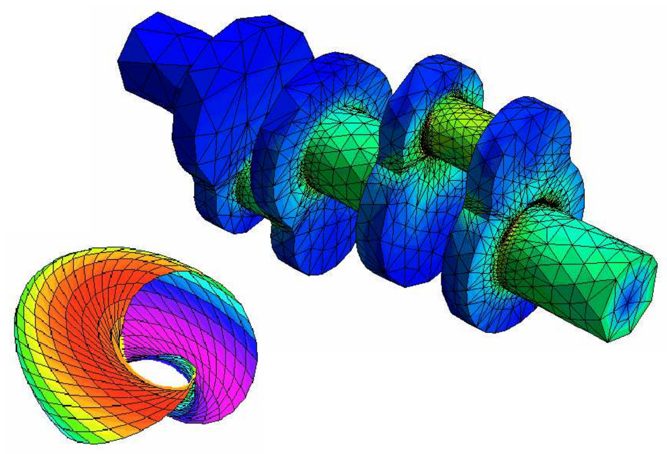
Special Research Program (SFB) F 013

Numerical and Symbolic Scientific Computing

Annual Report 2002

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. 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, F1317). Subproject F1301 is devoted to the coordination of the development of scientific computing tools such as visualization, solver and parallelization tools. 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,
- joint training of project co-workers,
- preparing the methods from symbolic computation in numerical computations and vice versa.

Now the integration of numerical and symbolic methods is present in all subprojects and leads to new a quality in scientific computing. A more precise discussion of this topic is given later in the presentation of the subprojects and 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”. Last but not least the international reputation of the computational and applied mathematics that was mainly established by the institutes participating in the SFB led to the foundation of the Johann Radon Institute for Computational and Applied Mathematics (RICAM) by the Austrian Academy of Sciences as a Center of Excellence in Applied Mathematics.

The following institutes of the University of Linz are currently involved in the subprojects of the SFB:

- Institute of Analysis,
- Institute of Computational Mathematics,
- Institute of Industrial Mathematics,
- Institute of Symbolic Computation.

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

`http://www.sfb013.uni-linz.ac.at`

or contact our office.

Acknowledgments: We express our thanks to the Austrian Research Fund (FWF), the University of Linz, the TNF, the Government of Upper Austria, and the City Linz for moral and financial support. Sincere thanks are also due to a.Prof.Dr. G. Haase and all SFB members and co-workers who helped preparing this booklet.

Linz, February 2003 Ulrich Langer

F 1301: Service and Coordination Project

Prof. Dr. U. Langer
Dr. G. Haase
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 and the parallelization tools. In 2002, we have been working on improving the mesh generator NETGEN, on redesigning the numerical software package FEPP resulting in the New Generation Solving Package NG-Solve (see subproject F1306), and we have continued our work on the algebraic multigrid package PEBBLES.

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 detailed description of the tools and packages developed in the SFB can be found on the SFB home page. This problem solving environment has been successfully applied to the simulation and optimization of many complicated problems including problems from mechanics, mechatronics, electrical engineering and life sciences (see F1306, F1309, [3] and [9] for some examples).

2 Algebraic Multigrid

In [3], we give an introduction to multigrid methods and describe the way from the geometrical version to algebraic version in detail. The Algebraic MultiGrid (AMG) methods are very powerful tools for solving large scale systems of algebraic equations arizing from the Finite Element (FE), Finite Volume (FV), Finite Integration Technique (FIT), Boundary Element (BE), or other discretizations of boundary value problems for elliptic Partial Differential Equations. We use AMG especially as preconditioners in a Krylov subspace iteration methods such as the CG-, QMR-, or the BiCGCRbi-methods. AMG methods are not only efficient, but also robust for broad classes of applications. The latter property is very important for hard practical applications. In 2002 we were working on the following topics:

1. AMG preconditioners for fully populated (dense) BE matrices and for sparse approximations to BE matrices: In 2002 we finished our paper on this topic and submitted it to the *International Journal for Numerical Methods in Engineering* that has recently accepted the paper for publication [5]. This paper already contains the first numerical results about AMG preconditioners for sparse BE matrices resulting form the Adaptive Cross Approximation to dense BE matrices. An original paper about these results is in work.
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 Parallel Solvers

The general parallelization strategies developed in previous years have been applied to our state-of-the-art algebraic multigrid solver (AMG). The contrast to other parallel AMG solvers consists in the fact that our sophisticated parallelization approach reuses 95% of the original sequential code which allows a very fast software development. The parallel scalabilily of that code is excellent, see also §4 and [2].

Some of the results obtained in F1301 and, especially, the parallelization techniques developed here were included in our book [1] that will be published by SIAM (USA) in 2003. We used typical domain decomposition data partitioning techniques for the parallelization of global multigrid methods. In [3] we describe how to carry over these parallelization techniques to algebraic multigrid methods. This new technology was the crucial point for developing the parallel version of the algebraic mulrigrid solver PEBBLES that was successfully applied to source reconstruction problem in life sciences described below.

The paper [4] is devoted to fast solvers for symmetric coupled finite and boundary element equations approximating static magnetic field problems in R^3 where the exterior magnetic field is modelled by means of scalar potential and the interior field is represented by a vector potential. In [7], we have recently introduced the Boundary Element Tearing and Interconnecting (BETI) methods as boundary element counterparts of the well-established Finite Element Tearing and Interconnecting (FETI) methods. The FETI methods are certainly the most successful parallel domain decompostion solvers, especially, for real-life engineering problems of very high complexity. In some practical important applications such as far field computations, handling of singularities and moving parts etc., BETI methods have certainly some advantages over their finite element counterparts. This claim is especially true for the sparse versions of the BETI preconditioners resp. methods. Moreover, we have developed an unified framework for coupling, handling, and analyzing both methods. In particular, the FETI methods can benefit from preconditioning components constructed by boundary element techniques. The first numerical results confirm the efficiency and the robustness predicted by our analysis.

4 Application to Life Sciences

The fast solution tools developed in this project outperformed professional software companies in a medical source reconstruction project guided by the Max-Planck-Institute of Cognitive NeuroScience in Leipzig, Germany. The reconstruction of the source distribution for epileptic fits from measurements of the electrostatic and/or magnetic field around the human head is an inverse problem. This special inverse problem requires a huge amount (appr. 10.000) of direct solves of the problem, i.e., simulation of the electric field when the source distribution is given. Therefore, we adapted our AMG solver to the specialities of the problem and achieved an acceleration factor 4 already on one processor. A test run on 12 processors resulted in an additional speedup of 10.

We wrote interfaces in order to integrate our parallel AMG solver [2] into the source reconstruction software and the results are very promising for a successfull clinical application of the source reconstruction [9]

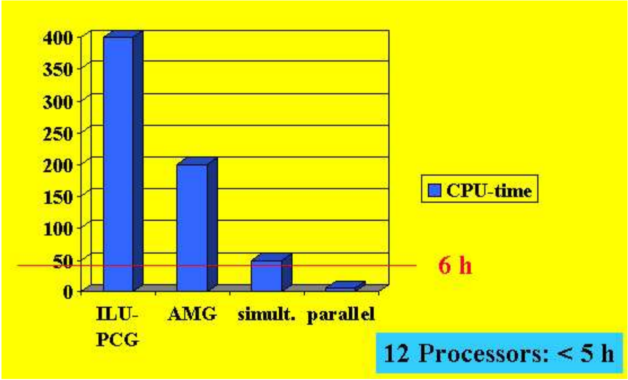


Figure 1: Solution time in houre for the source reconstruction.

References

[1] C. Douglas, G. Haase, and U. Langer. *A Tutorial on Elliptic PDE Solvers and Their Parallelization.* SIAM, Philadelphia, 2003. 135 pages.

[2] G. Haase, M. Kuhn, and S. Reitzinger. Parallel AMG on distributed memory computers. *SIAM Journal of Scientific Computing*, 24(2):410–427, 2002.

[3] G. Haase and U. Langer. Multigrid methods: From geometrical to algebraic versions. In A. Bourlioux and M. Gander, editors, *Modern Methods in Scientific Computing and Applications*, volume 75 of *NATO Science Ser. II, Mathematics, Physics and Chemistry*, pages 103–153. Kluwer Academic Press, Dordrecht, 2002.

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

[5] U. Langer, D. Pusch, and S. Reitzinger. An efficient preconditioner for boundary element matrices based on grey-box algebraic multigrid methods. *International Journal for Numerical Methods in Engineering*, 2003. (accepted).

[6] U. Langer, S. Reitzinger, and J. Schicho. Symbolic techniques for the element preconditioning technique. SFB-Report Nr. 02-03, University of Linz, 2002.

[7] U. Langer and O. Steinbach. Boundary element tearing and interconnecting methods. SFB-Report Nr. 02-41, University of Linz, 2002.

[8] S. Reitzinger, U. Schreiber, and U. van Rienen. Algebraic multigrid methods for complex symmetric matrices: Numerical studies. SFB-Report 02-01, University of Linz, 2002.

[9] C. Wolters, M. Kuhn, A. Anwander, and S. Reitzinger. A parallel algebraic multigrid solver for finite element method based source localization in the human brain. *Computing and Visualization in Sciences*, 5:165–177, 2002.

F 1302: Solving and Proving in General Domains

Prof. Dr. B. Buchberger

Prof. Dr. T. Jebelean, Dr. W. Windsteiger,
Dr. T. Kutsia, Dr. K. Nakagawa, Dr. J. Robu

D.I. F. Piroi, D.I. A. Craciun, D.I. N. Popov,
D.I. G. Kusper, D.I. M. Rosenkranz

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 2002, various components of the system have been improved and other new ones have been built on the foundations laid in the previous years of this SFB.

The improvements of previous existing components are:

- the set theory prover [12] is based now on the Zermelo-Frankel axioms;
- the geometry theorem prover has been extended to handle all the basic methods in the field, and was tested on a significant collection of examples [10];
- the prover for equational theories has been improved to handle sequence variables (including the novel theoretical work necessary to for unification of expressions with sequence variables) [5, 6];
- the presentation of proofs using focus windows, as well as interactivity, have been refined and improved [8, 9];
- the usage of the logico-graphical symbols has been enhanced [7];

Additionally, the proving power of Theorema is currently increased by incorporating a novel algorithm for solving the SAT problem [4, 3]. The SAT problem consists in finding a solution which satisfies a set of propositional formulae, or deciding that such a solution does not exist (the latter is a version of the problem of proving a propositional theorem). Essentially, the new algorithm developed in the Theorema group consists in trying to extend a given solution with several assignments and correcting the wrong ones – in contrast with the traditional Davis-Putnam method which tries to extend the current solution with one assignment at a time. Practical experiments show that the new method is faster in many situations.

Based on the progress in the implementation of the various components of Theorema, during the last year we started to use the system for approaching certain important activities in mathematics and computer science.

Study of Hilbert spaces theory. Using the capabilities of Theorema for representing and organizing mathematical theories, we started a comprehensive case study of the theory of Hilbert spaces. This led to an interesting characterization of some important functional operators in terms of non-commutative Groebner Bases [11]. Since this research is at the boundary between projects F1302 and F1308, full information on this topic is provided in the section concerning the cooperation between the subprojects. It should be noted that this research is a novel and significant breakthrough in an area situated at the intersection of symbolic and numeric computing, which shows the importance of the whole approach of this SFB project.

Study and verification of algorithms. One of the most important applications of automated reasoning is computer aided verification of algorithms and programs. In Theorema we started a very detailed case study concerning the properties of lists (tuples) and of various functions over lists. This allows the definition and study (proving correctness) of various sorting algorithms, and also stimulates further development of the special prover for the domain of lists [2, 1]. The possibility of describing both the algorithms and their properties in the *same language* is a distinctive feature of Theorema, which makes the system particularly attractive for the verification of programs written in functional style.

Other applications Additionally, we started to use *Theorema* for other applications: computer aided editing of mathematical texts (project Calculemus – combining computer algebra with automated reasoners), organization of mathematical knowledge (project MKM – Mathematical Knowledge Management), verification of procedural (imperative) programs (cooperation with Timisoara, Romania). More details about these activities are given in the section on international cooperation.

Related to editing of mathematical texts is the use of *Theorema* for computer aided teaching. Dr. Wolfgang Windsteiger used the system during his lectures (both at the University of Linz and at the Fachhochschule Hagenberg), both for preparing the lecture notes and for live examples illustrating the notions during the presentations. In particular, the lecture "Algorithmic Methods" for first-semester students of mathematics, is an interesting playground for the *Theorema* system, since the entire mathematical theory needed for polynomial interpolation and polynomial equation solving is built up in the algorithmic language of the *Theorema* system. In the same frame, all the mathematical knowledge needed in the algorithms could be proven using suitable provers in the *Theorema* system.

Using *Theorema* for various applications had of course an impact on increasing the efficiency of the respective activities (e.g. teaching), but also the reverse effect is important for our research: The various aspects of concretely using the system in a certain context of a certain application provides very useful feed-back about the capabilities of the system and leads to design and implementation decisions about various components.

References

[1] A. Craciun. The sequence provers in theorema. Joint AISC'02 - Calculemus '02 conference, Marseille, France, July 1-5, 2002; Appears in: Seki-Report Series Nr. SR-02-04, Calculemus 2002, Work in Progress Papers, Universitaet des Saarlandes, July 2002.

[2] A. Craciun and B. Buchberger. Proving the correctness of the merge-sort algorithm with theorema. In *Symbolic and Numeric Algorithms for Scientific Computing, Proceedings of the SYNASC02 Workshop*, pages 97–111, Timisoara, Romania, October 2002. ISBN 973-585-785-5.

[3] G. Kusper. Investigation of binary representations of sat, especially 2-literal representation. Conference of PhD Students in Computer Science, Szeged, Hungary, July 1-4, 2002, July 2002.

[4] G. Kusper. Solving the resolution-free sat problem by hyper-unit propagation in linear time. Fifth International Symposium on the Theory and Applications of Satisfiability Testing, Cincinnati, Ohio, USA, May 6-9, 2002, May 2002.

[5] T. Kutsia. *Solving and Proving in Equational Theories with Sequence Variables and Flexible Arity Symbols.* PhD thesis, Johannes Kepler University, Linz, 2002.

[6] T. Kutsia. Unification with sequence variables and flexible arity symbols and its extension with pattern-terms. In B. B. J. Calmet, O. Caprotti, L. Henocque, and V. Sorge, editors, *Artificial Intelligence, Automated Reasoning and Symbolic Computation. Proceedings of Joint AICS'2002 - Calculemus'2002 conference*, volume volume 2385 of *Lecture Notes in Artificial Intelligence*, pages 290–304, Marseille, France, July 2002. Springer Verlag. ISBN 3-540-43865-3.

[7] K. Nakagawa. *Supporting User-Friendliness in the Mathematical Software System Theroema.* PhD thesis, Research Institute for Symbolic Computation, January 2002.

[8] F. Piroi and B. Buchberger. Focus windows: A new technique for proof presentation. In J. Calmet, B. Benhamou, O. Caprotti, L. Henocque, and V. Sorge, editors, *Artificial Intelligence, Automated Reasoning and Symbolic Computation. Proceedings of Joint AICS'2002 - Calculemus'2002 Conference.*, volume 2385 of *Lecture Notes in Artificial Intelligence*, pages 290–304, Marseille, France, July 2002. Springer Verlag. ISBN 3-540-43865-3.

[9] F. Piroi and T. Jebelean. Interactive proving in theorema. Ninth Workshop on Automated Reasoning, AISB'02. 3-5 April, 2002, Imperial College of Science, Technology and Medicine, University of London. England. Appears in: Collected Abstracts, Toby Walsh editor., April 2002.

[10] J. Robu. *Geometry Theorem Proving in the Frame of the Theorema Project.* PhD thesis, Johannes Kepler University, Linz, 2002.

[11] M. Rosenkranz and H. W. Engl. Solving linear boundary value problems via non-commutative groebner bases. Symposium in Honor of Bruno Buchberger's 60th Birthday, Logic, Mathematics and Computer Science: Interactions (LMCS'2002) Hagenberg, Austria, October 20-22, 2002, October 2002.

