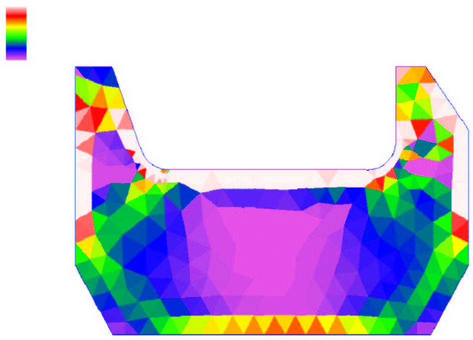

Figure 7: 449 design parameters

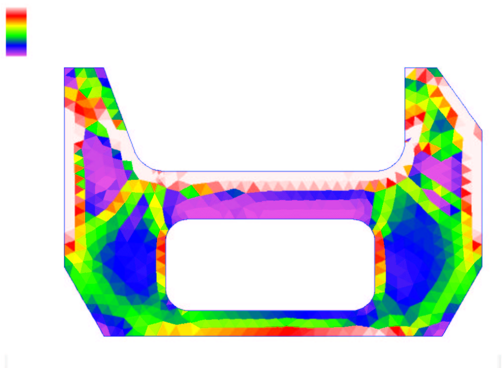

Figure 8: 1078 design parameters

3 Inverse Problems

In a close cooperation with Project F1308 we developed and worked out a method for the efficient solution of parameter identification problems. Our approach is based on iterative regularization using SQP-type methods and was described in two joint publications ([1, 2]). Our main goal during the development was a good numerical performance to be able to solve also large scale inverse problems. The first paper ([1]) introduces and analyzes the method which combines ideas from iterative regularization with ideas from sequential quadratic programming. This analysis is rather general and not restricted to a certain class of state problem. In the second paper ([2]) which is a follow-up we discussed the numerical approximation, but restricted ourselves to state problems of elliptic type. We presented a convergence analysis for the discretized method as well as error estimates. Besides, we focussed on the efficient numerical realization. Unlike classical approaches we do not introduce a solution operator for the underlying state equation but consider it as a constraint and apply SQP-techniques in the product-space for state and parameter. The numerical approximation leads to saddle point problems. These were solved by preconditioned Krylov sub-space correction methods. This allows us to solve also large scale parameter identification problems, as all occurring matrices are sparse. An implementation of the method in our abstract framework for optimal design problems and inverse problems showed the good numerical properties of our approach. Figure 9 shows the reconstruction of a two-dimensional parameter.

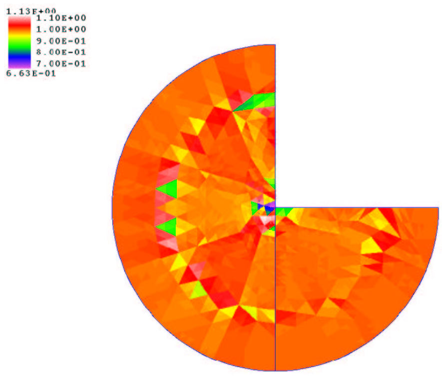

Figure 9: Reconstruction of a 2D parameter

Our method clearly outperformed classical solution methods for parameter identification problems as can be seen in Figure 10. The green line shows the runtime of the classical approach, the blue one of an approach developed by Kaltenbacher in project F1308 ([5]) and the red one of our new method. We could additionally accelerate our implementation using nested spaces for parameter and state variable. In Figure 11 a comparison of the original method with its nested version can be found.

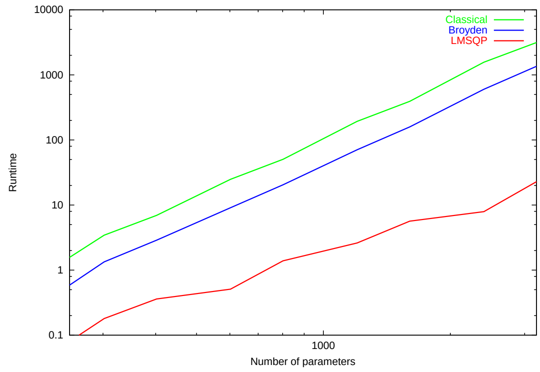

Figure 10: Comparison of runtimes

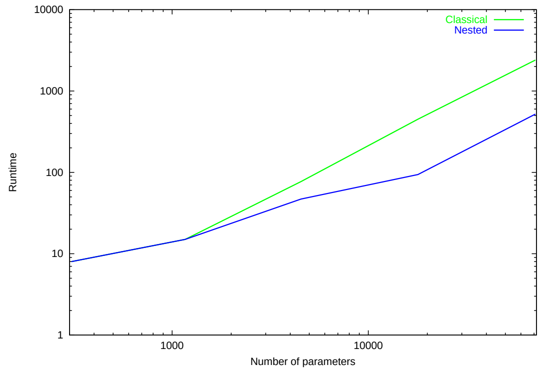

Figure 11: Acceleration using nested spaces

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F 1315: Numerical and Symbolic Techniques for Algebraic Spline Surfaces

Bert Jüttler, Josef Schicho
Pavel Chalmovianský, Johannes Gahleitner, Mohamed Shalaby

This is a new project of the second funding period. The three PhD students joined the project team in April, June, and October 2002.

1 Algebraic spline surfaces

The project aims to develop computational techniques for constructing and analyzing free-form shapes using algebraic spline curves and surfaces. A new method for algebraic surface fitting has been developed by Jüttler and Felis [6]. With the help of this methods one may generate surfaces from scattered data (point clouds), see Fig. 12. Unlike existing methods for parametric surface fitting, this methods does not need an auxiliary parameterization of the data, hence it can be applied to generate surfaces from more complex data sets. The potential applications include the reconstruction of free-form geometry in reverse engineering.

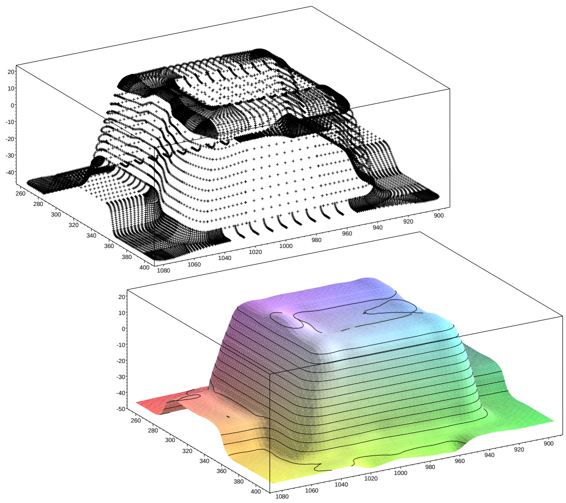

Figure 12: Algebraic spline surface fitting.

In order to improve the visualization of the implicitly defined surfaces, P. Chalmovianský implemented a variant of the marching triangle algorithm [1]. We modified the algorithm slightly, in order to obtain high–quality triangular meshes, see Fig. 12.

The algebraic order of the algebraic spline surfaces which are generated by the surface fitting technique is rather high (6), as they are based on a trivariate tensor–product representation. In order to generate algebraic spline surfaces of lower order, P. Chalmovianský used Hermite interpolation by 3D

Figure 13: Surface triangulation using marching triangles.

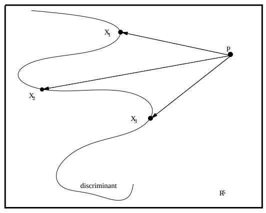

Figure 14: The general framework for robust parameterization

Clough–Tocher (CT) macro elements [5], producing a piecewise cubic algebraic spline surface. This surface can then be parameterized exactly (except for special cases, such as cones and cylinders), and it is easier to visualize it, e.g., via ray–tracing. The CT macro elements are defined over a suitable 3D triangulation which obtained as an two–sided offset of a coarse triangular mesh approximating the algebraic surface.

However, the conversion of the tensor–product high-degree spline surface into cubic CT elements led to unexpected problems, as the quality of the surfaces is not sufficient, due to unwanted oscillations [7]. We are now trying to detect the source of these problems, and to find ways to avoid them. Currently, P. Chalmovianský is exploring techniques for *fairing* algebraic spline curves. Here we use a local approach which is based on minimizing a suitable fairness functional, similar to the techniques developed in [4] for parametric spline curves. As the next step, we plan to apply these techniques to the CT spline surfaces.

2 Robust parameterization

In order to convert the algebraic spline curves and surfaces into a format that can be used in a CAD system, we need to develop techniques for parameterization. The existing methods rely mainly on symbolic methods. Consequently, they will fail if the coefficients of the algebraic curves or surfaces are floating point numbers, or if these curves/surfaces are not exactly rational, but only on in the neighbourhood of a rational curve or surface.

As the simplest possible case, J. Gahleitner is currently investigating methods for robustly parameterizing planar cubic curve segments. Here we use an algebraic condition for the rationality of a cubic curve [2]. This condition, the so–called discriminant (a polynomial of degree 8) describes a hypersurface in the space of Bézier coefficients space $\mathbb{R}^5$. We may formulate our problem as follows (cf. Figure 14): Given a point $P \in \mathbb{R}^5$, which corresponds to a cubic curve f, we want to find a a point X on the discriminant such that the corresponding curve has minimal distance (e.g., Hausdorff distance) from f within the region of interest. Here the region of interest is chosen as a triangle which is formed by two tangents of the cubic curve, and the line through the two points of contact. After some experiments with several methods for generating such a point X, J. Gahleitner developed an algorithm which is based on linear Chebyshev approximation. Using Remez' algorithm, he computes a direction d in Bézier coefficient space, such that the curves $P + \lambda d$ are highly accurate approximations for the given curve f within the triangle ABC, provided that the stepsize λ is sufficiently small. By intersecting this line with the discriminant hypersurface one obtains several candidates for rational curves which approximate the rational curve. An example is shown in Fig. 15. Currently we try to find an automatic procedure for

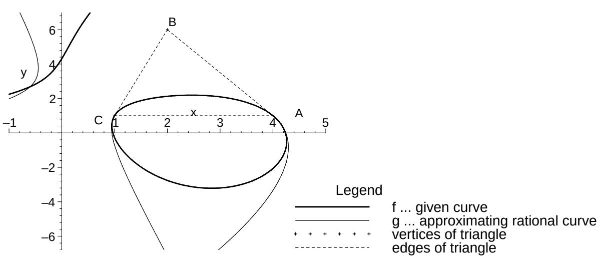

Figure 15: Robust parameterization of a planar cubic

picking an optimal solution. The next steps of this research include the generalization to higher degree curves and to algebraic surfaces.

Also, we gave symbolic and numeric algorithms for the parametrizations of pipe and canal surfaces [8].

3 Spline implicitization

As a theoretical result, any rational curve or surface can be equipped with an implicit representation. The exact implicit representation, however, is not very useful, as the number of coefficients is very high, even for relatively small degrees. In order to avoid these problems, and to make develop the implicit representations into a useful tool for applications, we propose to use approximate implicitizations by spline functions [3].

M. Shalaby is exploring methods for constructing algebraic spline curves by approximate implicitization. His research aims at generating low degree implicit spline representation of a given parametric planar curve. He developed an algorithm consisting of the following steps.

(1) Find a quadratic B-spline approximation of planar curves via orthogonal projection in Sobolev spaces, using a result by Reif. (2) Use adaptive knot removal, which is based on spline wavelets, in order to reduce the number of segments. (3) Implicitize the segments of the quadratic B-spline curve. (4) Find suitable "transversal lines" which can be used to join the bivariate quadratic polynomials which implicitize the segments, forming a continuous function.

As a subject of ongoing research, he is developing a

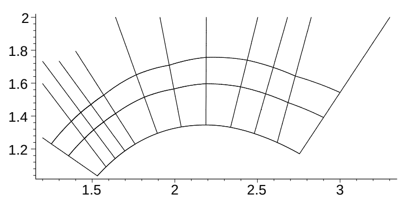

Figure 16: C^0 Spline implicitization of a planar curve. The original curve and two algebraic parallels $f(x, y) = c$ are shown

method for C^1 spline implicitization. Here, the main problem is to "localize" the construction, as otherwise the degree of the implicit representation would depend on the number of segments. Using results from classical differential geometry, the behaviour of the "transversal lines" for sufficiently small stepsize (segment length) has been analyzed by B. Jüttler. He showed that these lines are always well behaved, except at inflections of the original curve.

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F 1317: Estimation of Discontinuous Solutions of Ill-Posed Problems

Andreas Neubauer
Stefan Kindermann

Project F1317 has started in the second period of the SFB, i.e. in April 2001 with the objective to develop new and efficient methods for identifying discontinuous solutions in ill-posed problems. From its start until September 2001 it was run by the project leader A. Neubauer alone, from September 2001, S. Kindermann joined it on a PhD-position. This position has been changed to a Post-Doc after his graduation in December 2001 (cf. [4]).

The project is a continuation of the FWF-Project P13130-TEC *Regularization for Curve and Surface Representations.*

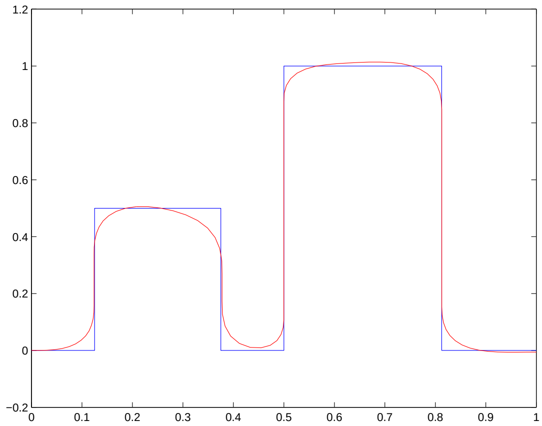

Figure 17: Graph of a discontinuous step function and corresponding curve regularization

1 Regularization by Curve and Surface Representations

We want to identify a discontinuous solution in an ill-posed equation. Such problem settings occur quite naturally in a wide range of important physical applications, such as nondestructive material testing, noninvasive medical imaging and related fields.

It has been observed that many existing regularization methods perform unsatisfactorily when applied to such type of problems due to the lack of smoothness of a discontinuous solution.

An interesting alternative to standard regularization schemes is regularization for curve and surface representations. Here, instead of viewing the discontinuous solution as unknown, its (continuous) graph is treated as unknown. Since a graph can be seen as parameterized curve or surface, we are applying regularization to the parameterization. This approach allows a greater flexibility in the representation of the solution and in its discretization. Moreover, we may use differentiable parameterizations even for graphs of discontinuous functions.

The regularization properties of this method have been analyzed in the FWF-project P13130-TEC. Although the starting point for the idea came from a different direction, it turned out, that regularization for curve and surface representations is closely related to BV-Regularization, a tool that has been investigated - amongst others - in the former SFB-project F1310 from the view point of diffusion equations (cf. [10, 12]).

Curve regularization has been sucessfully applied to one-dimensional linear (integral equations) and nonlinear ill-posed problems (e.g. parameter identification). Moreover, in two-dimensions, good results have been obtained for a special surface parameterization called Cartesian Product Parameterization (cf. [5, 6, 8, 7]).

Within the SFB we are interested in regularization using general two-dimensional surface parameterizations. We focus on an efficient numerical realization and its implementation for problems arising from application.

Following the basic idea of using parameterized curves and surfaces to represent discontinuous solutions, we numerically treated surface regularization by the method of Moving Grids [9]. In this framework, the discretized unknown solution is defined on an adaptive grid, which is deformed according to the smoothness of the computed solution.

The adaptive grid is the image of a uniform grid under an appropriately chosen deformation function. During each step of our regularization we remesh the grid in such a way that the gridsize is small whenever the approximate solution has large gradient and vice versa. The construction of such a deformation function is classical in geometry (cf. [11]).

Although adaptive grids are a quite common tool in various fields for direct problems (e.g. fluid dynamics, geometry), the combination of these with regularization incorporate new potential in the field of inverse and ill-posed problems.

The method of moving grids have been applied to two-dimensional integral equation of the first kind (cf. [9]). Using this technique we obtain a significantly better resolution of discontinuities than with a comparable fixed grid algorithm.

The application of moving grids to two-dimensional nonlinear parameter identification is in progress.

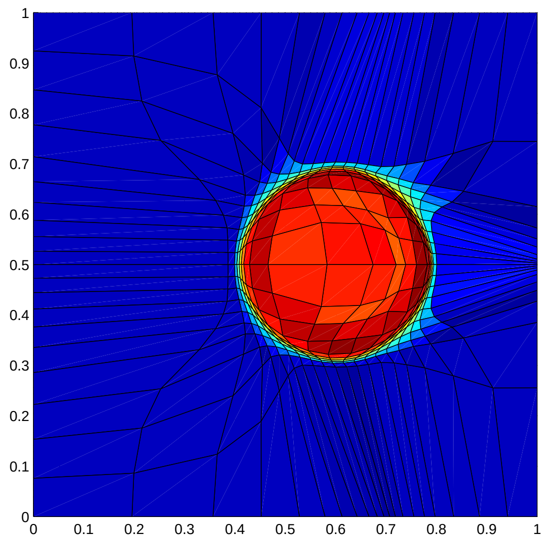

Figure 18: Identification of a function having discontinuities on a circle

2 Inverse Problems

In the field of general inverse problems there is a natural cooperation with Project F1309. In the context of discontinuous solutions for ill-posed equations a major challenge is to prove convergence rates of regularization schemes and to investigate approximation properties of appropriate discretizations. Some results for the former aim has been obtained in cooperation with project F1309, namely convergence rates for the continuously regularized Gauss-Newton method [3].

In cooperation with M. Burger, project F1309, interesting results concerning 'artificial intelligence' approximations have been found. Based on the work in [21], where approximation rates for this approach have been proven, the problem of function approximation by Neural Networks has been treated by Tikhonov regularization in [2]. This problem becomes ill-posed, when the number of network nodes becomes large. Thus, Tikhonov regularization gives rise to convergence and stable approximation even for large networks.

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SFB F013: Numerical and Symbolic Scientific Computing

Report on the SFB Conference "Symbolic and Numerical Scientific Computing (SNSC'01)" Hagenberg/Linz, 12–14 September 2001

In September 2001 we have again organized an international conference on *Symbolic and Numerical Scientific Computing (SNSC'01)*. As for SNSC'99, Franz Winkler served as the organizer and general chair of the conference. SNSC'01 was designed as an open conference of the SFB F013. The goal was to further the integration of methods in symbolic and numerical scientific computation. Topics of interest for the conference included all aspects of symbolic-numerical scientific computation, in particular:

- algebraic multigrid methods for FEM,
- computer aided geometric design,
- computer supported derivation of mathematical knowledge,
- constrain solving,
- regularization techniques,
- combinatorics and special functions,
- symmetry analysis of differential equations,
- differential geometry,
- visualization in scientific computation,
- symbolic and numerical methods in engineering sciences.

The following invited speakers addressed these topics:

- J. Apel (Leipzig, D), "Passive Complete Orthonomic Systems of PDEs and Riquier Bases of Polynomial Modules"
- M. Dellnitz (Paderborn, D), "Set-Oriented Numerical Methods for Dynamical Systems"
- E. Hubert (Sophia Antipolis, F), "Differential Equations from an Algebraic Standpoint"
- F. Schwarz (Bonn, D), "Algorithmic Lie Theory for Solving Ordinary Differential Equations"
- H.J. Stetter (Vienna, A), "Algebraic Predicates for Empirical Data"
- R. Walentyński (Gliwice, PL), "Solving Symbolic and Numerical Problems in the Theory of Shells with *MATHEMATICA*"

In addition to these invited presentations, 25 contributed talks were given at the conference. Abstracts of all these invited and contributed talks are available as [Wink01].

The more than 60 participants considered the confernce a great success. Proceedings of SNSC'01 will be published by Springer-Verlag Heidelberg.

The pictures below show the participants of SNSC'99 in front of the castle of Hagenberg, and Prof. Winkler during the opening ceremony of SNSC'01.

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SFB F013: Numerical and Symbolic Scientific Computing

Report on the Workshop "Numerical Simulation" Herrsching (Ammersee), April 29 – May 1 2001

In April 2001 we have co-organized a meeting of our SFB F013 with SFBs from Germany namely SFB 382, SFB 404, SFB 438 and the Stiftung Caesar. All of these institutions work on the field of numerical simulation which is often combined with life science or engineering applications. The main goal of this workshop was to inform each other on recent research in the SFBs and to find topics of common interest for cooperation between the SFBs in order to take advantage of synergetic effects. Another goal was to initiate personal relationships between the younger project workers of different SFBs which will simplify future cooperations.