[12] W. Windsteiger. An automated prover for zermelo-fraenkel set theory in theorema. Symposium in Honor of Bruno Buchberger's 60th Birthday, Logic, Mathematics and Computer Science: Interactions (LMCS'2002) RISC-Linz, Castle of Hagenberg, Austria, October 20-22, 2002. Appers in RISC-report nr. 02-60, October 2002.

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

Josef Schicho

Gábor Bodnár, Stefan Ratschan, Janka Pilnikova, Ibolya Szilagyi

1 Parametrization

Some algebraic curves admit polynomial parametrizations, i.e. it is possible to express the general solution of the corresponding algebraic equation in terms of polynomials in a single parameter. Up to now, the best known method to compute polynomial parametrizations is to compute a rational parametrization and then try to reparametrize in order to eliminate denominators. In [6], we devised a fast algorithm that computes the polynomial parametrizations directly, for the subclass of nonsingular algebraic curve.

The investigations on parametric surfaces have also been continued. In [10], we studied the possibility of inverting a parametrization as a rational map from the plane to the given surface. The paper [13] gives a method for simplifying a given parametrization of a fixed surface. The algorithm can be understood better when looking at it from the point of view of toric geometry. For example, a toric parametrization can be visualized as a convex lattice polygon. In the algorithm, we analyze this lattice polygon by passing repeatedly to the convex hull of interior points (see Figure 2). This shelling gives information that allows to find a unimodular transformation transforming the given polygon into another one which is as compact as possible (see Figure 3). The connection linking the method of adjoints for rational surfaces to lattice polygons is quite deep and will be investigated further.

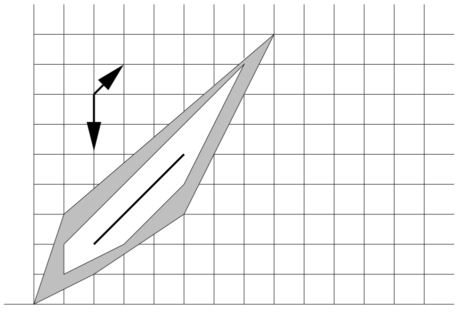


Figure 2: Shelling of a Convex Lattice Polygon.

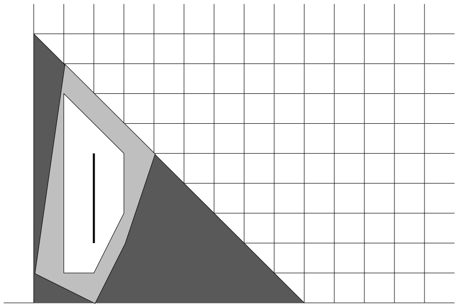


Figure 3: The Polygon After Transformation.

2 Box Approximation

Box approximation [11] is a method for computing approximate solution sets for first-order constraints over the reals, containing existential and universal quantifiers (see Fig. 4). We adapted the method in order to make it work under perturbations [12].

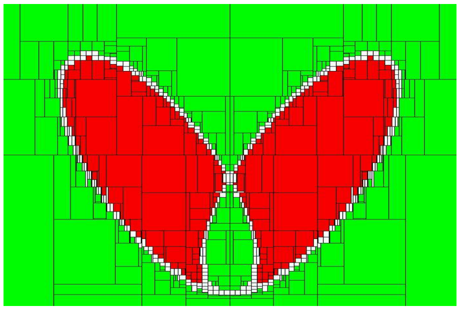


Figure 4: Box Approximation of an polynomial inequality.

3 Singularity Analysis

Resolution of singularities is a fundamental problem in algebraic geometry with several applications. An important area that benefits from the algorithm described in [4] is the computation of adjoints for hypersurfaces. Our computer program has been extended with this feature.

Since resolution of singularities is a complex problem, we investigated alternative techniques that can bring performance improvement in the relevant case of surfaces. A new algorithm for resolution of surface singularities and computation of adjoints has been proposed by J. Schicho and G. Brown, presented at [5]. This algorithm uses in its first phase toric modifications of the surface to transform its singularities into a special class, called quasi-ordinary. Then in the second phase these singularities are resolved via a generalization of the Newton-Puiseaux algorithm. The results are planned to be published in an forthcoming paper and the implementation of the algorithm in Magma is planned to be released this year.

An interesting problem related to resolution of singularities is to compute an ideal in the coordinate ring of the input variety, whose blowing up gives rise to the embedded resolution of the singularities of the variety. Relying on the algorithm of [4], we provided two methods for computing such an ideal in [2]. One of them relies on the sequence of blowing up transformations computed by the resolution algorithm, and the ideal is derived from the defining ideal of the blowing ups. The other relies on a "special" embedding of the nonsingular variety obtained by the resolution into projective space.

4 Exact Real Computation and Regularization

We have concluded our investigations in [3] in a discussion on the fundamentals of symbolic-numeric computation using the paradigm of exact real computation. We have proposed a framework for algorithms that encapsulate type-two machines which can compute arbitrarily accurate numerical approximations of compound mathematical objects (e.g. matrices, polynomials). This framework allowed us to formulate exact real solutions of certain ill-posed problems. One of them is the computation of pseudo-inverses of matrices with real or complex entries, using Tikhonov regularization [1]. Others are univariate polynomial GCDs, squarefree factorizations and root computations with dynamic root clustering.

5 Symbolic Methods in Numerical Algorithms

In the element preconditioning technique developed in [7], 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 [9], 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 [8].

References

[1] V. Arsenin and A. N. Tikhonov. *Solutions of ill-posed problems.* Wiley, 1977.

[2] G. Bodnár. Computation of blowing up centers. *J. Pure Appl. Alg.*, 2003. to appear.

[3] G. Bodnár, B. Kaltenbacher, P. Pau, and J. Schicho. Exact real computation in computer algebra. In U. Langer and F. Winkler, editors, *Proc. SNSC Hagenberg 2001.* Springer, 2002.

[4] G. Bodnár and J. Schicho. Automated resolution of singularities for hypersurfaces. *J. Symb. Comp.*, 30:401–428, 2000.

[5] G. Brown, J. Schicho, and G. Bodnár. Computation of adjoints for surfaces, 2002. talk on IMACS-ACA 2002, University of Thessaly, Volos, Greece.

[6] J. Gutierrez, R. Rubio, and J. Schicho. Polynomial parametrization of curves without affine singularities. *Comp. Aided Geom. Design*, 19:223–234, 2002.

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

[8] B. Kaltenbacher and J. Schicho. A multigrid method with a priori and a posteriori level choice for the regularization of non-linear ill-posed problems. *Num. Math.*, 93:77–107, 2002.

[9] U. Langer, S. Reitzinger, and J. Schicho. Symbolic methods for the element precondition technique. In U. Langer and F. Winkler, editors, *Proc. SNSC Hagenberg 2001.* Springer, 2002.

[10] S. Pérez-Díaz, J. Schicho, and J. R. Sendra. Properness and inversion of rational parametrizations of surfaces. *AAECC*, 13:29–51, 2002.

[11] S. Ratschan. Approximate quantified constraint solving by cylindrical box decompo sition. *Reliable Computing*, 8(1):21–42, 2002.

[12] S. Ratschan. Quantified constraints under perturbation. *Journal of Symbolic Computation*, 33(4):493–505, 2002.

[13] J. Schicho. Simplification of surface parametrizations. In *Proc. ISSAC 2002*, pages 229–237. ACM Press, 2002.

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 have been working on various issues involving algebraic curves and surfaces, from implicitization and parametrization, to the use of elliptic curves in cryptography, symbolic-numerical methods in the generation of minimal surfaces, and software design issues relating to algebraic computation, in particular geometric algebraic computation. In addition to these core topics, we have investigated modern methods in elimination theory such as the computation of involutive bases, and symbolic methods in the symmetry classification problem for 2nd order PDEs in one dependent and two independent variables.

1.1 Implicitization and parametrization of algebraic curves and surfaces

The old problem of implicitization of parametrically given algebraic varieties has been revisited by G. Landsmann, and new techniques of resultant theory and moving curves and varieties have been applied [16, 17]. We have further investigated the relation of parametrization of curves and surfaces to the 17th Hilbert problem of representing quadratic forms as sums of squares. The field in which such a representation is possible determines the field over which a parametrization can be found; [19, 20, 21, 22].

1.2 Elliptic curves in cryptography

R. Athale has worked on number theoretic problems [2, 3] and on the problem of determining elliptic curves with given rank. A preliminary report is available as [4]. Together with C. Aistleitner (a diploma student) we have created a new software package in the CASA system for computing and experimenting with elliptic curves. A report on this activity is in progress.

1.3 Symbolic-numerical methods in the generation of minimal surfaces

H. Gu has continued his work on symbolic-numerical methods for the generation of minimal surfaces, in particular the Plateau problem. He has presented his results at various conferences [7, 8, 9, 10, 12] and in an SFB report [11]. Gu is about to finish his PhD thesis on this topic. Recently there has been intensive discussion with colleagues from numerical projects (in particular Dr. M. Burger) towards application of these methods to level set problems. Joint papers on this topic are in preparation.

1.4 Elimination theory

In all aspects of algebraic geometry the theory of solving polynomial equations, i.e. elimination theory, plays a vital role. R. Hemmecke has made important progress in his research on involutive bases, a particular method in elimination theory [1, 13, 14]. Some of this work has been done in a cooperation with Prof. J. Apel of Leipzig University. Hemmecke is about to finish his PhD thesis on this topic.

1.5 Symmetry classification for PDEs

The work of E. Hillgarter on symmetry classification for PDEs is only weakly related to the core problems of the project. But algebraic surfaces play a role in understanding the geometric transforms and frames of such PDEs. Hillgarter has finished his PhD thesis on this topic [15].

1.6 Software design

The software system CASA (Computer Algebra Software for Algebraic Geometry) has been further improved and added to. New functionalities have been implemented (conf. subsection on elliptic curves) and modern tools of software design have been applied [5, 6, 18].

References

[1] Joachim Apel and Ralf Hemmecke. Detecting unnecessary reductions in an involutive basis computation. SFB F013 Report 02-13, Research Institute for Symbolic Computation, Johannes Kepler University, 4040 Linz, Austria, October 2002. Submitted to special issue of JSC.

[2] Rahul Athale. Verifying the jumping champion conjecture, August 2002. Talk presented at the Conference on Foundations of Computational Mathematics (FOCM02), Minneapolis, USA.

[3] Rahul Athale. Verifying the jumping champion conjecture. RISC Tech Report 02-17, Research Institute for Symbolic Computation, Johannes Kepler University, 4040 Linz, Austria, 2002. published in the informal proceedings of FOCM02.

[4] Rahul Athale and Franz Winkler. Curves in cryptography. RISC Tech Report 02-16, Research Institute for Symbolic Computation, Johannes Kepler University, 4040 Linz, Austria, 2002.

[5] Karoly Bosa and Wolfgang Schreiner. Tolerating stop failures in distributed Maple. In *Dapsys 2002*. Kluwer Academic Publishers, October 2002. 4th Austrian-Hungarian Workshop on Distributed and Parallel Processing, Linz, Austria.

[6] Olga Caprotti and Wolfgang Schreiner. Towards a mathematical service description language. In *ICMS 2002, International Congress of Mathematical Software*. World Scientific Publishers, 2002.

[7] Hong Gu. The finite element approximation to the minimal surfaces subject to the plateau problems. In *Proceedings of The Sixth International Conference on Computational Structure Technology*. Civil-comp Press, September 2002.

[8] Hong Gu. The finite element approximation to the minimal surfaces subject to the plateau problems, sep 2002. Talk at CST2002, Prague, Czech Rep.

[9] Hong Gu. Generating minimal surfaces subject to the plateau problems by finite element method. In *Lecture Notes on Computer Science—Proceedings for the fifth conference of Numerical Methods and Applications*, Borovets, Bulgaria, August 2002. Springer Verlag.

[10] Hong Gu. Graphical computation of the minimal surfaces problems by the symbolic-numerical method, june 2002. Talk at ACA'2002, Volos, Greece.

[11] Hong Gu. Graphical generating of minimal surfaces subject to the plateau problems. SFB F013 Report 02-24, Research Institute for Symbolic Computation, Johannes Kepler University, 4040 Linz, Austria, 2002. Submitted paper to the book "Computer and Structures", Elsevier Press, Oct. 2002.

[12] Hong Gu. Software generating of minimal surfaces subject to the plateau problems by the finite element method, aug 2002. Talk at NM-A'02, Borovets, Bulgaria.

[13] Ralf Hemmecke. Detecting unnecessary reductions in an involutive basis computation, June 2002. Talk presented at the Conference on Applications of Computer Algebra (ACA'02), Volos, Greece. Joint work with J. Apel.

[14] Ralf Hemmecke. An efficient method for finding a simplifier in an involutive basis computation (extended abstract). In Jacques Calmet, Marcus Hausdorf, and Werner M. Seiler, editors, *Proceedings of the Workshop on Under- and Overdetermined Systems of Algebraic or Differential Equations, March 18-19, 2002, Karlsruhe, Germany*, pages 87–95. Institut für Algorithmen und Kognitive Systeme, Universität Karlsruhe, March 2002. Local proceedings.

[15] Erik Hillgarter. A contribution to the symmetry classification problem for 2nd order pdes in one dependent and two independent variables. PhD Thesis, RISC Tech Report 02-26, Research Institute for Symbolic Computation, Johannes Kepler University, 4040 Linz, Austria, December 2002.

[16] Günter Landsmann. Implicitization of algebraic varieties. In N. Callaos, editor, *Proceedings of the SCI2002, Vol. 11*, July 2002.

[17] Günter Landsmann. Implicitization of algebraic varieties, September 2002. Talk at the 4th international Workshop on Automated Deduction in Geometry ADG2002, Hagenberg, Austria.

[18] Wolfgang Schreiner, Christian Mittermaier, and Karoly Bosa. Distributed Maple: Parallel computer algebra in networked environments. *Journal of Symbolic Computation*, 2002.

[19] Franz Winkler. Advances in Algebraic Geometric Computation. In *Proc. Internat. Conf. on Algebra and Its Applications (ICAA 2002)*, pages 107–120, 2002. ISBN 970-13-2182-1.

[20] Franz Winkler. Advances in Algebraic Geometric Computation, March 2002. Invited lecture at the Internat. Conf. on Algebra and Its Applications (ICAA 2002), Chulalongkorn Univ., Bangkok, Thailand.

[21] Franz Winkler. Quadratic Forms and the Parametrization Problem, April 2002. Invited lecture at the workshop "Applications of Commutative Algebra", Università di Catania, Italy.

[22] Franz Winkler. Quadratic Forms and the Parametrization Problem, August 2002. Talk at the Conference "Foundations of Computational Mathematics", Workshop on "Computational Algebraic Geometry", Minneapolis, USA.

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 2002 by the SFB project group F1305 is documented in the form of 10 publications: 2 articles came out in journals, 8 technical reports have been produced, half of them are already accepted for journal publication. 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 development of symbolic summation algorithms has been continued with respect to single as well as multiple sums. Particular emphasis has been put on special functions applications. For instance, the paper [3] presents a computer-assisted closed form evaluation of an integral arising in concrete statistical research. This has been achieved by an effective combination of different algorithms developed in SFB work; the original problem was not in the scope of the tools provided by systems like Maple or Mathematica. Another computer proof based on one of these algorithms has been published in [1].

A brief sketch of two major achievements on more general grounds is as follows. There is an algorithm, called WZ method, that in principle enables to compute linear recurrences with polynomial coefficients for any given multiple hypergeometric sum. The essence of the approach consists in transforming the problem into the task of solving a system of linear equations over multivariate rational functions. Despite its elegance and simplicity, in practice the computational bottle-neck of the method exactly is the problem to solve this linear algebra problem symbolically. So far the SFB group F1305 introduced various refinements to overcome this problem. But a real break-through has been achieved due to recent work of A. Riese and B. Zimmermann [7] which uses a modular approach. This extends the applicability of the method significantly; it already helped to solve problems that so far seemed to be intractable for symbolic computation procedures.