Topics of interest for the conference included all aspects of numerical scientific computation, in particular:

- parallel algebraic multigrid methods,
- modeling and simulation of shape memory alloys
- mathematical methods for the simulation in plastic surgery,
- algebraic geometry,
- computer aided geometric design,
- large scale inverse problems,
- constrain solving,
- contact problems and coupled field problems,
- sparse grids for mixed finite elements,
- symbolic and numerical methods in engineering sciences.

The following members and project workers of our SFB gave a presentation:

- U. Langer, "Introduction in SFB F013; Scientific Computing Tools"
- S. Reitzinger and G. Haase, "A General Concept for the Construction and Parallelization of Multigrid Methods"
- B. Kaltenbacher, "Large Scale Inverse Problems"
- B. Jüttler, "Computational Methods for Spline Surfaces"
- R. Hemmecke, "Computational Algebraic Geometry with CASA"

There where 30 contributed talks given at the workshop and more than 50 researchers from Germany, Austria, Russia and Czech Republic participated in it.

SFB F013: Numerical and Symbolic Scientific Computing

Coherence within the SFB

- **Symbolic Algorithms in Numerics:**
  In the element preconditioning technique developed in subproject F1306, the problem arises to construct an M-matrix that is as close as possible to a given symmetric positive definite matrix. The problem has to be solved for a large number of instances (the number of elements). The numerical solution of these optimazation problems are a critical bottleneck of the whole method.

  The idea of this cooperation was to solve this problem once symbolically and do the instantiations in the solution. For various element matrices involving only one symbolic parameter, we could find a closed form solution in terms of polynomials. A similar formula was given for general 2×2 matrices, but here there are several closed forms, and some inequalties need to be checked in order to determine which one has to taken. For general 3×3 matrices, a similar closed form would be theoretically possible, except that we need also square roots and – in one case – roots of higher degree polynomials. But such a closed formula would be too large to be useful, so we preferred to give a "formula" consisting of a program with arithmetic or square root (and in one case higher order root) assignments and **if then else** branches, but no loops. Using these formula, we can compute the optimal preconditioners faster and more accurately.

  Another cooperation was to use symbolic methods to make an optimal choice of the regularization parameter in a multigrid method for solving nonlinear ill-posed problems investigated in subproject F1308.

  In the other direction, we used some regularization techniques investigated in subproject F1308 in order to solve standard problems in computer algebra in exact real computation. This solution is integrated in our Maple implementation of exact real numbers, available under `http://www.risc.uni-linz.ac.at/-projects/basic/SFB/reals/themes/erna/`.

  We have also collaborated with several numerical projects on symbolic-numeric techniques for the analysis and solution of differential equations. Although we continue to be interested in this topic, it has been unfortunately cancelled from our project in the 2nd phase.

- **Parametrization:**
  There were also cooperations with the other subprojects dealing with symbolic computation, especially with subproject F1304, where new symbolic and numeric algorithms for the parametrization of pipe and canal surfaces have been developed.

  There has also been an intensive cooperation with subproject F1316, developing new symbolic and numerical algorithms for parametrization and implicitization of algebraic curves and surfaces.

- **International Conference:**
  In September 2001 we have again organized an international conference on *Symbolic and Numerical Scientific Computing (SNSC'01)*. As for SNSC'99, Franz Winkler (project F1304) served as the organizer and general chair of the conference. SNSC'01 was designed as an open conference of the SFB F013. The goal was to further the integration of methods in symbolic and numerical scientific computation.

  6 invited speakers elaborated on their view of the cooperation of symbolic and numerical scientific computation. Current research results were presented in 25 contributed talks. The more than 60 participants considered the confernce a great success. Proceedings of SNSC'01 will be published by Springer-Verlag Heidelberg.

- **Algebraic Packages:**
  Many of the results achieved with respect to summation methods are directly related to Project F1302 "Proving and Solving in General Domains". The packages developed by the project group F1305 are going to be integrated into THEOREMA as "black box" provers, for instance, C. Schneider's package "Sigma" developed in his PhD thesis. In addition, first attempts to combine summation tools with THEOREMA induction proof mechanisms have been made.

  Another application within the frame of Project F1302 is T. Kutsia's non-trivial use of the "Omega" package within the context of unification theory.

The wavelet collaboration between F1305 and the project F1310 of O. Scherzer (which has terminated after the first phase of the SFB) has been brought to its end by the production of a second paper "Wavelets with scale dependent properties" which will be completed soon.

- **Formalization of Hilbert Space Theory:**
  A big challenge of the SFB is the cooperation between the Numerics and the Symbolics groups. From the beginning of the SFB, both Prof. Buchberger and Prof. Engl envisioned a cooperation in the field of proving and solving in Hilbert spaces in connection with the theory of (first linear) inverse problems. In the second funding period Prof. Buchberger restructured F1302 in such a way that this is now a main effort for this period. To make this happen, regular meetings between the leaders and the staff of Projects F1302 and F1308 took place.

  To enable a deeper level of discussion, Prof. Buchberger and Prof. Engl started to give special lectures for the co-workers of each project on their respective fields of expertise as relevant for this cooperation. Up to now Prof. Buchberger gave a 4 times 3 hours lecture on *Introduction into Symbolics and Theorema* and Prof. Engl gave a 3 times 4 hours lecture on *Introduction into Regularization Theory.* The lectures are going to be continued.

  Furthermore two working groups have been introduced, both consisting of fellows of the numerics group and the symbolics group, and are supervised by Prof. Buchberger and Prof. Engl.

  To ensure an even more efficient cooperation Prof. Engl employed DI Markus Rosenkranz, a former student of Prof. Engl and the last two years a co-worker in Prof. Buchbergers Theorema group at RISC, in his Project F1308. DI Markus Rosenkranz has knowledge both on inverse problems and on symbolic methods and automatic proving.

  In the discussion so far, many points of possible promising (and challenging) cooperations could be identified.

- **All-at-once Approache to Iterative Regularization:**
  In cooperation between the Projects F1308 and F1309 an efficient all-at-once approach to the regularization of parameter identification problems, based on SQP techniques, was developed. Several numerical tests were performed using an optimization tool implemented in FEPP and developed by Project F1309. The numerical results were in good agreement with the theory developed in two joint publications and clearly outperformed standard approaches with respect to numerical efficiency, in particular if a multi-level optimization technique is used.

  The current research of the Projects F1308 and F1309 in this area deals with the improvement of the preconditioners for the indefinite problems arising in each step of the SQP-type iteration.

  Applications of the all-at-once approach to other inverse problems (arising e.g. from Inverse Scattering) as well as other improvements of the numerical methods (e.g. the use of non-conforming finite elements or parallel solution methods) are issues of future research.

- **Spline Surfaces:**
  During the last year a strong collaboration has been established between the teams of Project F1315 (Jüttler / Schicho) and F1303 (Schicho), aiming at the combination of numerical and symbolic techniques for algebraic spline surfaces. In addition to regular meetings, a weekly joint seminar took place during the winter semester 2001.

SFB F013: Numerical and Symbolic Scientific Computing

National and International Cooperations

1 Cooperations with other Research Institutions

- G. Haase (F1301) cooperates on Ocean Modelling with Prof. M. Iskanadarani from the **Miami State University (USA)** and Prof. C. Douglas from the **University of Kentucky (USA)**. Our contribution consists in the application of fast parallel preconditioners whose results can be found in joint publications.
- **University of Stuttgart (D):** Joint work by O. Steinbach, M. Kuhn (F1301) and Prof. U. Langer on coupling of boundary elements and finite elements, and their parallelization.
- **Wolfram Research** Developer of the mathematical software system *Mathematica*. We are in close contact by providing them with the results of our research and with suggestions about the existing and possible facilities of the Mathematica system (see also the section on technology transfer). In particular, the following aspects have been investigated: unification with sequence variables, logico-graphic symbols.
- **The CALCULEMUS Training Network** Consists of a net of universities and research institutes with the common goal of integrating the functionalities of existing mathematical software and theorem proving systems: IRST Trento Italy, Univ. Edinburgh UK, Univ. Karlsruhe Germany, RISC-Linz Austria, Univ. Nijmegen Netherlands, Univ. Eindhoven Netherlands, Univ. Genova Italy, Univ. Birmingham UK, Univ. Saarbrücken Germany, Univ. Bialystok Poland. The network is supported by the European Union in the frame of the Calculemus Training Network Project HPRN–CT–2000–00102. The yearly Calculemus Meeting evolved to a regular workshop, which is always co-located with one of the major conferences in the areas of Computer Algebra or Automated Deduction.
- **University of North Carolina:** Prof. H. Hong (Univ. North Carolina) and J. Schicho (F1303) have been working together on problem of quantifier elimination and on the generalization of resultants. Dr. J. Schicho visited the University of North Carolina in April 1999.
- **University of Passau:** In the winter term 99/2000, Prof. Volker Weispfenning (Univ. Passau) and J. Schicho (F1303) organized a joint seminar on computer algebra and quantifier elimination, taking place in Passau and in Hagenberg. The participants are: Prof. Volker Weispfenning (Univ. Passau), Dr. Isolde Mazucco (Univ. Passau), Hirokazu Anai (Univ. Passau), Andreas Dolzmann (Univ. Passau), Thomas Sturm (Univ. Passau), Dr. J. Schicho (SFB 1303), Dr. Stefan Ratschan (SFB 1303), Petru Pau (SFB 1303), Mohamed Shalaby (SFB 1303).
- We have invited Ron Goldman of **Rice University (USA)** to visit RISC-Linz for a week in November 2000. Ron Goldman is one of the leading experts in resultant based implicitization methods for algebraic curves and surfaces. He gave a talk on “Explicit Implicitization of Rational Surfaces by the Method of Moving Planes”.
- During the visit of Gert Vegter of the **University of Groningen (NL)** in February 2001 we have started a cooperation algebraic approaches to geometry whiochb was continued at the **Lorentz Center in Leiden (NL)**. He gave a talk on “Computational Topology”.
- D. Duval of the **University of Grenoble (FR)** and B. Mourrain of **INRIA at Sophia Antipolis (FR)** have presented their views of computer algebra and symbolic computation during their visits to RISC in two talks with the titles “Overloading, Coercions, Subsorts” and “Computation of Resultants”.
- With the visit of J. Kormos of the **University of Debrecen (H)** we have started a cooperation between our institutes and also our universities, respectively. Right now there is a university partnership between the University of Linz and the University of Debrecen, which is coordinated by RISC and the Mathematics Institute of Debrecen. Several colleagues from Debrecen participated in the conference SNSC’01. F. Winkler is invited as a guest professor at the University of Debrecen in April

2002, where he will lecture on symbolic computation in algebra, geometry, and logic.

- **Dresden University of Technology:** Joint book publication on finite elements and multigrid methods by M. Jung and Prof. U. Langer.

- **Texas A&M University:** Prof. J. Bramble, Prof. R. Lazarov, Prof. J. Pasciak: J. Schöberl joint the numerical analysis group as a Visiting Assistant Professor between Aug 2000 and June 2001, joint publication.

- **Texas Institute for Computational and Applied Mathematics (TICAM):** Prof. L. Demkowicz: J. Schöberl work together with L. Demkowicz on multigrid for *hp* finite elements and Maxwell equations, joint publication in preparation.

- **University Valenciennes, (F):** Prof. S. Nicaise: J. Schöberl work together with S. Nicaise on anisotropic finite elements for Maxwell equations, joint publications.

- J. Apel of the **University of Leipzig (D)** has visited our research group in September and collaborated with R. Hemmecke on the theory of involutive bases.

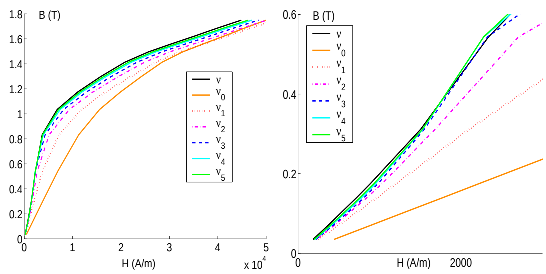
- A. Kondratyev, a doctoral student partially supported by our project, has collaborated intensively with H.-J. Stetter of the **Technical University of Vienna** on numerical schemes for Gröbner bases computation.

- **Pennsylvania State University:** In July 2001 Prof. Paule was visiting researcher at the Department of Mathematics at the Pennsylvania State University (USA), following an invitation of Prof. G.E. Andrews.

- **DLMF:** The cooperation of Prof. Paule with the National Institute of Standards and Technology (NIST, subdivision of the US Department of Commerce, Gaithersburg, USA) concerning the project of a "Digital Library of Mathematical Functions" (DLMF) has been continued. The goal of the project is the edition of a significantly revised version of the classical "Handbook of Mathematical Functions" (National Bureau of Standards, Applied Mathematics Series No. 55, Abramowitz and Stegun, Eds., 1964). Besides producing a hardcopy version, special emphasis is put on providing an electronic web version which is freely accessible to users world-wide. Prof. Paule is serving as Associate Editor, and as DLMF Author for the new chapter on computer algebra.

- **AMADEUS:** In November 2001 the Austrian OeAD has approved a two-years scientific exchange program between Austrian scientists and researchers at INRIA-Paris. Austrian partners: Prof. Paule (proposer), Prof. M. Drmota (TU Vienna), and Prof. C. Krattenthaler (University Vienna); French partners: Dr. F. Chyzak (Proposer), Prof. P. Flajolet, and Dr. B. Salvy (all INRIA-Paris).

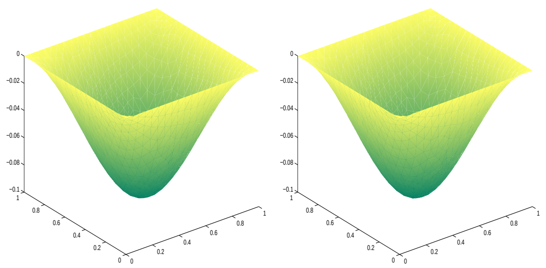
- **Department of Sensor Technology at the University Erlangen-Nürnberg:** Project F1308, in cooperation with project F1301 and the department of sensor technology in Erlangen, treated the problem of determining the nonlinear reluctivity curve of magnetic materials. The conventional method for doing so is to build up a special test sample (the so-called Epstein apparatus) from the material under consideration in order to achieve a magnetic field as uniform as possible. In that case the searched for relation between the magnetic field strength and the magnetic flux density (i.e., the reluctivity) can be computed by explicit formulas from the measured data, namely the magnetic flux corresponding to several values of the induced current in a coil. Since in many interesting applications, such as thin film magnetics, it is impossible to build up such an Epstein apparatus, though, it was our aim to develop a computational scheme that reconstructs the reluctivity in case of a non uniformly distributed magnetic field. In that general situation the physical proceedings are governed by Maxwell's equations, i.e., a system of partial differential equations, in which the reluctivity appears as a nonlinear parameter. We developed a Newton type iterative method for this purpose, where in each Newton step a multigrid method for the linearized (unstable) problem is used. Several algorithmic aspects of the proposed method were investigated and illustrated by numerical reconstruction results.



The above reconstruction result for an example of a $B-H$ curve whose curvature changes its sign close to the origin is typical for some magnetic materials: Convergence with noisy data ($\delta = 1$ % noise): full $H-B$ curves (left) and detailed view of curvature change (right).

- **Oxford Center for Industrial and Applied Mathematics:** This is a joint project with the Oxford Center and an English glass

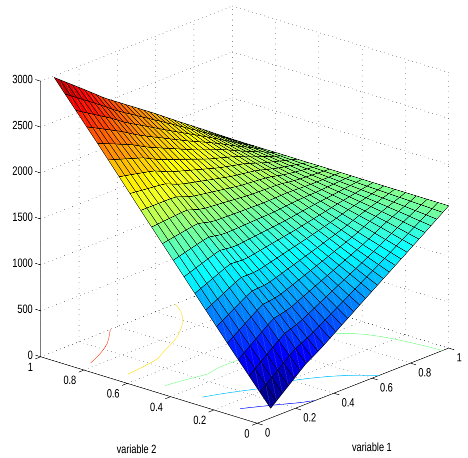
company whose name must be kept secret.
One main process for manufacturing car windshields is the sag bending process: Roughly speaking, a sheet of glass is put onto a frame and heated such that it sags under its own weight. Given a target windshield, the task is to find the right temperature distribution needed to achieve the target shape. This nonlinear material parameter identification problem could be tackled as a second order partial differential equation (pde) of mixed type (fully determined by the given target shape) for the parameter, then leading to enormous difficulties due to the lack of solution theories and methods. Following another approach based on research results of the Industrial Mathematics Institute at Linz, an iterative regularization algorithm was developed in joint work with the group of Dr. John Ockendon and meanwhile implemented, now allowing the computation of stable and reliable solutions.



Left: Given target shape. Right: Shape computed for the identified parameter

Nevertheless, although these techniques don't make use of the equation for the parameter, the numerical tests showed that the outcome is highly influenced by the type of the parameter pde. These phenomena as well as extensions to more complicated windshield models will be the issue of future collaborations with Oxford.

- **Regularization and Fuzzy Control:** In cooperation of Project F1308 with the Software Competence Center Hagenberg (SCCH), the problem of designing fuzzy controllers from example data was addressed. Martin Burger together with Josef Haslinger (from the Numerical Computation area of SCCH) and Ulrich Bodenhofer (from the Knowledge-Based Technology area of SCCH) show that for a special class of controllers (so-called *Sugeno controllers*), the design problem is equivalent to a nonlinear least squares problem, which turns out to be *ill-posed*. Therefore they investigate the use of regularization methods in order to obtain stable approximations of the solution. They analyze a smoothing method, which is common in spline approximation, as well as Tikhonov regularization with respect to stability and convergence.
In addition, an iterative method for the solution of the regularized problems was developed, which uses the special structure of the problem. It was tested both in some typical numerical examples and also on real-world data. They also compare the behavior of the iterations for the original and the regularized least squares problems. It turns out that the regularized problem is not only more robust but also favors solutions that are interpretable easily, which is an important criterion for fuzzy systems.



Control surface for resulting fuzzy controller using Tikhonov regularization

- **Dresden University of Technology:** Prof. Dr. A. Griewank, Dr. A. Walther and O. Vogel continued their cooperation with Wolfram Mühlhuber (F1309) on the efficient use of automatic differentiation for optimal design problems.

- **SINTEF Applied Mathematics (Norway):** Dr. T. Dokken (SINTEF, coordinator) and Prof. B. Jüttler and four other European partners were involved in the preparation of a IST–FET research project within the Fifth Framework Programme of the European Commission. After receiving a positive review by the referees, we are currently negotiating about the the details of the research contract.

- **Seoul National University (Seoul, Korea):** There is a close cooperation on issues of visualization and computer animation with Prof. Myung–Soo Kim (Seoul). Prof. Jüttler visited Seoul in September 2001 and worked with Prof. Kim on a joint project on real–time distance computation of ellipsoids for computer animation.

- **The University of Hong Kong (Hong Kong, China):** Prof. Jüttler visited Hong

Kong in September 2001 and worked with Professor Wenping Wang on shape analysis of spherical rational curves.

- **The University of California at Davis (Davis, USA):** Prof. Jüttler authored a joint survey paper with Prof. Farouki on "Geometric Design and motion control".