The second major achievement has been made with respect to summation using difference field methods. In a series of papers [6, 8, 9, 10, 11, 12], C. Schneider was able to extend Karr’s theory even further. A most remarkable achievement of his package Sigma was the computer proof of a long standing conjectured identity [2],

$$\boxed{\begin{aligned}&\sum_{k=0}^{m}(-1)^k\binom{m}{k}^3\\&\qquad\times\left[3(H_{m-k}-H_k)^2+H_{m-k}^{(2)}+H_k^{(2)}\right]=0,\end{aligned}}$$

where H_n and $H_n^{(2)}$ denote the nth harmonic number of the first and second kind, respectively. This settled the last missing link in a new approach to Padé approximation of the logarithm.

1.2 Partitions and Special Functions

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, that partition analysis is ideally suited for being supplemented by modern computer algebra methods. Applications range from the preprocessing for automatic theorem proving (Omega was used successfully in Project F1302) to enumeration problems in statistical physics. As an off-spring from the corresponding SFB work, various surprising new combinatorial results have been found. Corresponding research articles are in preparation.

Another work in progress concerns extensions of the so-called Extended Engel Expansion Algorithm due to A. and J. Knopfmacher. Recent results give new insight into approximation of (q-) hypergeometric series by rational functions. Related work, but using different methods, is the paper [4].

1.3 Symbolic Methods for Wavelet Construction

Wavelets are widely used in many practical applications such as data compression or image processing, or, more theoretically, in connection with partial differential equations. They are "non-standard" special functions with sort of 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 the first project phase, in cooperation with O. Scherzer and A. Schoisswohl, the SFB group F1305 has studied the basic equations for the filter equations from a symbolic computation point of view. 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. This work has been successfully extended, again with O. Scherzer and A. Schoisswohl [5]. Informally, it concerns the construction of new wavelets with scale dependent properties.

References

[1] A. Berkovich and A. Riese. A computer proof of a polynomial identity implying a partition theorem of Göllnitz. *Adv. in Appl. Math.*, 28:1–16, 2002.

[2] K. Driver, H. Prodinger, C. Schneider, and J. A. C. Weideman. Padé approximations to the logarithm II: Identities, recurrences, and symbolic computation. Preprint, 2003.

[3] R. Lyons, P. Paule, and A. Riese. A computer proof of a series evaluation in terms of harmonic numbers. *Appl. Algebra Engrg. Comm. Comput.*, 13:327–333, 2002.

[4] P. Paule and H. Prodinger. Fountains, histograms, and q-identities. SFB Report 02-34, J. Kepler University Linz, 2002.

[5] P. Paule, O. Scherzer, and A. Schoisswohl. Wavelets with scale dependent properties. SFB Report 02-4, J. Kepler University Linz, 2002.

[6] P. Paule and C. Schneider. Computer proofs of a new family of harmonic number identities. SFB Report 02-25, J. Kepler University Linz, 2002.

[7] A. Riese and B. Zimmermann. Randomization speeds up hypergeometric summation. Preprint, 2003.

[8] C. Schneider. Solving parameterized linear difference equations in $\Pi\Sigma$-fields. SFB Report 02-19, J. Kepler University Linz, 2002.

[9] C. Schneider. A collection of denominator bounds to solve parameterized linear difference equations in $\Pi\Sigma$-fields. SFB Report 02-20, J. Kepler University Linz, 2002.

[10] C. Schneider. Degree bounds to find polynomial solutions of parameterized linear difference equations in $\Pi\Sigma$-fields. SFB Report 02-21, J. Kepler University Linz, 2002.

[11] C. Schneider. A unique representation of solutions of parameterized linear difference equations in $\Pi\Sigma$-fields. SFB Report 02-22, J. Kepler University Linz, 2002.

[12] C. Schneider. How one can play with sums. RISC Linz Report Series 02-24, J. Kepler University Linz, 2002.

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

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

This project is concerned with the development 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 High Level High Performance Programming

This period was concerned with the redesign of the basic parts of our finite element software NGSolve. On one hand side, the high level features of the object oriented programming language C++ are an indispensable help for the development of complex software. On the other hand side, the functional programming language Fortran is often considered to be the first choice for high performance scientific software. In the new standard of C++, called the 99-standard, a few new features have been added to the language. But, this few features allow a complete new programming paradigm called 'Expression Templates'. We learned about that from two papers by Todd Veldhuizen, Univ. Bloomington, Indiana: One is called 'Why is C++ slower than Fortran', the other one 'How to make C++ faster than Fortran'. We explain the idea by the very frequent, simple assignment statement

$$x = y + M * z.$$

Here, x, y and z are vectors, and M is a matrix. The goal is to write the code exactly as this, and to obtain the high performance of a hand tuned special procedure for that. Fortran contains data types for vectors and dense matrices, and the compiler generates optimal code for that example. In a conventional performance oriented C++ approach one would write a function for that small task, and explicitly call it wherever it is needed. In a conventional textbook C++ approach one would define operators for vector plus vector, matrix times vector, and a few more, and write the statement as above. Both approaches have disadvantages. The first one needs a large number of procedures (VecPlusVec, VecMinusVec, VecPlusMatTimesVec, etc.). Since the possible combinations of expressions grow exponentially in the number of terms, the set of procedures will in practice not be sufficient for three and more terms. Then, several procedures have to be called. The textbook approach has a performance problem: Here, e.g., the result of $M * z$ has to be stored somewhere, i.e., a temporary vector has to be allocated. This temporary objects rule out the textbook approach for high performance applications.

The new expression template programming paradigm allows to write the statement as above, and to obtain hand tuned performance. The trick is that the result of $M * z$ is not a conventional vector, but it is an expression `Product<Matrix,Vector>`, and the result of the addition is `Plus<Vector,Product<Matrix,Vector>>`. Finally, in the assignment, the values of that object are evaluated and are assigned to the vector x.

J. Schöberl has rewritten the computational kernel of NGSolve based on such expression templates. They are not only useful for linear algebra terms as above, but also for many more finite element related tasks, such as the computation of gradients. The implementation of the finite element library is now much closer to the mathematical formulation, and, the performance of key components such as element matrix assembling increased by about a factor of 3.

2 3D Elasto-Plastic Simulation

Considering only purely elastic material laws in mathematical models does not suffice many real life applications. A modification to make the model more realistic is an additional term in the stress-strain relation describing plastic behavior. The governing equations describing this phenomenon are then 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.

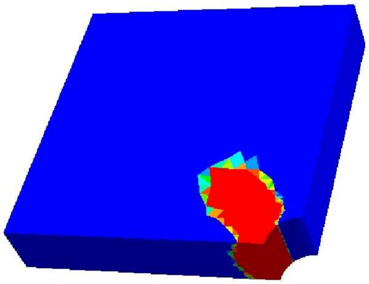
By discretizing the time derivatives occurring in the normality law and calculating the weak dual formulation, the problem can be considered as a variational inequality in each time step. An equivalent formulation to the variational inequality is the optimization problem in the displacement u and the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

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

under incompressibility constraints, with f being a non-differentiable function. The objective is regularized, the new $\tilde{f}$ is then piecewise quadratic and differentiable, thus standard methods apply.

This period, J. Kienesberger has extended her solver to 3D as well as to the quasi-static case [3]. The algorithm is a successive sub-space optimization method: In the first step, the Schur-Complement system for the displacement variable u is solved by a multigrid preconditioned conjugate gradient method. The second step, namely the minimization in the plastic part of the strain p, splits into a large number of local optimization problems. The linear incompressibility constraint is resolved by projecting the problem onto a hyperplane, where the constraint is satisfied exactly.

The algorithm was tested for a common benchmark example: A quadratic steel plate with a small circular hole in the middle with forces acting on the upper and lower edges. Due to the symmetry of the problem, only the upper left quarter is considered. The domain with plastic behavior is extending from the lower edge next to the hole:



The numerical tests show the fast convergence of the algorithm, it behaves almost linear with the number of unknowns.

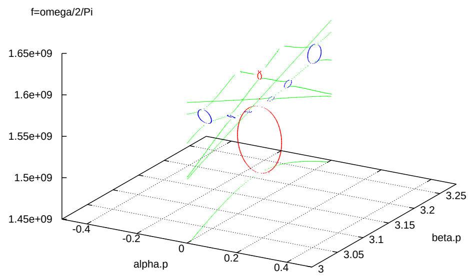
3 Piezo-Electric Device Simulation

S. Zaglmayr finished her Masters thesis on numerical methods for piezo-electric device simulation [4]. She worked together with Prof. U. Langer and J. Schöberl, and Prof. Lerch form the Institute for Sensor Technologies, University of Erlangen.

One application of interest are surface acoustic wave filters which are commonly used for frequency filtering in cell phones and TV-sets. We are interested in the dependency of the wave propagation on the excitation frequency. Since this device consists of 100s up to 1000s equidistantly arranged electrodes on its surface, we may assume a periodic domain. Floquet-Bloch theory reduces the infinite periodic computation-domain to the shifted unit-cell problem. This means we search for the solution $u = (u_{mech}, u_{elec})^T$ of the parameter-depending eigenvalue problem

$$\begin{aligned} Lu &= \omega^2 Mu \\ u_r &= e^{(\alpha+i\beta)p} u_l \\ \frac{\partial u_r}{\partial n_r} &= -e^{(\alpha+i\beta)p} \frac{\partial u_l}{\partial n_l}. \end{aligned}$$

Here, L is the piezo-electric differential operator coupling mechanical and electrical field, M the mechanical mass operator, u_l and u_r are the boundary values at the left and right boundary of the unit-cell. The parameter ω describes the frequency and $(\alpha + i\beta)p$ the propagation parameter, standing for damping factor (α) and phase shift (β) of the waves per cell. The solution can be shown in the dispersion diagram:



Direct and iterative solvers for the occurring quadratic parameter-dependent eigenvalue problems were developed by S.Zaglmayr. Earlier computations were restricted to pure propagating waves, that means no damping $(\alpha = 0)$. The new model is able to describe also damping effects. The figure above shows propagating modes in green, and damped modes in red and blue.

References

[1] J. Gerstmayr and J. Schöberl. A 3d finite element approach to flexible multibody systems. In *Proceedings to Fifth World Congress on Computational Mechanics (WCCM V)*, 2002.

[2] M. Hofer, R. Lerch, N. Finger, G. Kovacs, J. Schöberl, S. Zaglmayr, and U. Langer. Finite element calculation of wave propagation and excitation in periodic piezoelectric systems. In *Proceedings to Fifth World Congress on Computational Mechanics (WCCM V)*, 2002.

[3] J. Kienesberger. A multigrid preconditioned solver for elastoplastic problems. SFB-Conference on "Computational Methods for Inverse Problems", August 2002.

[4] S. Zaglmayr. Eigenvalue problems in SAW filter simulation. Master's thesis, Johannes Kepler University Linz, 2002.

F 1308: Large Scale Inverse Problems

Prof. Dr. Heinz W. Engl

Dr. Hend Benameur, Dr. Nicoletta Bila, Dr. Martin Burger,
Dr. Barbara Kaltenbacher

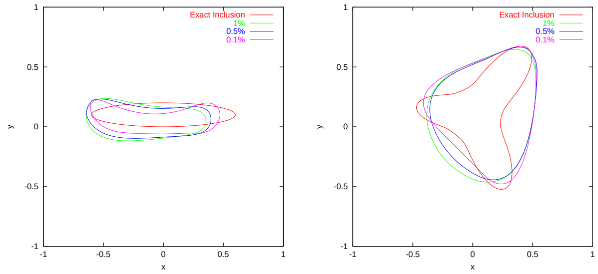
DI. Herbert Egger, DI. Benjamin Hackl, DI. Philipp Kügler, DI. Markus Rosenkranz

Andreas Hofinger

1 Level-Sets and Regularization

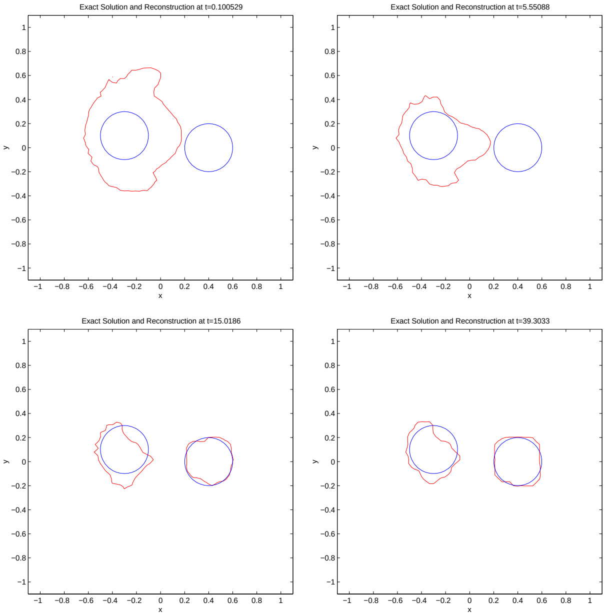
In the field of level set methods and regularization, several activities were carried out in the year 2002. M.Burger developed a functional-analytic framework for the construction of level set methods for inverse problems, with a velocity choice based on the shape gradient [2]. This paper and a previous publication of the author on this subject lead to a positive reaction both in the scientific community of inverse problems and level set methods, M.Burger was invited to give talks at a conference on geometric motion in the US, at a minisymposium on inverse obstacle problems at ICIAM 2003, and at University Graz. An extension of the paper [2] to choices of the velocity in a Newton-type way is in preparation.

In a joint work [1] H.Ben Ameur, M.Burger and B.Hackl investigated the application of level set methods as proposed in [2] for inverse problems in linear elasticity. Besides the application of this method, identifiability results as well as the regularizing and convergence properties of penaltization by perimeter were proven in a very general geometric setup, which corresponds well to the type of obstacles that can be reconstructed with the level set method.



Identified Inclusion for $1, 0.5, 0.1\%$ noise

M.Burger investigated the problem of regularity of curves and surfaces (the zero level set) obtained from a level set method in [3]. In general, the level set method does not provide information on regularity for the zero level set, but for a special class of first-order equations, local Lipschitz regularity almost everywhere in time could be shown. This type of regularity is crucial, when an elliptic or parabolic equation with boundary or interface conditions on the zero level set is coupled to the level set method - such a coupling typically occurs for inverse obstacle problems such as the ones investigated in [2] and [1].



Splitting of Domains with the Level-Set Method

Finally, a collaboration with the SFB F 003 was started in this subject, more details are given in the section on external collaborations below.

2 Neural Networks

In the field of neural networks, the diploma student Andreas Hofinger investigated the application of iterative methods for regularized training, under supervision of Prof. H.W. Engl and Dr. M. Burger, resulting in the diploma thesis [6].

As a consequence of this diploma thesis and a collaboration between A.Hofinger and M.Burger, two joint papers are in preparation. The first one is concerned with the application of the so-called *greedy algorithm* in presence of noise, for which a detailed convergence and stability analysis shall be carried out. The main idea of the greedy algorithm is to increase a neural network only by a single node in each step of the algorithm, and to train (i.e. optimize) only the parameters corresponding to this single node. Since the problem dimension of the optimization problem to be solved in each step of the algorithm is very small, this results in an efficient algorithm and moreover, it can be shown that standard iterative methods yield useful results when applied to the single node problem (cf. [6]).

A second paper shall be concerned with convergence problems of standard iterative methods, when applied to neural networks with more than one node without greedy approximation. It can be shown that the error is not decreasing monotonically during the iteration procedure in general (even in absence of data noise and for initial values arbitrarily close to the solution) and several numerical examples result in non-convergence. One of the iterative methods, where these convergence problems occur, is the frequently used *backpropagation* algorithm. Moreover, these results provide another strong argument in favour of greedy algorithms, where convergence and stability can be shown rigorously.