2 Guests

- **R. Krasauskas**, University of Vilnius, 22.10.-29.10.2001. He gave a talk on toric surfaces in the joint seminar of subprojects 1303 and 1316.
- **Prof. J. Kormos** , University of Debrecen (HU), 11.3.-14.3..2001. Joint research in project F1303.
- **Prof. H. Hauser**, University of Innsbruck, 12.3.-13.3..2001. He gave a survey talk on the resolution problem for singularities.
- **M. Minimair**, University of North Carolina, 25.1.2001. He gave a talk on efficient computation of resultants of composed polynomials.
- **M. Husty**, University of Innsbruck, 25.1.-26.1.2001. He gave a talk on symbolic methods in kinematics, especially parallel manipulators.
- **G. Brown**, University of Warwick, 3.9.-15.9.2001. We continued the project of implementing our surface parameterization algorithms in MAGMA.
- **V. Weisspfenning, I. Mazucco, A. Dolzmann, T. Sturm, A. Seidl**, University of Passau, 15.1.2001 and 5.7.2001. In the frame of a joint seminar with the University of Passau, they delivered various seminar talks.
- **Prof. Ron Goldman:** Rice University (USA), 12.11.2000–15.11.2000. Prof. Goldman gave a talk on "Explicit Implicitization of Rational Surfaces by the Method of Moving Planes".
- **Prof. Gert Vegter:** University of Groningen (NL), 12.02.2001. Prof. Vegter gave a talk on "Computational Topology".
- **Prof. D. Duval:** University of Grenoble (FR), 07.03.2001–11.03.2001. Prof. Duval gave a talk on "Overloading, Coercions, Subsorts".
- **Ass.-Prof. J. Robu:** University of Cluj-Napoca (RO), 22.04.2001–20.05.2001. Prof. Robu contributed to F1302.
- **Stefan Maruster:** University of Timisoara, Romania, June 2001.
- **Prof. Dr. Viorel Negru:** Western University, Timisoara, Romania, April 2001, January 27 – February 11 2002.
- **Dr. Dana Petcu:** Western University, Timisoara, Romania, January 25 – February 4 2002.
- **Dr. B. Konev:** University of St. Petersburg (RU), 05.06.2001–30.06.2001. Dr. Konev contributed to F1302.
- **Dr. B. Mourrain:** INRIA at Sophia Antipolis (FR), 16.03.2001. Dr. Mourrain gave a talk on "Computation of Resultants".
- **Prof. O. Biro:** University of Graz, 05.03-07.03.2001. Dr. Mourrain gave a talk on "Berechnung von Wirbelstromproblemen mit Potentialfunktionen".
- **Prof. V.G. Korneev:** University of Westminster (UK), 13.05.2001–20.05.2001. Prof. Korneev gave a talk on "May be solvers for the hp-version optimized?".
- **Prof. A. Ramm:** Kansas State University (USA), 01.07.2001–20.07.2001. Prof. Ramm gave a talk on "Dynamical Systems Approach for Solving Linear and Nonlinear Ill-Posed Problems".
- **Dr. M. Bischoff:** TU Munich (GE), 23.09.2001–25.09.2001. Dr. Bischoff gave a talk on "Stabilisierte dreidimensionale DSG-Schalenelemente".
- **Dr. R. Scheichl:** Institut Francais du Petrole (FR), 22.10.2001–25.10.2001. Dr. Scheichl gave a talk on "Entkopplungs- und Block-Vorkonditionierungsmethoden bei der Simulation sedimentärer Becken".
- **Prof. J. Haslinger:** Charles University of Praha (CZ), 20.11.2001–23.11.2001. Prof. Haslinger gave a talk on "Shape Optimization in Contact Problems with Coulomb Friction".
- **Prof. Z. Dostal:** VBS-Techn. University of Ostrava (CZ), 20.11.2001–23.11.2001. Prof. Dostal gave a talk on "Proportioning in Bound Constrained QP: Rate of Convergence and Finite Termination Property".
- **Prof. V. Capasso:** University of Milano (IT), 19.05.2001–22.05.2001. Prof. Capasso contributed to project F1308.
- **Dr. A. Micheletti:** University of Milano (IT), 19.05.2001–22.05.2001. Dr. Micheletti contributed to project F1308.

- **Dr. R. Falgout:** Lawrence Livermore National Laboratory (USA), 24.05.2001–25.05.2001. Dr. Falgout gave a talk on “New Advances in Algebraic Multigrid”.
- **Prof. A.-M. Sändig:** University of Stuttgart (GE), 09.06.2001–11.06.2001. Prof. Sändig gave a talk on “Spannungssingularitäten in heterogenen Materialien”.
- **Dr. J. Apel:** University of Leipzig, 17.9.2001–28.9.2001. Dr. Apel collaborated with R. Hemmecke on the theory of involutive bases.
- **Ing. D. Lukas:** VSB-Techn. University of Ostrava (CZ), 20.11.2001–30.11.2001. Ing Lukas collaborated with W. Mühlhuber on 3D optimal shape design of homogeneous electromagnets.
- **Prof. N. Sapidis:** University of the Aegean (GR), 30.11.2001–05.12.2001. Prof. Sapidis gave a talk on “Design Constraints in Solid Modelling”.
- **Dr. F. Chyzak:** INRIA-Paris, 17.–24.04.01. Dr. Chyzak, a former SFB F1305 member, visited Prof. Paule's group in order to continue joint research.
- **Dr. R. Vidunas:** University of Amsterdam, 20.–27.05.01. Talk on “Identities with nonterminating hypergeometric series”. Dr. Vidunas is member of Prof. Koornwinder's group; his visit intensified the good mutual scientic exchange.
- **Prof. C. Krattenthaler:** University Vienna, 20.–22.06.01. Joint research and survey talk on “Plane partitions and alternating sign matrices”.
- **Prof. H. Prodinger:** University of the Witwatersrand, Johannesburg, South Africa, 25.–29.06.01. Joint research on harmonic numbers and q-series; talk on “Mathematical analysis of algorithms for broadcast communication”.
- **Dr. D. Lozier:** NIST, Gaithersburg, USA, 24.–28.09.01. The general editor of the DLMF project, Dr. Lozier, visited the F1305 group for discussing cooperation. In addition, Dr. Lozier gave an invited talk at the occasion of Buchberger's conference MKM 2001 (“Mathematical Knowledge Management”).
- **Pavel Chalmovianský** (University of Bratislava, May 2001). Job interview for position of research assistant / PhD student
- **Szilagyi Ibolya** (University of Debrecen, May 2001). Job interview for position of research assistant / PhD student
- **Vejan Stoffa** (University of Nitra, May 2001). Job interview for position of research assistant / PhD student
- **Prof. Nikolaos Sapidis** (University of the Agean, December 2001). Prof. Sapidis gave a talk about “Design constraints in solid modelling.”
- **Dr. Tor Dokken** (SINTEF Applied Mathematics, September 2001). Dr. Dokken gave a talk about “Approximate implicitization” and prepared jointly with Prof. Jüttler a joint European grant proposal.
- **Prof. Rimmvydas Krausauskas** (University of Vilnius, Lithuania, October 22-27 2001). Professor Krasauskas gave a talk about “Toric surfaces in geometric modelling”.

3 Lectures at other Universities

- **Bruno Buchberger**, Theorema: Formale Mathematik. Universität Innsbruck, Institut fuer Mathematik, 14.3.2001.
- **Bruno Buchberger, Tudor Jebelean** Predicate Logic as a Working Language Using Theorema. Blockvorlesung (12 Stunden), University of the West, Timisoara, Romania, 19.-23.5.2001.
- **Bruno Buchberger**, The Didactics of Computer Mathematics. Short course for high school students and teachers, Konan High School, Kobe, 30.1.2001.
- **Bruno Buchberger**, Groebner Bases: A Practical Tool for Nonlinear Algebraic Equations. Kyushu University, Graduate School of Mathematics, Fukuoka, Japan, 2.7.2001.
- **Bruno Buchberger**, The Theorema System: A Frame for Formal Mathematics Kyushu University, Graduate School of Mathematics, Fukuoka, Japan, 3.7.2001.
- **Bruno Buchberger**, Logicographic Symbols: Combining Intuition and Formality. Lamar University, Computer Science Department, Beaumont, Texas, USA, 26.8.2001, 5.9.2001.
- **Bruno Buchberger**, Introduction to Groebner Bases: Theory and Applications. Texas A&M University, Dept. of Mathematics, 9.9.2001.
- **Bruno Buchberger**, Implementation of Groebner Bases: Using Functors in Theorema. Texas A&M University, Dept. of Mathematics, 11.9.2001.

- **Bruno Buchberger**, Mathematical Knowledge Management in Theorema. Texas A&M University, Dept. of Mathematics, 14.9.2001.

- **Bruno Buchberger**, Mathematical Knowledge Management in Theorema. 1st International Workshop on Mathematical Knowledge Management, RISC, Johannes Kepler Universitaet, Schloss Hagenberg, 24.9.2001.

- **Bruno Buchberger**, Groebner Rings and Modules. International Conference on Computational Methods in Algebraic Geometry, University of Hyderabad, Mathematical Department, India, 10.12.2001.

- **B. Buchberger and W. Windsteiger**, Organized a training week on "computer supported mathematical proving" for high school teachers (October 8-12, 2001).

- **F. Lichtenberger, W. Windsteiger**, Lectures on "Algorithmische Mathematik 1" and "Algorithmische Mathematik 2" by using *Theorema*, Regular Courses at the FHS-Hagenberg, 2 semesters.

- **W. Windsteiger**, Lectures on "Algorithmische Methoden 1" supported through using the *Theorema* software system, mandatory course in the first semester for mathematics students at the University of Linz.

- **Dr. J. Schicho** gave an invited talk on rational surfaces at the University of Cantabria (Santander, Spain), in January 2001.

- **Dr. J. Schicho** gave an invited talk on his surface parametrization algorithms at the University of Sydney, in February 2001.

- **Dr. J. Schicho** gave a survey talk on the surface parametrization problem at the University of Innsbruck, 23.5.2001.

- **Dr. J. Schicho** gave a talk on Villamayor's algorithm for the resolution of singularities at the University of Rennes, June 2001.

- **Dr. S. Ratschan** gave a talk on solving first order constraints at the Swiss Fed. IT, Lausanne, September 2001.

- **G. Bodnár, S. Ratschan and J. Schicho** delivered various seminar talks in the joint seminar with the University of Passau.

- **Prof. F. Winkler** was invited to give a minicourse on *Computer Algebra in Geometric Computing* at the workshop of the European project ECG (Effective Computation Geometry). The workshop took place at the Lorentz Center at the University of Leiden.

- **R. Hemmecke** presented the software system CASA at the meeting of several German SFBs at Herrsching/Ammersee, April 2001

- **Prof. Winkler** was one of the invited lecturers at the Workshop on "Systems Theory and Computer Algebra" at the Royal Dutch Academy of Sciences in Amsterdam, Nov. 2001

- **Prof. F. Winkler** was invited to give a short course on "Gröbner Bases and Algebraic Computation in Geometry" at a workshop of the European project ECG at the Lorentz Center in Leiden, The Netherlands, Oct. 2001

- **Prof. P. Paule:** "Symbolic Computation and Wavelets", Special Session Symbolic and Numerical Scientific Computation, IMACS conference on applications of Computer Algebra (ACA 2001), Albuquerque, USA, 31.5–3.6.01.

- **Prof. P. Paule:** "Computeralgebra und Kombinatorik: der Omega-Kalkül von MacMahon", Naturwissenschaftliches Kolloquium, University Innsbruck, Austria, 25.4.01.

- **Prof. P. Paule:** "The WZ Method — A Contiguous Approach", Number Theoretical Colloquium, Department of Mathematics, Pennsylvania State University, USA, 27.7.01.

- **Prof. P. Paule:** "Computer Algebra and Combinatorics: MacMahon's Partition Analysis Revisited", General Mathematics Colloquium, Korteweg-de Vries Institute for Mathematics, University Amsterdam (UvA), The Netherlands, 31.10.01.

- **Prof. P. Paule:** "Contiguous Relations and Creative Telescoping", Stieltjes Analyse Colloquium, Thomas Stieltjes Institute for Mathematics, Amsterdam, The Netherlands, 2.11.01.

- **Prof. P. Paule:** "Plane Partition Diamonds", 46th Sém. Lothar. Combin., Lyon, France, 18.–21.3.01.

- **Dr. A. Riese:** "qMultiSum – A package for proving q-hypergeometric multi-sums", 46th Sém. Lothar. Combin., Lyon, France, 18.–21.3.01.

- **Dr. C. Schneider:** "Symbolic summation in difference fields", Conference Symbolic and Numerical Scientific Computation (SNSC'01), Hagenberg, Austria, 12.–14.9.01.

- **Prof. H.W. Engl:** Lectures on "Introduction into Inverse Problems", given in Hagenberg, October 31, November 16, December 7, 2001, each 4 hours.

- **Prof. H.W. Engl:** Graduate Course on "Inverse Problems", Trinity Term 2001, Mathematical Institute, University of Oxford.
- **Prof. H.W. Engl:** Lecture on "Regularization of inverse problems: mathematical methods and applications" at OCIAM, University of Oxford, January 25, 2001.
- **Prof. H.W. Engl:** Lecture on "Regularization of inverse problems: mathematical methods and applications", Strathclyde University, March 2001
- **Prof. H.W. Engl:** Lecture on "An inverse problem from nondestructive testing", Strathclyde University, March 2001
- **Prof. H.W. Engl:** Talk at the British Inverse Problems Day, "Iterative regularization of nonlinear inverse problems", Loughborough, March 2, 2001
- **Prof. H.W. Engl:** Lecture on "Computational methods for inverse problems" at Computing Laboratory, University of Oxford, April 26, 2001
- **Prof. H.W. Engl** Colloquium talk, "'Iterative regularization of nonlinear inverse problems", Gregynog, Wales, May 22, 2001.
- **Prof. H.W. Engl:** Talk at the British Inverse Problems Day, "Inverse Problems in Industry", University College London, May 29, 2001
- **Prof. H.W. Engl:** Invited Talk, "Iterative Methods for Nonlinear Inverse Problems: Theory and Numerical Examples", Applied Inverse Problems: Theoretical and Computational Aspects, Montecatini, Italy, June 18-22, 2001
- **Prof. H.W. Engl:** Invited Talk, "Identification of Parameters in Polymer Crystallization, Semiconductor Models and Elasticity via Iterative Regularization", Berkeley, USA, November 1-9, 2001
- **Dr. J. Schöberl** gave an invited talk on "Multigrid Methods for Anisotropic Mesh Refinement" at the University of Texas, Austin in April 2001.
- **Dr. J. Schöberl** gave an invited talk on "Mesh Generation Algorithms" at the FH Salzgitter-Wolfenbüttel in December 2001.
- **Dr. J. Schöberl** gave an invited talk on "Multigrid Methods for Anisotropic Mesh Refinement" at the University Hannover in December 2001.
- **Dr. G. Haase** gave an invited talk on "Allgemeine und spezielle Lösungskonzepte für gross dimensionierte Probleme" at the University of Salzburg in May 2001.
- **Dr. G. Haase, Prof. U. Langer and Dr. S. Reitzinger** gave an invited talk on "A General Concept for the Construction and Paralleization of Algebraic Multigrid Methods" at the Int. Conf. on Fast Solvers for PDEs in Oberwolfach, May 2001.
- **Dr. G. Haase** gave an invited talk on "Allgemeine und spezielle Lösungskonzepte für gross dimensionierte Probleme" at the University of Erlangen-Nürnberg in May 2001.
- **Prof. U.Langer** gave an invited keynote talk on "Scientific Computing Tools in Computational Sciences and Engineering" at the IFIP WG2.5 Workshopin Amsterdam, May 2001.
- **Prof. U.Langer** gave an invited keynote talk on "Applications of Multigrid Methods to 3D Magneto-Mechanical Field Problems" at the GAMM-Workshop on Computational Electromagnetics, Kiel in January 2001.
- **Prof. U.Langer** gave an invited keynote talk on "On the Use of Multigrid Methods in Magneto-Mechanics" at the Second IMACS Conference MODELLING 2001 on Mathematical Modelling and Computational Methods in Mechanics, Physics, Biomechanics and Geodynamics in Pilsen, Czech Republic, June 2001.
- **Prof. Jüttler:** Talk on "Algebraic Spline Surface Fitting" given at the University of Hong Kong, Hong Kong, August 2001.
- **Prof. Jüttler:** Talk on "Algebraic Spline Surface Fitting" given at the Seoul National University, September 2001.
- **Prof. Jüttler:** Talk on "The shape of spherical quartics" given at Dresden University of Technology, December 2001.

SFB F013: Numerical and Symbolic Scientific Computing

Transfer of Knowledge and Technologies

1 Software Competence Center Hagenberg

The strong cooperation between the *Theorema* Group and Wolfram Research International, and the planned integration of the software system *Theorema* within *Mathematica* led Wolfram Research International to join the SWCC (Software Competence Center Hagenberg). The work program of the SWCC section related to Wolfram Research includes practical applications of the models developed using the *Theorema* system.

2 Wolfram Research

Through close contact our group is influencing the development of the Mathematica software in order to include facilities which are useful for automatic reasoning, improved graphical interface, mathematical training, etc. We are official beta testers of versions 4 and 5 and also accredited Mathematica developers (access to the Mathematica Developers Kit).

3 Unisoftware Plus

Official Austrian *Mathematica* resellers. Contacts with the *Theorema* group for using the *Theorema* software system in order to produce educational software.

4 Digital Library of Mathematical Functions

The cooperation of Prof. Paule with the National Institute of Standards and Technology (NIST, subdivision of the US Department of Commerce, Gaithersburg, USA) concerning the project of a "Digital Library of Mathematical Functions" (DLMF) has been continued. The goal of the project is the edition of a significantly revised version of the classical "Handbook of Mathematical Functions" (National Bureau of Standards, Applied Mathematics Series No. 55, Abramowitz and Stegun, Eds., 1964). Besides producing a hardcopy version, special emphasis is put on providing an electronic web version which is freely accessible to users world-wide. Prof. Paule is serving as Associate Editor, and as DLMF Author for the new chapter on computer algebra.

5 Simulation of Injection Moulding Machines

In this project with the company ENGEL in Schwertberg (in cooperation with the SCCH) we are developping a mathematical model of existing injection moulding machines using the simulation language Modelica. This model is then simulated in a specially designed and implemented simulation environment incorporating an SPS interface. The simulation of such devices with electrical and hydraulic components requires the dynamical solution of algebraic differential equations. The working group of Prof. Winkler (at RISC-Linz) is investigating practical project-oriented problems in this area, and is also developing new algebraic approaches to the theory of differential equations. This cooperation of theory and practice is currently being supported in a project "Algebraische Analyse von Differentialgleichungen" by the government of Upper Austria.

6 Design and Implementation of a System for Driverless Transport

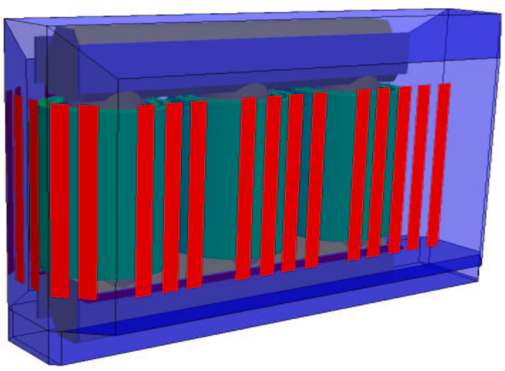
In this project with the company VA-Tech the goal is to design an implement algorithms for steering driverless vehicles along efficient routes. Various problems in geometry and optimization theory have to be solved toward this goal. In addition to the development of new algorithms, we will also create a simulation for analyzing and optimizing the throughput of such a system. One of the central geometric problems is the determination of traction curves and surfaces covered by the vehicles. During the last year Ms. Elisabeth Schoegler has contributed to these investigations in the frame of her diploma thesis, under the direction of Prof. Winkler.

7 Shape Optimization in Machine Construction

The tools developed in projects F1309 and F1306 proved their correctness in practical applications for the last years. Therefore, our industrial partner, the ENGEL Group Schwertberg, decided to use our competence in shape optimization software already in the construction process of injection moulding machines. We designed several support frames of the recent production line with a minimal weight under certain constraints taking into account critical stresses, deflections, etc.. This cooperation will be continued.

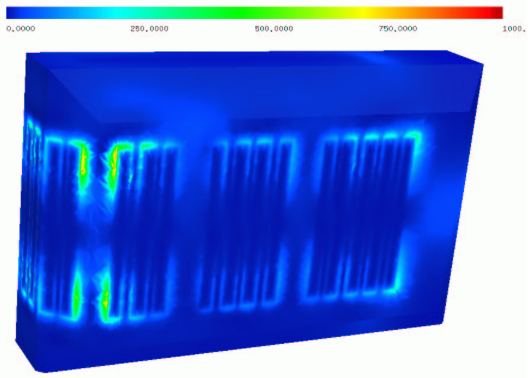
8 Eddy Current Simulation in Power Transformers by Multigrid Methods

This is a joint project of VA TECH EBG Transformatoren GmbH, MathConsult GmbH, and performed by Joachim Schöberl. Here, the potential of modern numerical methods as multigrid algorithms and adaptive mesh refinement enables the accurate simulation of a whole transformer in less than 30 minutes. In contrast, attempts with commercial finite element software required 12 hours computing time, or even failed.



Transformer geometry with shields

In the transformer, the stray flux enters the tank wall, and induces eddy currents which result in eddy losses. Thus, the designer places shields in front of the wall. The goal of the simulation is to provide a design tool telling the engineer where to place efficient shields.