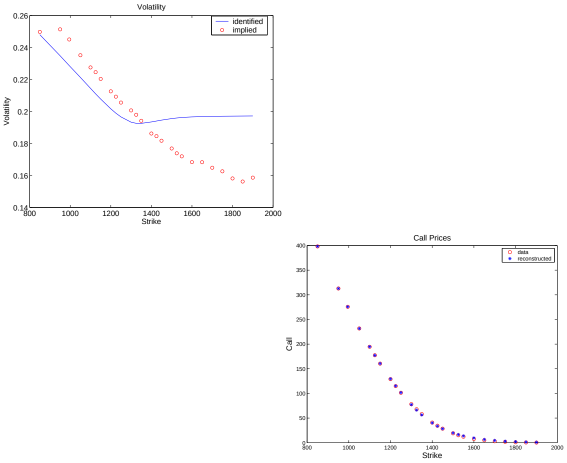
3 Inverse Problems in Mathematical Finance

The Black-Scholes model is a frequently used and standard stochastic model for stock price evolution in mathematical finance. The important parameter in this model is the so called *volatility*, which corresponds to the magnitude of fluctuations in the stock price movement or the standard deviation of underlying stochastic process.

In an idealized market, i.e. under absence of arbitrage and transaction costs, where unlimited continuous trading is possible, a variety of derivative instruments, e.g. all sorts of options, can be priced by solving partial differential equations of usually parabolic type, where volatility appears as a diffusion coefficient. In fact, the pricing equations, and thus prices of derivatives, depend only on the a-priori unknown and not directly observable level of volatility.

It is a well known observation that market prices of frequently traded options disagree with the constant volatility assumption of the Black-Scholes model, but quite the contrary, implied (by the market prices) volatilities show a distinct dependence on strike and time, known as the *smile*- and *term*-structure. Possible generalizations of the Black-Scholes stock price evolution model include stochastic volatility, jump-diffusion and deterministic-volatility-function models, the latter having the advantage that essential features of the Black-Scholes model, e.g. the market completeness and pricing equations are preserved.

The identification of volatility surfaces out of given option prices (model calibration to market prices) is essential for derivative pricing. In the case of of European Vanilla option prices as data, an adjoint parabolic equation (Dupire equation) can be derived. In this framework, volatility identification corresponds to parameter estimation in a degenerate parabolic pde in non-divergence form on unbounded domain by means of given state observation, which is a nonlinear inverse and ill-posed problem, i.e. approximately the same option prices may imply very different volatilities. The problem can successfully be regularized in the framework of Tikhonov regularization [5].



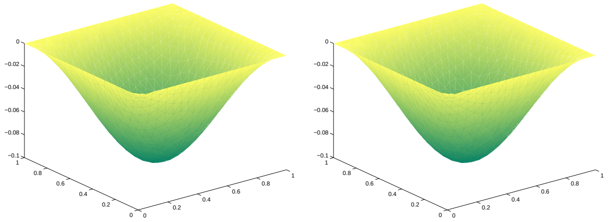
Identified vs. implied Black-Scholes volatility and recovered option prices

Besides stability and convergence, convergence rates can be proven for the case when only the smile structure of volatilities is unknown. The convergence rate result further indicates global uniqueness of the solution but also difficulties with the identification in certain regions; both can be observed in numerical experiments. A careful inspection of the convergence rate statement reveals that under incorporation of derivative data (i.e. market prices of digital options) more details, i.e. non-smooth parts, of the volatility can be identified with rates [4].

4 Derivative Free Landweber Iteration

Identifying a physical parameter in an elliptic state equation from knowledge of the state is a nonlinear inverse and ill-posed problem, i.e. its solution, may be highly sensitive to data perturbations. Common regularization techniques for computing approximations of the solution in a stable way are - both from the theoretical and the numerical point of view - based on Fréchet derivatives of the nonlinear forward operator. The conditions on the derivative that guarantee convergence of the methods are usually hard to verify in the context of parameter identification.

Within the Project F1308, an iterative regularization method was developed not at all involving the derivative of the parameter-to-output map. Thereby, convergence of the iterates as well as rate estimates can be given under natural assumptions only related to the solvability of the underlying direct problem. Our theory allows the latter to be itself nonlinear and this nonlinearity even to be due to the unknown parameter. Considering the numerical realization, the avoidance of using derivatives significantly reduces the computational efforts compared to the classical Landweber method since auxiliary direct problems and derivatives of the parameter with respect to the physical state become unnecessary. The algorithm has be successfully applied to the inverse windshield problem introduced in last year's report.



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

5 Moore-Penrose Inverse and Symbolic Methods

A new approach for symbolically solving linear boundary value problems was found. Seen from an operator-theoretic viewpoint, the differential equation poses the problem of finding a right inverse of the given differential operator, while the boundary conditions serve to select one particular right inverse out of infinitely many. This interpretation is in contrast to the usual formulation, where the boundary conditions serve to define the domain of the differential operator such that its right inverse is uniquely determined (provided that the BVP has a unique solution).

The oblique Moore-Penrose equations are invoked for finding a right inverse, using the freedom of choice in the nullspace projector for ensuring the boundary conditions. The resulting system of equations is conceived as a non-commutative polynomial system, having such indeterminates as the Green's operator G, differentiation D, antiderivative A, boundary operators, and multiplication operators. Saturated by suitable interaction equations expressing the analytical relations of these indeterminates, one ends up with a system that can be solved for G with computer algebra methods like Gröbner bases.

The new approach was originally presented as a heuristic method that needed "creative" steps at some critical points in the computation; this stage of research is presented in [8]. Due to some recent findings, it is now possible to use an alternative method that is algorithmic at least for the case of linear differential operators with constant coefficients (again provided that the solution is unique); this is described in [9]. In the latter case, the costly use of Gröbner bases can be dispensed with.

References

[1] H. Ben Ameur, M. Burger, B. Hackl, *On some inverse problems in linear elasticity*, University Linz, (2003), Preprint.

[2] M. Burger *A framework for the construction of level set methods for shape optimization and reconstruction*, University Linz, (2002), SFB-Report 02-12, submitted.

[3] M. Burger, *Growth fronts of first-order Hamilton-Jacobi equations*, University Linz, (2002), SFB Report 02-8, submitted.

[4] H. Egger. *Tikhonov Regularization Applied to the Inverse Problem of Option Pricing: Convergence Analysis and Rate Results*, University Linz, (2002), Preprint.

[5] H. Egger. *Identification of Volatility Smile in the Black Scholes Equation via Tikhonov Regularization*, Master's thesis, University Linz, November 2001.

[6] A. Hofinger, *Iterative Regularization and Training of Neural Networks*, University Linz, (2003).

[7] P. Kügler, *A Derivative Free Landweber Iteration for Parameter Identification in Elliptic PDEs*, University Linz, (2003), Preprint.

[8] M. Rosenkranz, B. Buchberger, H.W. Engl, *Solving Linear Boundary Value Problems via Non Commutative Gröbner Bases*. Accepted in the journal *Applicable Analysis*.

[9] M. Rosenkranz. *Symbolic Solution Methods for Linear Boundary Value Problems* (working title). PhD Thesis, in preparation.

F 1309: Multilevel Solvers for Large Scale Discretized Optimization Problems

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

1 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, flexibility is needed 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 5 and Figure 6 (white indicates the thick part, violet the thin one). For details see [3], [6].

2 Topology Optimization

We began to investigate topology optimization problems which are very familiar with sizing problems. The main difference is the fact that in sizing the thickness can vary between given upper and lower bounds, whereas in topology optimization intermediate values for the thickness are not wanted because here the thickness is interpreted as material density. Currently, we use the *Method of moving asymptotes* – a well-known optimization method in this area – for solving these problems. We mainly focus on the introduction of multilevel solution ideas to these established optimization methods and test our routines with model problems from literature (see e.g. Figure 7 for the material distribution for a 2D benchmark example). For the future we want to introduce ideas developed in the frame of inverse problems also to this field. We mainly think of all-at-one approaches similar to the ideas presented in the con-

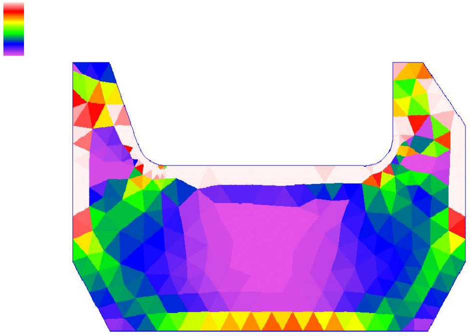


Figure 5: 449 design parameters

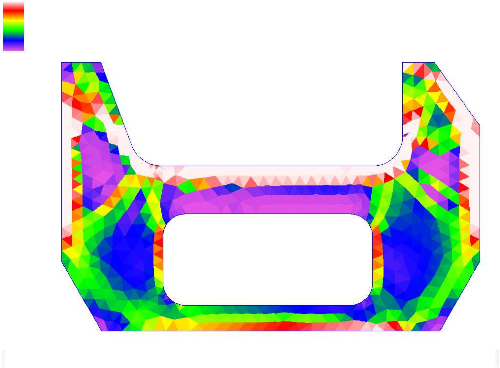


Figure 6: 1078 design parameters

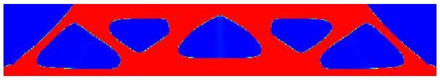


Figure 7: Material distribution

text of inverse problems ([1, 2]). These ideas should allow us to reduce the current runtimes of topology optimization codes dramatically.

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, see also [4]. Our approach is based on iterative regularization using SQP-type methods ([1, 2]) and puts special emphasis on 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 focused on the efficient numerical realization. Unlike classical approaches we treat the state equation as a constraint for the underlying optimization problem and apply SQP-techniques in the product-space for state and parameter. This leads to saddle point problems which were solved by iterative methods allowing us to solve also large scale parameter identification problems. An implementation of the method showed the good numerical properties of our approach. Our method clearly outperformed classical solution methods for parameter identification problems as can be seen in Figure 8. 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 9 a comparison of the original method with its nested version can be found. Currently we focus our work on problem adapted and more efficient preconditioners for two important model problems which we also continue in the future.

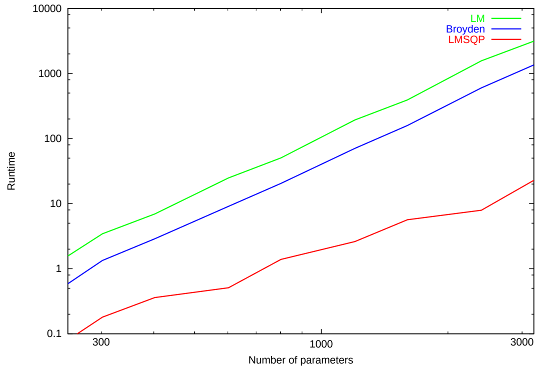


Figure 8: Comparison of runtimes

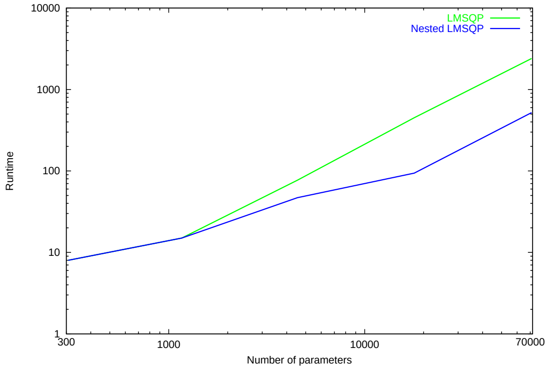


Figure 9: Acceleration using nested spaces

References

[1] M. Burger and W. Mühlhuber. Iterative regularization of parameter identification problems by SQP methods. *Inverse Problems*, 18:943 – 970, 2002.

[2] M. Burger and W. Mühlhuber. Numerical approximation of an SQP-type method for parameter identification. *SIAM J. Numer. Anal.*, 40(5):1775 – 1797, 2002.

[3] G. Haase, U. Langer, E. H. Lindner, and W. Mühlhuber. Optimal sizing of industrail structural mechanics problems using automatic differentiation. In G. Corliss, C. Faure, A. Griewank, L. Hascoët, and U. Naumann, editors, *Automatic Differentiation of Algorithms: From Simulation to Optimization*, pages 181 – 188, New York, 2002. Springer.

[4] H.W.Engl and P. Kuegler. Identification of a temperature dependent heat conductivity by tikhonov regurlaization. *J. of Inverse and Ill-Posed Problems 10*, 10:67–90, 2002.

[5] B. Kaltenbacher. On Broyden's method for the regularization of nonlinear ill-posed problems. *Numer. Funct. Anal. and Optimiz.*, 19:807–833, 1998.

[6] W. Mühlhuber. *Efficient Solvers for Optimal Design Problems with PDE Constraints.* PhD thesis, JK University of Linz, Austria, 2002.

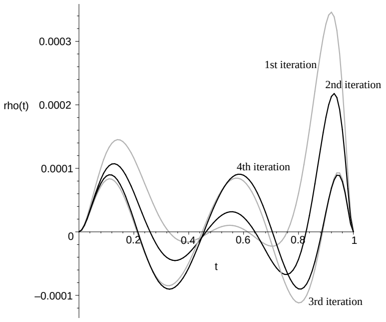
F 1315: Numerical and Symbolic Techniques for Algebraic Spline Surfaces

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

This project is devoted to computational techniques for implicitly defined curves and surfaces. The first two subprojects deal with conversion methods between implicit and parametric representations.

Approximate parameterization

J. Gahleitner developed a method for approximately parameterizing planar rational cubics [3]. After deriving a condition for rationality, he formulated this task as an best approximation problem, which can then be solved using a Remes–type algorithm in coefficient space (Fig. 10). The local and global existence of solutions to this best approximation problem has been analyzed using the classical theory of Meinardus and Schwedt



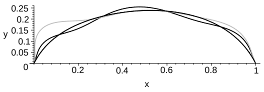


Figure 10: Using a Remez-type algorithm for approximate parameterization. Left: error functions; above: curves.

Currently, the research focuses on the use of monoid curves and surfaces, which are a special class of rational surfaces which are characterized by the presence of a single singular point with high multiplicity. It is expected that this leads to simpler computational algorithms.

Approximate implicitization

M. Shalaby developed several methods for approximate implicitization of planar curves [6, 7, 10], which are an alternative to exact methods (such as resultants or Gröbner bases) which have many associated problems, e.g., a high number of coefficients and the presence of unwanted branches. The methods consist of four steps:
(1) Find a quadratic B-spline approximation of planar curves via orthogonal projection in Sobolev spaces, using results from approximation theory.
(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) Join the segments according to the desired level of differentiability (C^0 or C^1).
An example for C^1 spline implicitization is shown in Figure 11. Note that the distribution of the algebraic parallels $f(x,y)=c$ depends on the parametric speed of the initial curve.

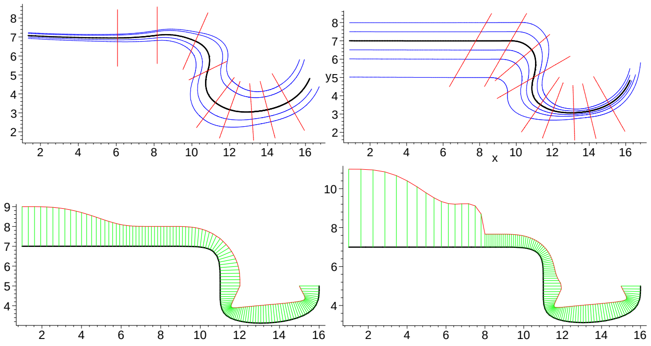


Figure 11: C^1 spline implicitizations (top) and parametric speed distribution (bottom).

The results of the implicitization process will now be exploited in order to generate a hierarchy of shapes, which may be useful for applications in FEM simulation.