Visualization of eddy currents in the transformer

The model contains the high permeable core, magnetic pressing plates, the magnetic tank wall, and high permeable shields. Cylindrical coil currents are prescribed. Highlights of the finite element solver are second order Nedelec elements, anisotropic multigrid methods, and a-posteriori error control. Currently, we work on a refined model for the laminated core. The concept is the two-level FEM homogenization to capture the strong microscopic variations on a macroscopic mesh.

9 Parallelization

Our knowledge from project F1301 on parallelization, code acceleration and usage of workstation clusters enabled us to support the parallelization of an industrial FEM code. Together with the engineers from the Engineering Center Steyr, Steyr-Daimler-Puch AG we found a way to parallelize their FEM postprocessing code on all sorts of computers ranging from an inhomogeneous workstation cluster to supercomputers with several hundreds of processors.

10 Algebraic spline surfaces for reverse engineering

The reverse engineering of geometric objects, where a CAD model is generated automatically from a point cloud (measurement data), has become a valuable alternative to the standard top–down construction process in Computer Aided Design. Our industrial partner Holometric Technologies (Aalen, Germany) produces one of the most advanced commercial software packages in this market. In a master thesis, we explored the potential of algebraic spline surfaces for this specific application, and produced some promising results. Due to internal reasons of our partner, however, this development has temporarily come to an halt, but we hope to continue the cooperation soon.

11 Algebraic spline surfaces in CAD

Based on our results on algebraic spline surface fitting, the group of Prof. Jttler became a partner in the consortium of an IST-FET proposal within the Fifth Framework programme of the EU. The proposal, entitled GAIA II "Intersection algorithms for geometry-based IT-applications using approximate algebraic methods" aims at developing a new generation of intersection algorithms for Computer Aided Design. The consortium includes 6 partners, including the (mainly) French company think3. In January 2002, we were informed that the proposal has been evaluated positively by the reviewers. We are currently negotiating with the European commission about the details of the contract.

SFB F013: Numerical and Symbolic Scientific Computing

Statistical Appendix

1 Monographs, PhD Theses, Diploma Theses

[1] EGGER, H. Identification of Volatility Smile in the Black Scholes Equation via Tikhonov Regularization. Master's thesis, Johannes Kepler University Linz, Industrial Mathemtics Institute, November 2001.

[2] HAASE, G. *Parallele Algorithmen für Partielle Differentialgleichungen.* Habilitation, Technisch-Naturwissenschaftliche Fakultät, Johannes Kepler Universität Linz, April 2001.

[3] KIENESBERGER, J. Multigrid preconditioned minimization algorithms for elastoplastic problems. Master's thesis, TNF, Johannes Kepler University of Linz, June 2001.

[4] REITZINGER, S. *Algebraic Multigrid Methods for Large Scale Finite Element Equations.* PhD thesis, University of Linz, 2001.

[5] SCHNEIDER, C. *Symbolic Summation in Difference Fields.* PhD thesis, RISC, Johannes Kepler University Linz, 2001.

[6] WEIXLBAUMER, C. Solutions of difference equations with polynomial coefficients. Master's thesis, RISC, Johannes Kepler University Linz, 2001.

[7] WINDSTEIGER, W. *A Set Theory Prover in Theorema: Implementation and Practical Applications.* PhD thesis, RISC Institute, May 2001.

2 Publications

[1] ANDREWS, G., KNOPFMACHER, A., PAULE, P., AND PRODINGER, H. q-Engel series expansions and Slater's identities. *Quaestiones Math. 24* (2001), 1–14.

[2] ANDREWS, G., KNOPFMACHER, A., PAULE, P., AND ZIMMERMANN, B. Engel expansions of q-series by computer algebra. In *Symbolic Computation, Number Theory, Special Functions, Physics and Combinatorics* (2001), F. Garvan and M. Ismail, Eds., vol. 4 of *Developments in Mathematics*, Kluwer, pp. 33–57.

[3] ANDREWS, G., PAULE, P., AND RIESE, A. MacMahon's partition analysis III: The Omega package. *European J. Combin. 22* (2001), 887–904.

[4] ANDREWS, G., PAULE, P., AND RIESE, A. MacMahon's partition analysis IX: k-Gon partitions. *Bull. Austral. Math. Soc. 64* (2001), 321–329.

[5] ANDREWS, G., PAULE, P., AND RIESE, A. MacMahon's partition analysis VII: Constrained compositions. In *q-Series with Applications to Combinatorics, Number Theory, and Physics* (2001), B. Berndt and K. Ono, Eds., vol. 291 of *Contemp. Math.*, Amer. Math. Soc., pp. 11–27.

[6] ANDREWS, G., PAULE, P., AND RIESE, A. MacMahon's partition analysis VIII: Plane partition diamonds. *Adv. in Appl. Math. 27* (2001), 231–242.

[7] ANDREWS, G., PAULE, P., RIESE, A., AND STREHL, V. MacMahon's partition analysis V: Bijections, recursions, and magic squares. In *Algebraic Combinatorics and Applications* (2001), A. Betten et al., Eds., Springer, pp. 1–39.

[8] APEL, T., NICAISE, S., AND SCHÖBERL, J. Crouzeix-Raviart type finite elements on anisotropic meshes. *Numerische Mathematik 89*, 2 (2001), 193–223.

[9] APEL, T., NICAISE, S., AND SCHÖBERL, J. A non-conforming finite element method with anisotropic mesh grading for the stokes problem in domains with edges. *IMA Journal of Numerical Analysis 21* (2001), 843–856.

[10] BAUMEISTER, J., AND LEITAO, A. Iterative methods for ill-posed problems modeled by pde's. *Journal of Inverse and Ill–Posed Problems 9*, 1 (2001), 1–17.

[11] BERKOVICH, A., AND PAULE, P. Lattice paths, q-multinomials and two variants of the Andrews-Gordon identities. *Ramanujan J. 5* (2001), 409–424.

[12] BERKOVICH, A., AND PAULE, P. Variants of the Andrews-Gordon identities. *Ramanujan J. 5* (2001), 391–404.

[13] Bodnár, G., and Schicho, J. Two computational techniques for singularity resolution. *Journal of Symbolic Computation 32*, 1-2 (2001), 39–54.

[14] Borges-Quintana, M., Borges-Trenard, M., and Winkler, F. An Application of the FGLM Techniques to Linear Codes. In *Proc. 4th Italian-Latin American Conference on Applied and Industrial Mathematics, Inst. Cybern. Math. Phys., Havana, Cuba, 2001* (Inst. Cybern. Math. Phys., Havana, Cuba, CMP 1 830 504, 2001), pp. 280–286.

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[16] Burger, M. A level set method for inverse problems. *Inverse Problems 17* (2001), 1327–1356.

[17] Burger, M., Bodenhofer, U., and Haslinger, J. Data-driven construction of Sugeno controllers: Analytical aspects and new numerical methods. In *Proc. Joint 9th IFSA World Congress and 20th NAFIPS Int. Conf.* (Vancouver, July 2001), pp. 239–244.

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[20] Burger, M., Engl, H., Markowich, P., and Pietra, P. Identification of doping profiles in semiconductor devices. *Inverse Problems 17* (2001), 1765–1795.

[21] Burger, M., and Neubauer, A. Error bounds for approximation with neural networks. *Journal of Approximation Theory 112* (2001), 235–250.

[22] Burger, M., and Scherzer, O. Regularization methods for blind deconvolution and blind source separation problems. *Mathematics of Control, Signals and Systems 14* (2001), 358–383.

[23] Chyzak, F., Paule, P., Scherzer, O., Schoisswohl, A., and Zimmermann, B. The construction of orthonormal wavelets using symbolic methods and a matrix analytical approach for wavelets on the interval. *Experiment. Math. 10* (2001), 67–86.

[24] Engl, H., and Felici, T. On shape optimization of optical waveguides using inverse problems techniques. *Inverse Problems 17* (2001), 1141–1162.

[25] Engl, H., and Kügler, P. On the identification of a nonlinearity in heat conduction by tikhonov regularization. *Journ. of Inverse and Ill-Posed Problems* (2001). To appear.

[26] Engl, H., and Leitao, A. A Mann iterative method for elliptic Cauchy problems. *Numer. Funct. Anal. and Optimiz. 22*, 7-8 (2001), 861–884.

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[29] Haase, G., Langer, U., Reitzinger, S., and Schöberl, J. Algebraic multigrid methods based on element preconditioning. *International Journal of Computer Mathematics 78*, 4 (2001), 575–598.

[30] Haase, G., U.Langer, Lindner, E., and Mühlhuber, W. Various methods for structural optimization problems with industrial applications. In *Trends in Computational Structural Mechanics* (May 2001), W. Wall, K.-U. Bletzinger, and K. Schweizerhof, Eds., CIMNE, pp. 623–636.

[31] Kuhn, M., and Steinbach, O. Symmetric coupling of finite and boundary elements for exterior magnetic field problems. *Math. Methods Appl. Sci. 25* (2002), 357–371.

[32] Landsmann, G., Schicho, J., and Winkler, F. The Parametrization of Canal Surfaces and the Decomposition of Polynomials into a Sum of Two Squares. *J. of Symbolic Computation 32*, 1-2 (2001), 119–132.

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[35] MICHELETTI, A., AND BURGER, M. Stochastic and deterministic simulation of nonisothermal crystallization of polymers. *Journal of Mathematical Chemistry 30* (2001), 169–193.

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[47] WINKLER, F. *Proc. of Coll. on Systems Theoy and Computer Algebra.* Royal Dutch Academy of Science, M. Hazewinkel (ed.), 2001, ch. Computer Algebra and Geometry - Some Interactions.

3 Conference Talks

[1] BODNÁR, G., KALTENBACHER, B., PAU, P., AND SCHICHO, J. Exact real computation in computer algebra. SNSC 2001, Johannes Kepler University, Linz, Austria, September 2001.

[2] BODNÁR, G., AND SCHICHO, J. Algorithmic resolution of singularities after villamayor. Singularities of algebraic varieties and desingularization, University of Versailles-Ecole Polytechnique, France, June 2001.

[3] BODNÁR, G., AND SCHICHO, J. Eroc: A maple library for exact real object computation. IMACS-ACA 2001, Albuquerque, NM, June 2001.

[4] BURGER, M. Inverse problems for semiconductor devices. 15th Congress of the Austrian Mathematical Society, Vienna, Austria, September 2001.