Fairing and Fitting

P. Chalmovianský developed a method for variational design algebraic curve segments, via numerical minimization of appropriate functionals [1], using an SQP-type technique. The functional is based on the bending energy of a curve segment. In order to avoid singularities along the segment he used a suitable

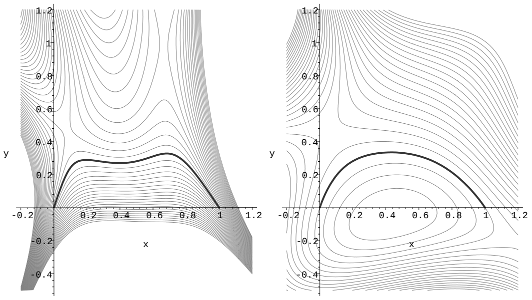


Figure 12: Fairing algebraic curve segments.

penalty function. As an application he described and implemented a “pulling tool”, which pulls the curve segment towards a fixed point in the plane. He also developed a method for detecting and filling holes in point clouds [2, 4]. Here, the aim is to improve the data generated by a 3D scanner, which may contain a lot of holes not present in the scanned solid. The algorithm consists of three steps: 1. identifying the neighborhood of an unwanted hole; 2. fitting an algebraic surface to those (G^1) data; 3. generating of points in the hole as sample points of the surface. The last step requires an approximation (triangulation) of the implicit surface and the detection of the part of the surface contained in a hole.

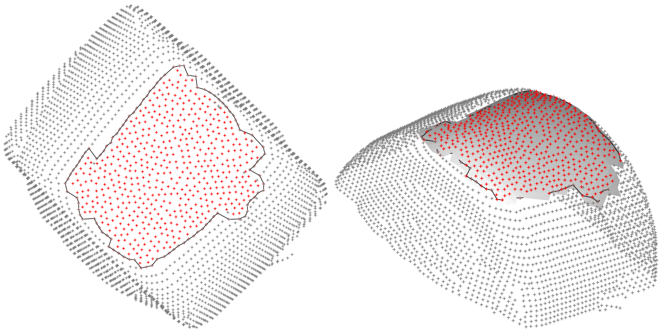


Figure 13: Filling holes via algebraic fitting.

Other activities

Related to previous work on so–called universal parameterizations, we constructed and analyzed special rational mappings for parameterizing cubic ruled surfaces [5], via line geometry. The different types of cubic ruled surfaces can be identified with a special line congruence, see Fig. 14. This leads to an associated rational mapping which can be used for parameterizing these surfaces (Fig. 15). Other activities include work on Hermite subdivision schemes, kinematics and computer animation [8, 9, 11].

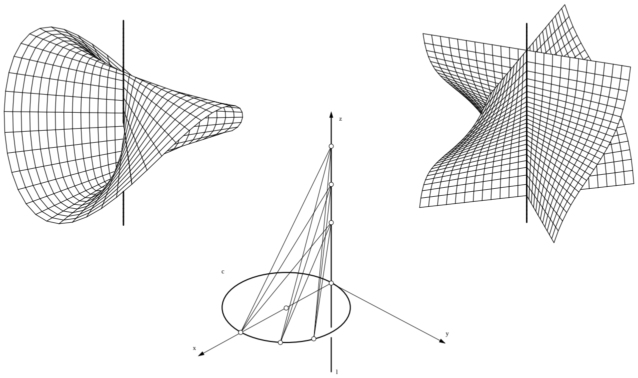


Figure 14: Types of cubic ruled surfaces and line congruence.

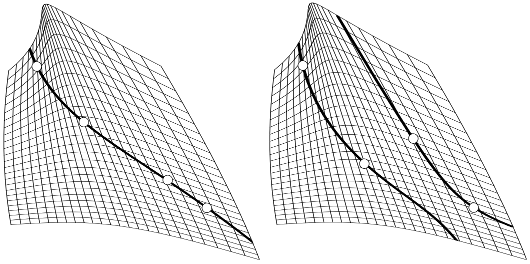


Figure 15: Interpolation on cubic ruled surfaces.

References

[1] P. Chalmovianský and B. Jüttler. Fairness criteria for algebraic curves. Dagstuhl Seminar on Geometric Modeling, submitted; also presented as talk at Austrian Conference on Geometry, St. Vorau, 2002.

[2] P. Chalmovianský and B. Jüttler. Filling holes in point clouds. manuscript, 2003.

[3] J. Gahleitner, B. Jüttler, and J. Schicho. Approximate parameterization of planar cubics. submitted to: Curves and Surfaces - St. Malo 2002, also presented as talk, 2003.

[4] B. Jüttler and A. Felis. Least–squares fitting of algebraic spline surfaces. *Advances in Computational Mathematics*, 17:135–152, 2002.

[5] B. Jüttler and K. Rittenschober. Using line congruences for parameterizing special algebraic surfaces. Submitted to Mathematics of Surfaces X, 2003.

[6] B. Jüttler, J. Schicho, and M. Shalaby. Spline implicitization of planar curves. Technical report, SFB Technical Report 02-23, 2002.

[7] B. Jüttler, J. Schicho, and M. Shalaby. Spline implicitization of planar curves. to appear in: Curves and Surfaces - St. Malo 2002, 2003. (also presented as talk).

[8] B. Jüttler and U. Schwanecke. Analysis and design of hermite subdivision schemes. *The Visual Computer*, 18:326–342, 2002.

[9] B. Jüttler and M. Wagner. Kinematics and animation. In *Handbook of Computer Aided Geometric Design (G. Farin et al., eds.)*, pages 723–748. Elsevier, Amsterdam, 2002.

[10] M. Shalaby, B. Jüttler, and J. Schicho. C1 spline implicitization of planar curves. Submitted to Automated Deduction in Geometry, 2002.

[11] K.-A. Sun, B. Jüttler, M.-S. Kim, and W. Wang. Computing the distance between two surfaces via line geometry. In *Proceedings of 10th Pacific Conference on Computer Graphics and Applications (S. Coquillart et al.,eds.)*, pages 236–245. IEEE Press, Los Alamitos, 2002.

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

Andreas Neubauer
Stefan Kindermann

1 Regularization by Surface Representations via the Moving Grid Approach

It is the aim of this project to develop efficient methods to identify discontinuous solutions in ill-posed equations. 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.

Due to the ill-posed nature, the solutions do not depend continuously on the data. Therefore, the problems have to be regularized. Most of the 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. This method has similar regularization properties as the well-known bounded variation regularization, as has been analyzed by us in the FWF-project P13130-TEC.

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 surfaces to represent discontinuous solutions, we numerically treated surface regularization by the method of Moving Grids. 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 grid size is small whenever the approximate solution has large gradient and vice versa. The construction of such a deformation function is classical in geometry (cf. [5]).

The combination of adaptive moving grids with regularization have been successfully applied to two-dimensional integral equations of the first kind (cf. [3]). With this technique the resolution of discontinuities was significantly better than with a comparable fixed grid algorithm.

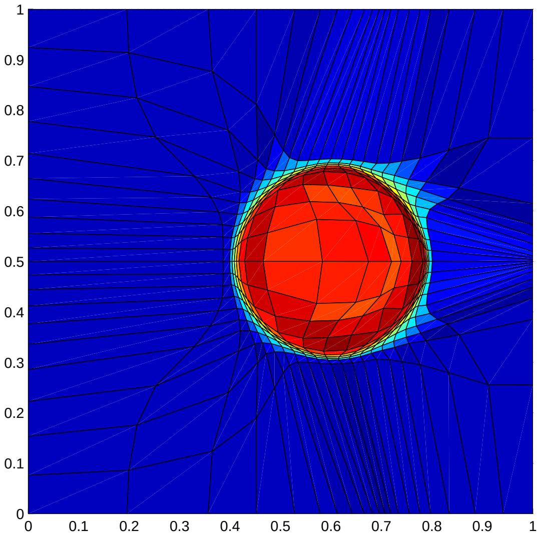


Figure 16: A solution of a linear integral equation having discontinuities on a circle

The project leader, Andreas Neubauer, was invited to present these new results at the Inverse Problems Conference in Hong Kong in January 2002.

As a further step, we applied this new approach also to two-dimensional nonlinear parameter identification problems. Since the combination with moving grids is not restricted to a special regularization method, we tried different ones. In view of an efficient numerical realization it turned out that it is better not to use Tikhonov regularization but iterative regularization methods. The iterative regularized Gauss-Newton method in combination with a conjugate gradient method yielded excellent results [2].

2 Regularization by Equations of Hamilton-Jacobi type

Starting from regularization for curve and surface representations an unexpected and interesting relation to recently developed and popular methods for

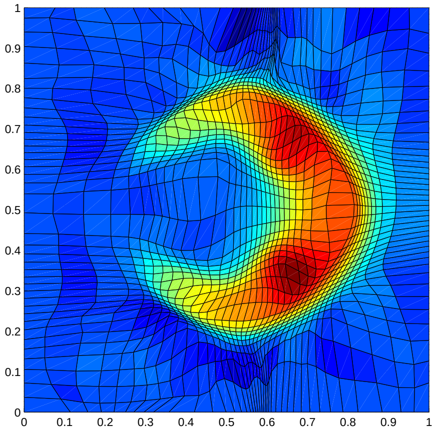


Figure 17: Identification of a function having discontinuities on a moon-shaped region

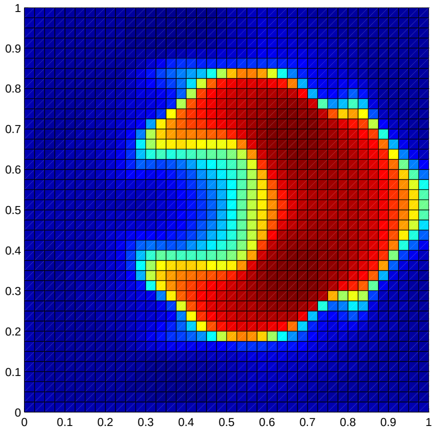


Figure 18: Same as Figure 17 using Regularization by HJ-Equation

ill-posed problems with discontinuous solutions popped up: instead of using the Lagrangian viewpoint of curve and surface representations as it has been done in the previous work we can look at the corresponding regularization in Eulerian variables.

For the Lagrangian variables approach the parameterization of the curve and surfaces are defined on a reference domain on which also the discretization and computation is done. Hence, the computed solution will always live on an adaptive grid. In contrast, in the Eulerian viewpoint we consider the evolution of the unknown solution itself on the domain where it is defined.

Taking the evolution equation of steepest descent for the regularization for curve and surface representations in Eulerian variables leads to an evolution equation of Hamilton-Jacobi type, which can be considered as a generalization of both the level-set method (cf., e.g., [1, 4]) and the well-known Landweber iteration.

Although this new method implicitly uses curve and surface parameterizations the resulting equation can be discretized on a fixed grid due to the Eulerian variables. For its discretization we used recently developed ENO-Schemes (cf. [6]) tailored to Hamilton-Jacobi equations.

Comparing this fixed-grid method to the adaptive grid method by moving grids we have the advantage that the numerical implementation becomes more simple and the new algorithm can quite easily be embedded into existing code for standard regularization methods. On the other hand, of course, an adaptive grid still allows more flexibility in the approximation of discontinuities.

This new approach has been presented at the Conference on Computational Methods for Inverse Problems in Strobl, August2002. Moreover, the method has been successfully applied to linear and nonlinear inverse problems. A report describing the results and the central ideas is in preparation.

References

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

[2] S. Kindermann and A. Neubauer. Parameter identification by regularization for surface representations via the moving grid approach. SFB-Report 02-10, University of Linz, 2002. submitted.

[3] A. Neubauer. Estimation of discontinuous solutions of ill-posed problems by regularization for surface representations: numerical realization via moving grids. In B. Hon, L. Cheng, J. Lee, and M. Yamamoto, editors, *Proceedings for International Conference on Inverse Problems*. World Scientific Publisher, 2003. to appear.

[4] F. Santosa. A level-set approach for inverse problems involving obstacles. *ESAIM, Control Optim. Calc. Var.*, 1:17–33, 1996.

[5] B. Semper and G. Liao. A moving grid finite element method using grid deformation. *Numer. Methods of PDEs*, 11:603–615, 1995.

[6] J. A. Sethian. A fast marching level set method for monotonically advancing fronts. *Proc. Natl. Acad. Sci. USA 93*, 4:1591–1595, 1996.

Report on the SFB Conference
“Computational Methods for Inverse Problems”
St.Wolfgang, August 25th – 31st, 2002

In August 2002 we organized an international conference on *Numerical Methods for Inverse Problems* in St.Wolfgang (Austria). Besides the conference we organized also a Mini-symposium on *Parameter Identification in Plasticity.* Both events were chaired by Prof. Heinz W. Engl who was also in charge for the organization.

The main goal of the conference on *Numerical Methods for Inverse Problems* was to present the newest results in

- Inverse Problems in Elasticity
- Inverse Problems in Imaging
- Medical Imaging
- Shape Optimization
- Inverse Scattering
- Level Set Methods
- Numerics for Inverse Problems
- Discrete Inverse Problems

and to give young scientists (mainly from the SFB) the chance to present their newest results to the acknowledged scientists in this field.

To reach this aim we invited 18 experts in the field *Numerical Computation and Inverse Problems*:

- U. Ascher (University of British Columbia, Canada), “Computational methods for large distributed parameter estimation problems in 3D”
- H.T. Banks (North Carolina State University, USA), “Incorporation of Uncertainty in Inverse Problems”
- M. Bendsøe (Technical University of Denmark, Denmark), “Inverse Homogenization - On the Design of Periodic Composites”
- M. Bertero (University of Genova, Italy), “An overview of image restoration in astronomy”
- L. Borcea (Rice University, USA), “Optimal finite difference grids for direct and inverse Sturm Liouville problems”
- D. Calvetti (Case Western Reserve University, USA), “Iterative Methods for Tikhonov Regularization”
- M. Hanke (Tomography University of Mainz, Germany), “Reconstructing smaller and larger inhomogeneities with Electrical Impedance”
- T. Hohage (University Göttingen, Germany), “Regularization of Large-Scale Exponentially Ill-Posed Problems”
- C. Johnson (University of Utah, USA), “Inverse Bioelectric Field Problems: Modeling, Simulation, and Visualization”
- J. McLaughlin (RPI, USA), “Finding Stiffness Variations in Human Tissue”
- R. Plemmons (Wake Forest University, USA), “Integrated Optics for Image Quality Control”
- L. Reichel (Kent State University, USA), “Iterative Methods for Large-Scale Non-Selfadjoint Ill-Posed Problems”
- W. Rundell (Texas A&M University, USA), “Some new inverse eigenvalue problems”
- E. Sachs (University of Trier, Germany), “Inverse Problems in Financial Applications of Optimization”
- O. Scherzer (University of Innsbruck, Austria), “Non-convex regularization”
- J. Schicho (Johannes Kepler University of Linz, Austria), “Parameterization, an Ill-Posed Problem in Computer Algebra”
- E. Somersalo (Helsinki University of Technology, Finland), “Structural Prior Information in Computational Inverse Problems”
- X-C. Tai (University of Bergen, Norway), “Level-set method with TV-norm regularization for the identification of some discontinuous coefficients”

and placed 17 (10 SFB talks) contributed talks of young scientists between the invited talks. The abstracts of all talks are available as a booklet [1]. Abstracts as well as the slides of most talks are available at our conference page:
http://www.sfb013.uni-linz.ac.at

⟶ **SFB Conferences**

⟶ **SFB-Conference on ”Computational Methods for Inverse Problems”**

As a second event at the conference we had the mini-symposium about *Parameter Identification in Plasticity*, also organized and chaired by Prof. Heinz W. Engl together with Dr. N. Petrinic (Oxford, England). This mini-symposium intended to present a quite new and challenging practical problem from engineering science to mathematicians. The following invited speakers addressed this new field.