[5] BURGER, M., LINDNER, E., AND MÜHLHUBER, W. Automatic differentiation and optimal sizing of industrial components. Optimization 2001, Aveiro, Portugal, July 2001.

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[7] BURGER, M., AND MÜHLHUBER, W. Simultaneous SQP-methods for parameter identification problems. SFB-Workshop, Strobl, Austria, June 2001.

[8] ENGL, H. Inverse problems in industry. British Inverse Problems Days, University College London, May 2001.

[9] ENGL, H. Iterative methods for nonlinear inverse problems: Theory and numerical examples. Applied Inverse Problems: Theoretical and Computational Aspects, Montecatini, Italy, June 2001.

[10] ENGL, H. Iterative regularization of nonlinear inverse problems. University of Loughborough, March 2001.

[11] ENGL, H. Parameters in polymer crystallization, semiconductor models and elasticity via iterative regularization methods. Berkeley, USA, November 2001.

[12] HAASE, G. An additive schwarz preconditioner in an ocean modeling code. FEM Symposium 2001, Sept 19-21, 2001 in Chemnitz, 2001.

[13] HAASE, G. Simultaneous iterations in ocean modeling. 2001.

[14] HAASE, G., LANGER, U., AND REITZINGER, S. A general concept for the construction and paralleization of algebraic multigrid methods. May 27 - June 2, 2001 in Oberwolfach, Germany,, 2001.

[15] HAASE, G., LANGER, U., AND REITZINGER, S. A general concept for the construction and parallelization of algebraic multigrid. Int. Conf. on Fast Solvers for PDEs, Oberwolfach, May 26 - June 2, May 2001.

[16] HAASE, G., AND REITZINGER, S. Simultaneous and parallel algebraic multigrid in applications. Workshop on Large Sparse Linear Systems, March 1 - 2, 2001 in Toulouse, 2001.

[17] HAASE, G., U.LANGER, LINDNER, E., AND MÜHLHUBER, W. Various methods for structural optimization problems with industrial applications. Int. Conf. on Trends in Computational Structural Mechanics, Schloß Hofen, May 20-23, 2001, May 2001.

[18] HEMMECKE, R. Computational Algebraic Geometry with CASA. Talk at a German SFB Workshop in Herrsching/Ammersee (Germany), April 2001.

[19] HEMMECKE, R. Dynamical Aspects of Involutive Bases Computations. SFB Workshop SNSC'01 (September 12, 2001 - September 14, 2001 in Hagenberg, Austria), September 2001.

[20] HEMMECKE, R. Dynamical Aspects of Involutive Bases Computations. Talk at the IMACS-ACA conference in Albuquerque, New Mexico, USA, June 2001.

[21] KÜGLER, P. The influence of the equation type on iterative parameter identification problems which are elliptic or hyperbolic in the parameter. ÖMG - Tagung, September 2001.

[22] LANGER, U. Applications of multigrid methods to 3d magneto-mechanical field problems. Invited keynote talk at the GAMM-Workshop on Computational Electromagnetics, Kiel, Germany, January 26 - 28 2001.

[23] LANGER, U. On the use of multigrid methods in magneto-mechanics. Invited keynote talk at the Second IMACS Conference MODELLING 2001 on Mathematical Modelling and Computational Methods in Mechanics, Physics, Biomechanics and Geodynamics, Pilsen, Czech Republic, June 25 - 29 2001.

[24] LANGER, U. Scientific computing tools. Gemeinsamer Workshop der SFB 438 mit der Forschungstiftung caesar und den SFBs F013, 382 und 404, Herrsching, Deutschland., April 29 - May 1 2001.

[25] LANGER, U. Scientific computing tools in computational sciences and engineering. Invited keynote talk at the IFIP WG2.5 Workshop, May 28 - 29 2001.

[26] MÜHLHUBER, W. Optimal design of industrial components. SIAM-EMS Conference, Berlin, September 2001.

[27] MÜHLHUBER, W. Optimal design of industrial components. Workshop on Adjoints - Analysis and Applications, Decin, Czech Republic, September 2001.

[28] MÜHLHUBER, W. Triangulation and mesh generation for FE-problems. SFB-Workshop, Strobl, Austria, June 2001.

[29] PAULE, P. Symbolic computation and wavelets. Invited talk at the IMACS conference on applications of Computer Algebra, Albuquerque, New Mexico, June 2001.

[30] RATSCHAN, S. Computing approximate solutions of first-order constraints over the reals. Workshop on Solving First-Order Constraints in Various Structures, Marseille, 2001.

[31] RATSCHAN, S. Quantified constraints under perturbation. Invitational Special Session, Seventh International Conference on Applications of Computer Algebra, Albuquerque, 2001.

[32] RATSCHAN, S. A symbolic-numeric algorithm for computing approximate solutions of first-order formulae over the reals. Talk at SNSC, 2001.

[33] REITZINGER, S. Algebraic multigrid methods for large scale finite element equations. Defense of the PhD Theses, March 2001.

[34] REITZINGER, S. A general approach to amg methods. June 2001.

[35] REITZINGER, S., AND HAASE, G. A general concept for algebraic multigrid methods and their parallelization. April 2001.

[36] REITZINGER, S., AND HAASE, G. A general concept for the construction and parallelization of algebraic multigrid methods. FEM Symposium Chemnitz, 2001.

[37] REITZINGER, S., AND KALTENBACHER, M. Algebraic multigrid methods for magnetostatic field problems. Poster Presentation, June 2001.

[38] REITZINGER, S., AND SCHÖBERL, J. An algebraic multigrid method for 3d magnetic field problems. January 2001.

[39] RIESE, A. qMultiSum — A package for proving q-hypergeometric multi-sums. Contributed talk at "46th Sém. Lothar. Combin.", Lyon, France, March 2001.

[40] S. REITZINGER, G. HAASE, U. L., AND SCHÖBERL, J. A general concept for algebraic multigrid methods. May 2001.

[41] SCHNEIDER, C. Symbolic summation in difference fields. Talk at the "Conference Symbolic and Numerical Scientific Computation (SNSC'01)", Hagenberg, Austria, September 2001.

[42] SCHÖBERL, J. Algebraic multigrid methods for edge elements. Copper Mountain Multigrid Conference, Colorado, April 2001.

[43] SCHÖBERL, J. Algebraic multigrid methods for edge elements. Livermore workshop on AMG, June 2001.

[44] SCHÖBERL, J. Commuting quasi-interpolation operators for mixed finite elements. European Conference on Computational Mechanics, June 2001.

[45] SCHÖBERL, J. Multigrid methods for anisotropic meshes. Finite Element Rodeo, Dallas TX, March 2001.

[46] SCHÖBERL, J. Multigrid methods for anisotropic meshes. Finite Element Circus, Newark DE, March 2001.

[47] SCHÖBERL, J. Multigrid methods for parameter dependent problems. Oberwolfach meeting on Mixed Finite Element Methods and Applications, February 2001.

[48] SCHÖBERL, J. Netgen: Algorithms and visions. 17th GAMM-Seminar Leipzig on Construction of Grid Generation Algorithms, Jannuary 2001.

[49] SCHÖBERL, J. A posteriori error estimates for reissner mindlin plate models. Jahrestagung ÖMG / DMV, Wien, September 2001.

[50] SCHÖBERL, J. A posteriori error estimates for reissner mindlin plate models. Chemnitzer FEM Symposium, September 2001.

[51] SENDRA, J., AND WINKLER, F. Computation of the Degree of Rational Maps between Curves. ISSAC'01, University of Western Ontario, London, Ontario, Canada, July 2001.

[52] WINKLER, F. Faithful and Reliable Plotting of Curves by Symbolic-Numerical Methods. IMACS Conf. on Applications of Computer Algebra, Albuquerque, NM, USA, May 2001.

[53] WINKLER, F. Gröbner Bases and Algebraic Computation in Geometry. Workshop "Computer Algebra in Geometric Computing", Lorentz Center, Univ. Leiden, Niederlande, Oct. 2001.

4 SFB Reports

2001

01–1 Sendra, J.R., Winkler, F.: *Tracing Index of Rational Parametrizations.* January, 2001. Eds.: P. Paule, J. Schicho

01–2 Ratschan, S.: *Quantified Constraints Under Perturbation.* January, 2001. Eds.: P. Paule, J. Schicho

01–3 Burger, M., Engl, H.W., Markowich, P.A., Pietra, P.: *Identification of Doping Profiles in Semiconductor Devices.* January, 2001. Eds.: U. Langer, R. Lerch

01–4 Andrews, G.E., Paule, P., Riese, A.: *MacMahon's Partition Analysis VI: A New Reduction Algorithm.* February, 2001. Eds.: J. Schicho, F. Winkler

01–5 Andrews, G.E., Paule, P., Riese, A.: *MacMahon's Partition Analysis VII: Constrained Compositions.* February, 2001. Eds.: J. Schicho, F. Winkler

01–6 Andrews, G.E., Paule, P., Riese, A.: *MacMahon's Partition Analysis VIII: Plane Partition Diamonds.* February, 2001. Eds.: J. Schicho, F. Winkler

01–7 Riese, A.: *`qMultiSum` — A Package for Proving q-Hypergeometric Multiple Summation Identities.* February, 2001. Eds.: P. Paule, F. Winkler

01–8 Berkovich, A., Riese, A.: *A Computer Proof of a Polynomial Identity Implying a Partition Theorem of Göllnitz.* February, 2001. Eds.: B. Buchberger, P. Paule

01–9 Burger, M., Haslinger, J., Bodenhofer, U.: *Regularized Optimization of Fuzzy Controllers.* February, 2001. Eds.: J. Schicho, F. Winkler

01–10 Andrews, G.E, Paule, P., Riese, A.: *MacMahon's Partition Analysis IX: k-Gon Partitions* March, 2001. Eds.: B. Buchberger, F. Winkler

01–11 Zauner, J.: *Immersive Visualization of Adaptive Grids based on CAVE-Technology* March, 2001. Eds.: U. Langer, J. Volkert

01–12 Burger, M., Neubauer, A.: *Analysis of Tikhonov Regularization for Function Approximation by Neural Networks* March, 2001. Eds.: H. Engl, J. Schicho

01–13 T. Kutsia: *Unification in the Empty and Flat Theories with Sequence Variables and Flexible Arity Symbols* April, 2001. Eds.: B. Buchberger, P. Paule

01–14 M. Burger: *A Level Set Method for Inverse Problems* April, 2001. Eds.: H. Engl, U. Langer

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