- I. Herle (University of Innsbruck, Austria), "Calibration of hypoplastic constitutive equations"
- R. Kreißig (University of Chemnitz, Germany), Parameter identification of elastic-plastic deformation laws by the analysis of inhomogeneous strain states"
- N. Petrinic (University of Oxford, England) "Multi-Action Inverse Modeling of Material Response to Impact Loading"

The more than 50 participants of the conference on *Computational Methods for Inverse Problems* and the mini-symposium on *Parameter Identification in Plasticity* considered the conference a great success. Let us conclude wit the remark by Prof. Joyce McLaughlin: *It is a good idea to give young scientists the chance to talk in front of so many experienced scientists.*

References

[1] H. Engl, *Abstracts of the Conference "Computational Methods for Inverse Problems"*, St. Wolfgang, August 25-31, 2002.

- **Symbolic Methods in Numerics and Geometry:**
  In the element preconditioning technique developed in subproject 1306, 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 optimization 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 inequalities 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 1308.

  In the other direction, we used some regularization techniques investigated in subproject 1308 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/`.

  There has also been an intensive cooperation with subproject 1316, developing new symbolic and numerical algorithms for parameterization and implicitization of algebraic curves and surfaces: we developed symbolic-numerical methods for spline implicitizations of parametric curves, and for the approximate parameterization of planar cubic curves.

- **Curves and Surfaces:**
  Within the SFB we have had an intensive cooperation with U. Langer in editing the proceedings of SNSC’01. With B. Jüttler and J. Schicho we have cooperated on research on algebraic curves and surfaces. The work on generating minimal surfaces has led to an intensive cooperation with M. Burger.

- **Summation in Theorema:**
  Most of the results achieved with respect to summation methods are directly related to Project F1302 “Proving and Solving in General Domains”. The general object is to integrate the software packages developed by the SFB group F1305 into the Theorema system as “black box” provers. A major step forward into this direction has been achieved by C. Schneider. He has been invited to the IMA Minneapolis Conference “Special Functions in the Digital Age” where he presented a talk and a computer demo illustrating the interaction of his summation package Sigma with Theorema.

- **Wavelets:**
  The wavelets collaboration of the first SFB period between F1305 and the project F1310 of O. Scherzer (which has terminated after the first phase of the SFB) emerged in a second publication “Wavelets with scale dependent properties”. There, motivated by the previous work, new types of wavelets are introduced.

- **Orthogonal Polynomials in Numerics:**
  Within the context of finite element methods and related to U. Langer’s SFB group F1306, a very promising collaboration has been started. An important subproblem of a particular approach is the following. One chooses a suitable polynomial basis on the face of a tetrahedron. If one simply took monomials, the corresponding matrices would be badly conditioned. A better choice are suitable families of orthogonal polynomials. The main task then is to ex-

tend the ansatz from the face to the interior of the tetrahedron. To this end, various transformations of orthogonal polynomials can be applied. Since such polynomials have a representation in the form of terminating hypergeometric sums, it is a natural idea to apply tools developed in the SFB group F1305. Indeed, first results show that the package MultiSum, in particular, its refined version due to A. Riese and B. Zimmermann, does play a substantial role in discovery and proving. Moreover, it seems that by using recurrences delivered by MultiSum, one can compute "good" basis functions in a simple and fast manner. Currently further, more detailed investigations are on their way.

- **Summation in Finite Elements:**
  Prof. P. Paule and Dr. J. Schöberl started to apply hypergeometric summation techniques as developed in F1305 for the construction of high order finite elements as used in F1306. High order finite elements are usually defined by recursive polynomials, e.g. Legendre polynomials. Often, some operations such as differentiation or averaging is needed. By now, it was good luck to find a recursive representation of the result. Hypergeometric summation provides a systematic way to derive recursive formulas for the desired operations.

- **Symbolic Methods in Hilbert Spaces:**
  The symbolic-numerical cooperation within the SFB F013 has entered a new stage in October 2001, when the project group F1302, as a typical representative of the "symbolic side", and the project group F1308, as a typical representative of the "numerical side", have started a series of joint seminars, soon to be known by the picturesque name *Hilbert seminars.* In fact, the name of Hilbert is a very adequate metaphor of the symbolic-numerical cooperation, since this outstanding German mathematician has achieved enormous progress on both sides alike.

  It was in the stimulating atmosphere of these Hilbert seminars that we came across an interesting topic linking our fields on a nontrivial basis, namely *operator theory via noncommutative polynomials.* But before we go into the details of this topic, let us briefly outline the chronological development leading to it.

  The Hilbert seminars were initiated through a *series of lectures* given by the two principal investigators. Prof. Buchberger talked about "Predicate Logic as a Working Language", explaining the practical aspects of symbolic logic and as the linguistic framework underlying both traditional mathematics and automated proof assistants such as the Theorema system [1], developed within F1302. Prof. Engl gave a short "Introduction to Regularization Theory" [5], focusing on the role of the Moore-Penrose inverse as a convenient formulation for the most common regularization strategies. The ensuing discussions on linking the potential of both groups received a new impetus when Prof. Buchberger suggested the *operator paper* [6] for closer investigation.

  The essential point of this paper is the usage of non-commutative Gröbner bases for *simplifying* complicated terms arising in operator theory. In the next seminar, Markus Rosenkranz presented a new approach that uses Gröbner bases for *solving* linear boundary value problems; the whole procedure was exemplified in the simple classical BVP $y'' = f, y(0) = y(1) = 0$, see Section 2 in [13]. In principle, this turn was rather consequent: If powerful (non-commutative) polynomial methods from computer algebra, like Gröbner bases [2], can be used for simplifying terms, why not use them also for solving equations? The crucial question was how to bridge the gap between operator-based equations and non-commutative polynomial theory. This missing link between operator theory and computer algebra was provided through the oblique Moore-Penrose equations. A detailed exposition of the theory can be found in Section 1 of [13]; see also [8, 10, 11, 12].

  The unique feature in our method is that we approach BVP *on the level of operators* rather than functions. To our knowledge, all the traditional methods (for example, see page 189 in [7]) compute the Green's function g directly, essentially by evaluating certain functional determinants containing the fundamental system and the boundary conditions. This approach, though elegant and self-contained, has at least two drawbacks:

  - On the theoretical side, one often gets *more insight* by understanding the structure of the operators rather than that of the functions that may be used to define them. In some sense, the "real" solution of a BVP is the Green's operator G; the Green's function g (if available!) is merely one way to describe G, namely as an integral operator with kernel g.
  - On the practical side, the costs for computing functional determinants soon become prohibitive. We have not yet started to analyze the *complexity* of our method, but there is some hope that it will outperform the determinant-based approach

at least for the case of linear differential operators with constant coefficients.

Viewing *BVP in an operator setting* is very much in the spirit of numerical analysis. Many convergence proofs use powerful results from functional analysis, which typically involve operators on suitable Sobolev spaces. The operator-theoretic viewpoint, however, is equally useful for making BVP amenable to effective methods of computer algebra: Interpreting the Moore-Penrose equations as non-commutative polynomial equations with certain operators as indeterminates, one gains safe ground for symbolic methods. In particular, many crucial questions about (commutative as well as non-commutative) polynomials are answered exhaustively by the powerful theory of Gröbner bases [2].

The operator-theoretic viewpoint has been introduced into other parts of computer algebra as well, notably in the field of special functions and differential equations, where it is intimately associated with the *theory of holonomy* [4]. It has proven to be a powerful computing and proving tool in this field, which is also strongly linked to the subproject F1305. The main difference to the approach described here is that solving a differential equation means "hunting" for a function; operators are only used as an intermediate device for specifying this function, the functional coefficients of the differential operator, and other relevant functions. The basic idea of holonomy is that many special functions—the holonomic ones—can be defined by stating suitable operators that annihilate them. Solving a BVP, however, means "hunting" for an operator and studying questions of inversion rather than annihilation.

Looking at the introductory chapter of [13], one may actually wonder why this simple but powerful link has not been perceived clearly before. Such a question is of course always difficult to answer. However, one thing seems to be quite clear: Due to the *traditional separation of the symbolical and numerical communities*, there is a certain lack of knowledge about the material from the "other" side. On the one hand, the numerical analysts know—among many other things— the power of the Moore-Penrose theory, but they might fail to appreciate the far-reaching polynomial methods available to modern computer algebra. The mathematicians from the side of symbolic computation, on the other hand, do know a lot about polynomial algorithms—and numerous other algebraic manipulations—while they often have a rather limited knowledge about the tools of functional analysis relevant for numerical mathematics. This may at least serve as a partial explanation.

Finally, we should also mention that in the meantime, there are already promising new results [9], to be presented in the ongoing PhD thesis [14]. The article [13] describes the state of research as of summer 2002, offering a solution "method" that needed some creative input at critical stages of the computation. Using our new results, this method can be greatly simplified and turned into a *full algorithm*, at least for the case of differential operators with constant coefficients. In fact, Markus Rosenkranz has implemented the whole algorithm for this case within the frame of Theorema system [1].

- **Algebraic Spline Curves and Surfaces:** We continued the collaboration 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 entitled "Algebraic Spline Curves and Surfaces" took place during both semesters.
- **Automatic Simplification of Domains:** We started to establish a cooperation with between G. Haase and B. Jüttler, about automatic simplification of domains for FEM. This will be further pursued in the final year of the second funding period.

References

[1] B. Buchberger, C. Dupre, T. Jebelean, F. Kriftner, K. Nakagawa, D. Vasaru, W. Windsteiger. *The THEOREMA Project: A Progress Report.* In: M. Kerber and M. Kohlhaase (Eds.), Symbolic Computation and Automated Reasoning (Proceedings of the Calculemus 2000 Conference, August 6-7, 2000, St. Andrews, Scotland), A. K. Peters, Natick, Massachusetts, 98–113.

[2] B. Buchberger, Franz Winkler (Eds.), Groebner Bases and Applications. London Mathematical Society, Lecture Note Series 251, Cambridge University Press 1998.

[3] M. Burger, R. Pinnau, *Fast optimal design of semiconductor devices*, University Linz, (2002), SFB Report 02-29, submitted.

[4] Frédéric Chyzak, Bruno Salvy. Non-commutative Elimination in Ore Algebras Proves Multivariate Identities, *Journal of Symbolic Computation*, **11**, 1997.

[5] Heinz W. Engl. Regularization methods for the stable solution of inverse problems, *Sur-*

veys on Mathematics for Industry, **3**(1993), 71–143.

[6] J. William Helton, Mark Stankus, John Wavrik. Computer Simplification of Engineering Systems Formulas, *IEEE Trans. Autom. Control* **43**(3), 1998, 302–314.

[7] Erich Kamke. Differentialgleichungen, Volume I. Teubner, Stuttgart, tenth edition, 1983.

[8] Markus Rosenkranz. *A Gröbner Bases Approach Towards Solving Linear BVP.* Statusquo report in: SFB Status Seminar, Strobl, Austria, April 26, 2002.

[9] Markus Rosenkranz. *Green Polynomials*, talk given in the Hilbert Seminar, Johannes Kepler University, January 15, 2003.

[10] Markus Rosenkranz, Bruno Buchberger, Heinz W. Engl. *Computing the Moore-Penrose-Inverse by Gröbner Bases.* Contributed Talk in: Conference on Computational Methods for Inverse Problems, Strobl, Austria, August 27, 2002.

[11] Markus Rosenkranz, Bruno Buchberger, Heinz W. Engl. *Solving Linear Boundary Value Problems via Non-Commutative Gröbner Bases.* Contributed Talk in: Fourth International SYNASC Workshop, Timisoara, Romania, October 9-12, 2002

[12] Markus Rosenkranz, Heinz W. Engl. *Solving Linear Boundary Value Problems via Non-Commutative Gröbner Bases.* Contributed Talk in: Symposium in Honor of Bruno Buchberger's 60th Birthday, Logic, Mathematics and Computer Science: Interactions (LMCS'2002). Hagenberg, Austria, October 20-22, 2002.

[13] Markus Rosenkranz, Bruno Buchberger, Heinz W. Engl. Solving Linear Boundary Value Problems via Non Commutative Gröbner Bases. Accepted in the journal *Applicable Analysis.*

[14] Markus Rosenkranz. *Symbolic Solution Methods for Linear Boundary Value Problems* (working title). PhD Thesis, in preparation.

[15] Franz Winkler and Manasi Athale. ADG'2002 – Automated Deduction in Geometry – Abstracts Booklet. RISC Tech Report 02-20, Research Institute for Symbolic Computation, Johannes Kepler University, 4040 Linz, Austria, 2002.

[16] Winkler, F., and Langer, U. (eds.). Symbolic and Numeric Scientific Computation. Proceedings of the Conference SNSC'01. To appear.

SFB F013: Numerical and Symbolic Scientific Computing

National and International Cooperations

1 Cooperations with other Research Institutions

- **Institute e-Austria Timisoara.**
  The Theorema group is currently involved in a project consisting of the design and implementation of methods for program verification using automated reasoning. This project is developed in cooperation with the Institute e-Austria in Timisoara, on the period Oct.2002 - Sep.2003. The results of this research are to be applied in concrete industrial environments inside software companies in Romania and Austria. Currently we are in contact with Alcatel-Timisoara and Sanguaro-IBM-Timisoara for a possible application of program verification techniques during software development and testing.

- **Mathematical Knowledge Management.**
  Theorema is involved in an European project concerning this subject. In the frame of this project we are also contacting industrial partners which are interested to apply MKM techniques for solving certain problems which occur in their area of activity: publishing houses, creators of mathematical software, etc. (See more details in the section on international cooperation.)

- **SSWCC.**
  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 included practical applications of the models developed using the *Theorema* system.

- **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).

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

- **Texas A&M University, College Station, USA:** U. Langer (F1301, F1306) visited the Texas A&M University (TAMU) in the Summer semester (February - May 2002) as guest professor. He cooperated with J. Bramble, R. Lazarov, J. Pasciak from the TAMU on different topics.

- **St. Petersburg State Polytechnical University, Russia:** V.G. Korneev (St. Petersburg), G. Haase (F1301), and U. Langer (F1301) worked on domain decomposition methods in the Research-in-Pairs Program of the Mathematical Research Institute Oberwolfach (28 July - 21 September 2002). Several publication are in work.

- **University of Kentucky, Lexington, USA:** C. Douglas (Lexington), G. Haase (F1301), and U. Langer (F1301) finished their work on a book about elliptic PDE solvers and their parallelization. The book will be published by SIAM (USA) in 2003.

- **University of Erlangen, Germany:** U. Langer (F1301), J. Schöberl (F1301), M. Hofer (Erlangen) and R. Lerch (Erlangen) continued their cooperation on piezo-electric device simulation. Several joint talks and proceedings papers were presented.

- **University of Stuttgart, Germany:** O. Steinbach (Stuttgart) and U. Langer (F1301) are cooperating on boundary element domain decomposition methods. They gave a joint talk at the Oberwolfach conference on "New Trends in Boundary Elements" (December 2002) and published a first joint paper as SFB-Report Nr. 02-41. Further publications are in work.

- 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 Innsbruck, University of Sevilla:**
  The algorithms and programs for singularity analysis developed in our subproject are of great interest and relevance for the current attempts to solve long-open problems in this field. In order to intensify the research on this important matter, we have started an OeAD project together with F. Paco-Jímenez from the university of Sevilla and an FWF project together with H. Hauser from the university of Innsbruck. G. Bodnár is now working in this FWF project, but he will of course continue to work in close cooperation with the SFB.

- **University of Sydney:**
  We started to implement our algorithms for surface parametrization in the computer algebra system MAGMA, which is maintained and distributed by J. Cannon. This cooperation will continue in 2002, also jointly with G. Brown from the University of Warwick.

- **University of Passau:**
  Since 1999, there is a joint seminar with the Computer Algebra group around V. Weispfenning, which was continued.

- **Workshop on Automated Deduction in Geometry:**
  In September 4–6, 2002, F. Winkler has organized and chaired the *International Workshop on Automated Deduction in Geomety (ADG'02)*. This series of workshops, started in 1992 in Schloss Weinberg in Käfermarkt (Austria), and continued in Toulouse (1996), Beijing (1998), and Zürich (2000), has become an important forum for presenting new computational methods in geometry and for demonstrating geometric software tools. Applications to computer aided geometric design, computer vision, and geometry education are discussed in these workshops. A booklet of abstracts is available [15]. We have an agreement with Springer Heidelberg to publish proceedings of the conference in the series Lecture Notes in Computer Science.

- **Editing proceedings of SNSC'01:**
  In September 2001 F. Winkler has organized and chaired the SFB Conference *Symbolic and Numerical Scientific Computing (SNSC'01)*. The proceedings are currently being edited by F. Winkler and U. Langer [16], and will be published by Springer Heidelberg as Lecture Notes in Computer Science 2630.

- **Diophantine analysis:**
  In the frame of this project we have had intensive cooperations with Prof. J.R. Sendra (Madrid), Prof. H.J. Stetter (TU Wien), Prof. J. Apel (Leipzig), and the Department of Mathematics of the University of Debrecen (Hungary). Our parametrization algorithms have led to applications in Diophantine analysis, and we have had Profs. D. Poulakis and E. Voskos from Thessaloniki, Greece, as guests to discuss these common interests.

- **University of Waterloo:**
  During September 2002, Prof. Paule was ORCCA Chair Professor at the Department of Computer Science at the University of Waterloo (Ontario, Canada), following an invitation of Prof. Keith Geddes.

- **University of the Witwatersrand:**
  During September 2002, Dr. Schneider was visiting researcher at the John Knopfmacher Centre for Applicable Analysis and Number Theory at the University of the Witwatersrand (Johannesburg, South Africa), following an invitation of Prof. Helmut Prodinger.

- **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). In 2002 the first scientific exchange visits started: L. Meunier to RISC (November), and P. Paule to INRIA (December).

- **Texas Institute for Computational and Applied Mathematics (TICAM):**

Prof. L. Demkowicz: Joachim Schöberl works together with L. Demkowicz on multigrid for *hp* finite elements and Maxwell equations, a joint publication is in preparation. Visit of J.S. in Texas.

- **University Valenciennes, France:**
  Prof. S. Nicaise: J. Schöberl works together with S. Nicaise on anisotropic finite elements for Maxwell equations, joint publications, joint publication in preparation. Visit of J.S. in Valenciennes.
- **ETH Zürich:**
  Prof. Ch. Schwab: J. Schöberl works together with Ch. Schwab and his coworkers on *hp* finite elements. Visit ov J.S. in Zürich.
- **Technical University of Dresden:**
  Prof. Dr. Andreas Griewank, Dr. Andrea Walther and Olaf 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 **(University of Cantabria, Spain; University of Nice and INRIA, France; think3, Italy, University of Oslo, Norway)** are involved in a IST–FET research project within the Fifth Framework Programme of the European Commission. After completing the contract negotiations, the projected has started on July 1st, 2002.
- **Seoul National University (Korea):**
  We continued the cooperation on issues of visualization and computer animation with Prof. Myung–Soo Kim (Seoul). This lead to a joint publication "Computing the distance between two surfaces via line geometry" which was presented at the 10th Pacific Conference on Computer Graphics.
- **The University of Hong Kong (China):**
  Prof. Jüttler authored a joint paper with Prof. Wenping Wang on "The shape of spherical quartics".
- **Arizona State University (USA):**
  Prof. Jüttler authored a joint paper with Prof. Wagner on "Kinematics and Animation".
- **Daimler Chrysler Research (Germany)**
  Prof. Jüttler authored a joint paper with Dr. Schwanecke on "Analysis and Design of Hermite subdivision schemes".

2 Guests

- **Dr. Li Deng:** Japan Research Institute, Ltd., Japan, January 5 - 9,2002. Talk on "Perturbation Analysis of Eigenvalue Problem for Structural-Acoustic Coupled System".
- **Dr. Viorel Negru:** Western University of Timisoria, RO, January 25 - Feb 4. Cooperation with F1302.
- **Dr. Dana Petcu:** Western University of Timisoria, RO, January 25 - Feb 4. Cooperation with F1302.
- **Dipl.-Math. Günther Of:** University of Stuttgart, Germany, March 10 - 15, 2002. Talk on "Die Multipolmethode für die symmetr. Randintegralformulierung".
- **Dr. Manfred Kaltenbacher:** University of Erlangen, Germany, March 18 - 22, 2002. Talk on "Numerische Simulation mikromechanischer, elektrostatischer Sensoren und Aktoren".
- **Prof. Dr. Roman Chapko:** University of Liv, Ukraine, May 2 - 31,2002. Talk on "Über die numerische Lösung von direkten und inversen Anfangs-Randwertproblemen mit Hilfe der Integralgleichungsmethode".
- **Dr. Kim Knudsen:** University of Aalborg, Denmark, May 9 - 14, 2002. Talk on "Reconstruction of Conductivities from Boundary Measurements".
- **Prof. Dr. Craig Douglas:** University of Kentucky, USA, May 14 - 20, 2002. Talk on "Modeling and Computation of Sea Surface Heights in Complex Domains".
- **S. Encinas:**, University of Valladolid, 7.3.2002-14.3.2002, and 11.12.2002-18.2.2002. He worked together with G. Bodnár and J. Schicho on an new implementation of the *desing* package in the computer algebra system Singular. S. Encinas was here on behalf of the ÖeAD project.
- **S. Basu:**, University of Atlanta, **R. Pollack**, University of New York, and **M.-F. Roy**, University of Rennes, 25.5.2002-6.6.2002. They delivered various talks on the field of real algebraic geometry.
- **G. Brown:**, University of Warwick, September 2002. He worked together with J. Schicho on an algorithm for computing adjoints of surfaces based on toric resolution. This is ongoing research. He also gave a talk at the conference LMCS 2002.

- **V. Weispfenning, I. Mazucco, A. Dolzmann, T. Sturm, A. Seidl:**, University of Passau, 4.6.2002. In the frame of a joint seminar with the University of Passau, they delivered various seminar talks.

- **Prof. E. Neuwirth:** University Vienna, Austria, 16.1.02. Talk on "Extending Galton's board: Recursive combinatorial functions and Linear Algebra".

- **Dr. J. Lebrun:** Sophia Antipolis, France, 12.–15.3.02. Talk on "Balancing multiwavelets using Gröbner bases".

- **Prof. H. Prodinger:** University of the Witwatersrand, Johannesburg, South Africa, 16.–22.6.02. Joint research; talk on "Digits and Beyond".

- **Prof. J. Louck:** Los Alamos National Laboratory, USA, 2.–6.9.02. Joint research.

- **Prof. D. Zeilberger:** Rutgers University, USA, 19.–23.10.02. Invited participant at the "LMCS '02" conference.

- **L. Meunier:** INRIA-Paris, France, 18.11.–6.12.02. Joint research; talk on "The Encyclopedia of Special Functions".

- **Dr. Olaf Steinbach:** University of Stuttgart, Germany, July 10 - 14,2002. Talk on "Hybride Gebietszerlegungsmethoden".

- **Prof. Dr. G. C. Hsiao:** University of Delaware, USA, July 10 - 14,2002. Talk on "On the Two-dimensional Inverse Scattering Problems in Electromagnetics".

- **Prof. Dr. V. G. Korneev:** St. Petersburg State University, Russia, July 17 -28,2002. Talk on "Fast Domain Decomposition Solvers for hp-Finite Element Version".

- **DI Dalibor Lukas:** University of Ostrava, Czech Republic, August 18 - 25,2002. Talk on "On a Numerical Solution to a 3-D Optimal Shape Design Problem of Homogeneous Electromagnets and the Existence Result".

- **Dr. Rene Pinnau:** TU Darmstadt, Germany, September 23 - 28, 2002. Talk on "Optimale Randsteuerung in der Glasproduktion".

- **Dr. Nicoleta Bila:** University of Cambridge, UK, October 7 - 31,2002. Cooperation with F1308.

- **Prof. Dr. Hoon Hong:** October 19 - 23, 2002. Cooperation with F1302.

- **D.Phil. Benjamin Elliott:** University of Oxford, UK, November 17 - 30, 2002. Talk on "Parameter Optimisation in Material Constitutive Models - Background and the Engineering Perspective".

- **Prof. Dr. Dimitrios Poulakis:** Aristotle University, Thessaloniki, Greece, November 17 - 24,2002. Cooperation with F1304.

- **Dr. Evaggelos Voskos:** Aristotle University, Thessaloniki, Greece, November 17 - 24,2002. Cooperation with F1304.

- **Dr. Zbynek Sir** (Charles University, Prague, January 2003). Dr. Sir worked with Prof. Jüttler on Pythagorean hodograph curves.

- **Prof. Gershon Elber** (Technion, Haifa, January 2003). Prof. Elber gave a talk about "Adaptive Isocurves Based Rendering" and discussed with Prof. Jüttler about a possible joint attempt towards a EU project.

- **Mag. Katharina Nevrla** (Charles University of Prague, March 2002), Cooperation

- **Mag. Elmar Wurm** (TU Graz, Austria), March 2002, Talk on "Four bar mechanisms"

- **Mag. Zbynek Sir** (Charles University of Prague, April, 2002) Talk on "The Penrose transformation")

- **Mag. M. Hofer** (University of Vienna, Austria, April 2002) Talk on "Geometric Positioning Problems",

- **Dr. Martin Peternell** (TU Vienna, Austria, November 2002), Research (implicitization in line space)

- **Prof. Dr. Alexander Pasko** (Hosei University, Japan, September 2002), Talk on "The Hyperfun Project"

3 Lectures at other Universities

- **Tudor Jebelean,** University of Timisoara, Romania. 11 - 15 Feb 2002. Blocked lecture (8 hours) on automated reasoning techniques and their implementation in Theorema.

- **Tudor Jebelean**, University of Cluj, Romania. 18 - 23 Feb 2002. Blocked lecture (8 hours) on automated reasoning techniques and their implementation in Theorema.

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

- **J. Schicho** gave a lecture "Algebraic Geometry on the Computer" at the university of Innsbruck, winter term 2002/03.
- **Prof. P. Paule:** Symbolic Summation: Creative Telescoping Revisited", University of Waterloo, Ontario, September 2002.
- **Prof. P. Paule:** "MacMahon's Partition Analysis and the Omega Package", University of Waterloo, Ontario, October 2002.
- **Dr. C. Schneider:** "Symbolische Summation in Differenzen-Körpern, University Leoben, Austria, January 2002.
- **Dr. C. Schneider:** "Sigma: A Summation Package for Discovering Sum Identities", University of Stellenbosch, South Africa, September 2002.
- **Dr. C. Schneider:** "Sigma: A Summation Package for Discovering Sum Identities", University of the Witwatersrand, Johannesburg, South Africa, September 2002.
- **Dr. C. Schneider:** "Sigma: A Summation Package for Discovering Sum Identities", University Graz, Austria, December 2002.
- **Prof. H.W. Engl**: Identification of parameters in polymer crystallization, semiconductor models and elasticity via iterative regularization methods. Lomonossov University Moskow, Russia, Juli/Augusust 2002.
- **Dr. G. Haase** was instructor at the "Int. Workshop on Industrial Mathematics" (modelling week) held in Bombay (India), Dec. 2-6, 2002.
- **Prof. U. Langer** delivered three lectures on "Computational Electromagnetics" in the lecture series "Frontiers in Mathematics" at the Taxas A&M University, College Station, USA, March 19-21, 2002.
- **Prof. U. Langer** delivered seven lectures on "The Schwarz Machinary and Domain Decomposition Methods" at the Technical University Dresden, Dresden, Germany, June 27 - July 5, 2002.

SFB F013: Numerical and Symbolic Scientific Computing

Transfer of Knowledge and Technologies

1 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.

2 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. The project is organized into several tasks, and our group plays an important role in two tasks *(a) enhancing computer algebra systems with reasoning power* and *(b) computer aided editing of mathematical texts.* In the frame of task *(a)* we enhanced our existing provers and added new ones to the *Theorema* system (see section describing the subproject F1302), which is implemented on top of the computer algebra system *Mathematica.* In the frame of task *(b)* we continued to include in the *Theorema* system the appropriate capabilities concerning: display of mathematical formulae in natural style (including two dimensional notations and even the possibility of defining new logico-graphic symbols), organization of mathematical knowledge, display of mathematical proofs in natural style and in natural language. We are currently developing several case studies (theory of Hilbert spaces, theory of tuples, theory of integers) which are written in the style of mathematical textbooks, including (besides explanatory texts) the complete formalization of the notions in higher-order logic, as formulae which can be used by the system for computations and for proving.

As a special Calculemus-activity, the Calculemus Autumn School was held in Pisa, Italy, from September 23 till October 4, 2002. The school consisted of several introductory lectures in the area of Computer Algebra and Automated Deduction and was accompanied by tutorials of available software systems in the two fields. The event did bring together an impressive number of experts from the research field of Computer Algebra and Deduction Systems. The goal was to train young researchers, high school teachers, and representatives from industry on the state-of-the-art research and current systems in this field. All together, there were 72 participants at the school. The *Theorema* group was actively present by two lectures (B. Buchberger and W. Windsteiger), a system tutorial by W. Windsteiger, and 4 students among the regular participants.

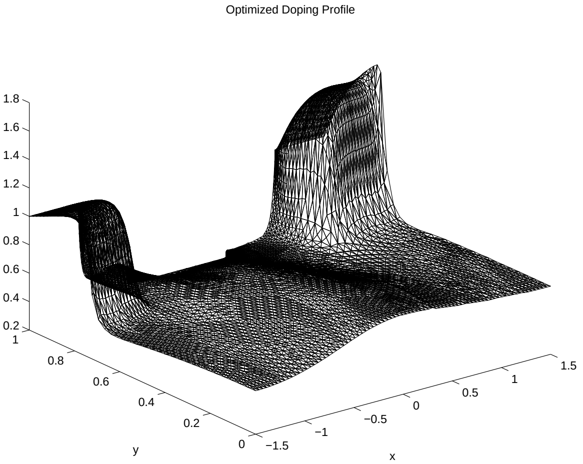
3 Mathematical Knowledge Management

This is a new field in mathematics with high potential of becoming one of the crucial prerequisites for the further development of mathematics: A significant amount of effort and money is spent for the invention of new mathematical facts and methods but it becomes harder and harder to organize and retrieve what had been invented and, thus, lots of efforts and funds are spent in vain. Knowledge management on the basis of the textual presentation of mathematical knowledge is not the answer. It becomes clear that sophisticated mathematical methods based on automated theorem proving and symbolic computation are necessary in order to provide a new generation of mathematical knowledge management systems. The work done within the SFB 1302 project (Theorema) appears to become an important basis for the new field of mathematical knowledge management. As a consequence, the first international workshop on Mathematical Knowledge Management (a term coined by B. Buchberger at the occasion of organizing this workshop) was organized at RISC, Hagenberg, Austria, in September 2001. This workshop did not only attract respresentatives of the international groups that represent the various possible mathematical and logical approaches to the area of mathematical knowledge management but also representatives of the publishing industry and institutions who organize mathematical indices, handbooks, and libraries. Also, at this occasion and subsequent meetings, a Thematic Network on Mathematical Knowledge Management within the EU was created and it was decided to organize international conferences on Mathematical Knowledge Management on a regular basis. Correspondingly, already a second international conference on Mathematical Knowledge Management took place (Bologna, February 15 - 19). Furthermore, by the efforts of B. Buchberger as a delegate of the Theorema Group, Mathematical Knowledge Management was introduced as an official theme in the formulation of the document on 'Future RTD Work in the Field of Digital Content, Knowledge, and Interface Technologies' of the EU Directorate-General on Information Society.

4 Inverse Problems for Semiconductor Devices

In collaboration of the project F 1308 with Peter Markowich (University Vienna), Paola Pietra (CNR Pavia) and Rene Pinnau (Technical University Darmstadt), inverse problems appearing in the design and characterization of semiconductor devices are investigated. M.Burger and P.Markowich are currently preparing a paper on the identification of doping profiles from transient measurements of the currents and capacitances in a device. The transient identification process is an inverse problem of extremely large-scale, already the direct problem consists in a several (stiff) nonlinear systems of parabolic and elliptic equations.

Another aspect of inverse dopant profiling was investigated in a collaboration between M.Burger and R.Pinnau [3], namely the optimal design of devices.



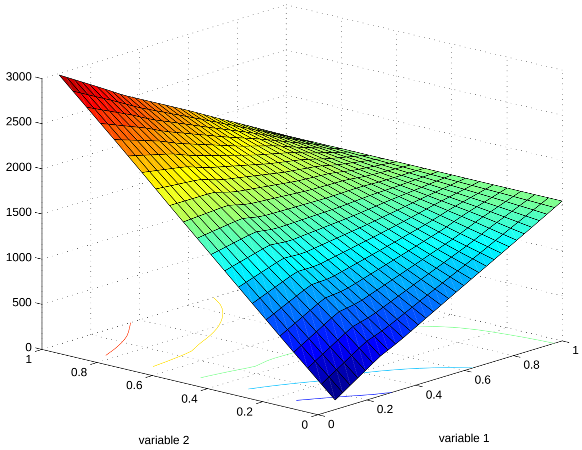
Optimized Shape of a Doping Profile

By reinterpreting the doping profile as a state variable and the potential as the design variable, the authors were able to obtain an efficient design algorithm of the same effort as a single forward simulation of the device, and therefore improving by far existing methods for this problem. A second paper on the exponentially fitted discretization of adjoint equations appearing both in the design and identification problem, is in preparation.

5 Regularized Data-Driven Construction of Fuzzy Controllers

In collaboration of the project F 1308 with Josef Haslinger and Ulrich Bodenhofer (both SCCH Hagenberg), the use of regularization theory and numerical analysis in the data-driven construction of Sugeno controllers has been investigated. This topic is closely related to the activity on neural networks in project F 1308.

In a journal paper by M.Burger, U.Bodenhofer, H.W.Engl and J.Haslinger [43], the use of different regularization approaches to fuzzy control has been investigated. Besides the typical improvements when using regularization methods, such as convergence and stability in presence of data noise, an approach based on Tikhonov regularization also lead to an improvement with respect to the *interpretability*, i.e. the separation of the elements in the solution vector, which is a fundamental property for reasonable fuzzy control.



Control surface for resulting fuzzy controller using Tikhonov regualrization

6 Level Set Methods

Recently, a collaboration between project F 1308 (Dr. Martin Burger) and the SFB 003 at University Graz (Dr. Michael Hintermüller, Dr. Wolfgang Ring) on level set methods for optimal design has been started. The aim of this collaborations are the use of second order shape derivatives for Newton-type and Lagrange-Newton-type methods based on the level set approach for computing the shape. A problem of particular importance arises in the application of SQP-type methods to shape optimization problem, where the concept of *linearized state equations* seemed not to be well-understood before, since

Fréchet-derivatives for the state have to be mixed with shape derivatives for the parameter. The authors developed a novel approach for a class of shape optimization problems, a paper on this subject is in preparation.

Moreover, in the framework of SQP-type and level set methods, the use of all-at-once approaches to shape optimization is planned in this collaboration. This provides a strong link to a previous internal collaboration between the projects F 1308 and F 1309 on all-at-once approaches for distributed parameter identification.

7 Parameter Identification in Plasticity

In cooperation with the Department of Engineering Science, University of Oxford, England and project F 1308 the identification of material parameters of (visco)-plastic materials from boundary measurements is investigated. Especially the parameters determining the yield surface are of main interest.

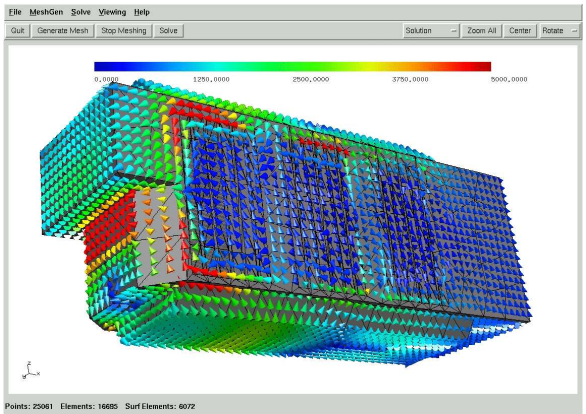
(Visco)-plastic materials are described via variational inequalities, which are not differentiable (with respect to the parameter) in general. Standard regularization techniques therefore do not apply due to lack of existence of derivative of the objective function. Existing results in control theory for variational inequalities do also not apply since there distributed parameters given in the PDI are considered, whereas in our problem the parameters (yield surface) describe the convex set for the PDI. Inspired by heuristic arguments, we developed an algorithm based on Landweber iteration, replacing the derivative by an approximate derivative. Testing the algorithm on real data and a rigorous mathematical analysis of the algorithm will be the aim of further cooperation.

8 Mathematical Optimization supports Strategic Decisions

The long term cooperation with our industrial partner, the ENGEL AUSTRIA GmbH Schwertberg, is based on the fast tools developed in projects F1309 and F1306. Our goal was the optimization of the very heavy supporting frames of the injection moulding machines produced by the company. The optimizaion was done with respect to a minimal weight under certain constraints taking into account critical stresses, deflections, etc.. After finishing several shape optimizations for the steel frame with constant thickness and optimal design problems for the cast iron fram with variable thickness we were involved in the strategic decision which frame out of the two sorts will be used for the new production line. Our fast tools allowed several optimization runs for various materials, different design variants and technical constraints. We could show that the previously prefered cast iron frame has no advantages in comparison to the steel frame. This result and the cheaper production costs for steel frames were the basis for the company's decision to use that sort of frame. This cooperation will be continued.

9 Eddy Current Simulation in Power Transformers with Multigrid Methods

MathConsult GmbH, VA TECH EBG Transformatoren GmbH, and Dr. Joachim Schöberl are working on the simulation of Power Transformers with modern numerical methods such as multigrid solvers and automatic mesh size control. The goal is the accurate computation of the losses due to eddy currents. The first part of the project has been successfully completed beginning 2002. The developed software (based on Netgen/NGSolve) can simulate quite complicated models in about 30 minutes. The picture below shows the computed eddy currents in the casing:



Points: 25061 Elements: 16695 Surf Elements: 6072

Being able to compute all the electromagnetic fields, we could detect the major influence of the simplified model a posteriori. A too strong simplification was the assumption of an isotropic iron core. In reality, the core is a laminate of highly permeable, highly conducting metal sheets, and insulation in between. This year, we have benen developing a homogenization method for the laminated core. Indeed, the model is very simple, namely just setting isotropic conductivity and permeability. But, the standard finite element Method for Maxwell does not perform well: These finite elements combine all three components of the vector field, and cannot handle the highly different (about a factor of 10^6) conductivities in the sheet planes and across. A discretization scheme in the core, plus the coupling to the rest of the domain has been developed by Joachim Schöberl. First computational results are promising.

10 Algebraic Spline Surfaces in Reverse Engineering

The use of algebraic spline surface for reverse engineering has been explored in cooperation with Holometric Technologies GmbH, Aalen. This company develops software for constructing a CAD model of an object from measurement data (point clouds). Often, however, these data have holes, due to problems of the measurement process (optical properties of the surface, difficult access to the object, etc.). Thes holes may cause problems for the surface reconstruction process, and need to be repaired.

Dr. Chalmoviansky is working on methods for detecting and filling holes in point clouds. After the boundary of the hole is found, it is filled by approximating the boundary with an algebraic surface patch. Finally, the point is filled by sampling points from the surface.

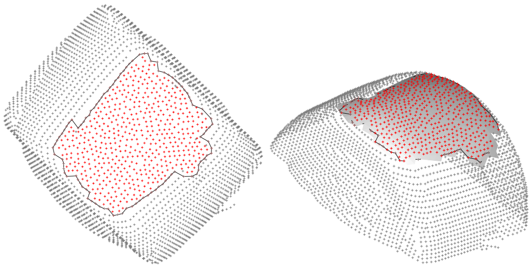


Figure 19: Fairing algebraic curve segments.

The results on algebraic spline surfaces have contributed to the formulation of a European RTD project entitled "Intersection algorithms for geometry based IT-applications using approximate algebraic methods" (GAIA II, 2002-2005) which is is funded by the European commission through its Fifth Framework Programme (IST–FET). The project involves partners from Norway, Spain, France, Italy and Austria. It will explore the more practical aspects of the use of these surfaces in CAD, especially for robustly detecting self–intersections, and for the improvement of algorithms for surface–surface–intersection.

11 Mathematics helps in the Development of Combustion Engines

Numerical simulation plays a growing role in the development of engines. Individual components of the engine can be analyzed and improved by computer experiments.

In this project special air-conducting components are considered, see figure 20. Numerical methods have been developed to optimize the design of such components with respect to certain criteria, like the minimal loss of total pressure, under certain constraints, like prescribed geometric bounds. So far only a few variants of the design could be analyzed in several development cycles.

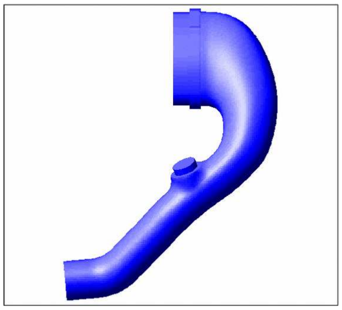


Figure 20: component

By using mathematical methods it is possible for several situations to compute the optimal design in a systematic manner and with an acceptable amount of computational work.

The start design and the total pressure, which is relevant for the quality of the component, is shown in figure 21. The calculated optimal design, see figure 22, leads a reduction of the pressure drop by 10 percent.

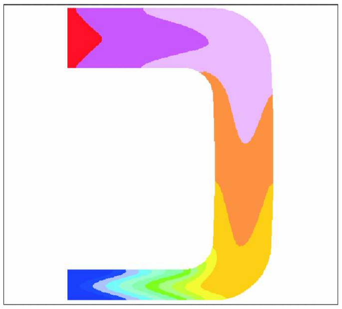


Figure 21: start design

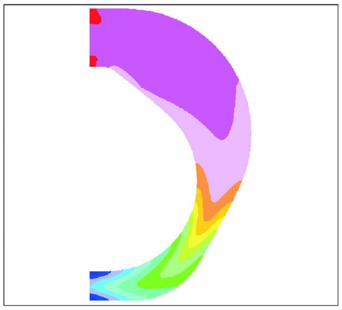


Figure 22: optimal design

This is a joint project of the Institute of Computational Mathematics, Johannes Kepler University Linz and the department Simulation/CAE of BMW Motoren GmbH Steyr.

SFB F013: Numerical and Symbolic Scientific Computing

Statistical Appendix

1 Monographs, PhD Theses, Diploma Theses

[1] Caruso, F. *Polynomial Arithmetic and Linear Systems in Symbolic Summation.* PhD thesis, RISC, Johannes Kepler University Linz, 2002.

[2] Chalmoviansky, P. *Mathematical Methods in Subdivision Surfaces.* PhD thesis, Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava, 2002.

[3] Gerhold, S. Uncoupling systems of linear Ore operator equations. Master's thesis, RISC, Johannes Kepler University Linz, 2002.

[4] Kutsia, T. *Solving and Proving in EquationalTheories with Sequence Variables and Flexible Arity Symbols.* PhD thesis, Johannes Kepler University, Linz, 2002.

[5] Mühlhuber, W. *Efficient Solvers for Optimal Design Problems with PDE Constraints.* PhD thesis, University of Linz, Inst. for Computational Math., April 2002.

[6] Nakagawa, K. *Supporting User-Friendliness in the Mathematical Software System Theroema.* PhD thesis, Research Institute for Symbolic Computation, January 2002.

[7] Rathberger, C. Fast product design with modern optimization software: Shape optimization. Master's thesis, University of Linz, Inst. for Computational Math., July 2002.

[8] Robu, J. *Geometry Theorem Proving in the Frame of the Theorema Project.* PhD thesis, Johannes Kepler University, Linz, 2002.

[9] Zaglmayr, S. Eigenvalue problems in saw filter simulation. Master's thesis, Johannes Kepler University Linz, 2002.

2 Publications

[1] *Integrating Temporal Assertions into a Parallel Debugger* (2002). Proceedings of the 8th International Euro-Par Conference, Paderborn, Germany, 2002.

[2] Apel, T., and Schöberl, J. Multigrid methods for anisotropic edge refinement. *SIAM J. Numer. Anal 40*, 5 (2002), 1993–2006.

[3] Benameur, H., and Kaltenbacher, B. Regularization of parameter estimation by adaptive discretization using refinement and coarsening indicators. *Journal of Inverse and Ill-Posed Problems* (2002). to appear.

[4] Berkovich, A., and Riese, A. A computer proof of a polynomial identity implying a partition theorem of Göllnitz. *Adv. in Appl. Math. 28* (2002), 1–16.

[5] Bodnár, G. Unification of blowing up sequences. In *Actas del EACA–2002* (2002), P. Giménez, Ed., University of Valladolid, Spain, pp. 111–115.

[6] Bodnár, G., Kaltenbacher, B., Pau, P., and Schicho, J. Exact real computation in computer algebra. In *Proc. SNSC Hagenberg 2001* (2002), U. Langer and F. Winkler, Eds., Springer.

[7] Bosa, K., and Schreiner, W. Tolerating stop failures in distributed Maple. In *Dapsys 2002* (Oct. 2002), Kluwer Academic Publishers. 4th Austrian-Hungarian Workshop on Distributed and Parallel Processing, Linz, Austria.

[8] Burger, M., Engl, H. W., and Markowich, P. Inverse doping problems for semiconductor devices. In *Recent Progress in Computational and Applied PDEs* (2002), Kluwer Academic/Plenum Publishers. To appear.

[9] Caprotti, O., and Schreiner, W. Towards a mathematical service description language. In *ICMS 2002, International Congress of Mathematical Software* (2002), World Scientific Publishers.

[10] Craciun, A., and Buchberger, B. Proving the correctness of the merge-sort algorithm with theorema. In *Symbolic and Numeric Algorithms for Scientific Computing, Proceedings of the SYNASC02 Workshop* (Timisoara, Romania, October 2002), pp. 97–111. ISBN 973-585-785-5.

[11] Douglas, C. C., Haase, G., and Iskandarani, M. An acceleration procedure for the spectral element ocean model formulation

of the shallow water equations. In *Fluid Flow and Transport inPorous Media: Mathematical and Numerical Treatment* (Providence, 2002), Z. Chen and R. E. Ewing, Eds., American Mathematical Society, pp. 153–158.

[12] ECMI. *Parameter identification in industrialproblems via iterative regularization methods* (2003).

[13] Gahleitner, M., Jüttler, B., and Schicho, J. Approximate parametrization of planar cubics. In *Curve and Surface Fitting. St. Malo 2002* (2002), Nashboro Press.

[14] Gerstmayr, J., and Schöberl, J. A 3d finite element approach to flexible multibody systems. In *Proceedings to Fifth World Congress on Computational Mechanics (WCCM V)* (2002).

[15] Gu, H. The finite element approximation to the minimal surfaces subject to the plateau problems. In *Proceedings of The Sixth International Conference on Computational Structure Technology* (Sept. 2002), Civil-comp Press.

[16] Gu, H. Generating minimal surfaces subject to the plateau problems by finite element method. In *Lecture Notes on Computer Science—Proceedings for the fifth conference of Numerical Methods and Applications* (Borovets, Bulgaria, Aug. 2002), Springer Verlag.

[17] Gutierrez, J., Rubio, R., and Schicho, J. Polynomial parametrization of curves without affine singularities. *Comp. Aided Geom. Design 19*, 3 (2002), 223–234.

[18] Haase, G., Kuhn, M., and Reitzinger, S. Parallel amg on distributed memory computers. *SIAM Jouranal of Scientific Computing 24*, 2 (2002), 410–427.

[19] Haase, G., and Langer, U. *Multigrid Methods: From Geometrical to Algebraic Versions*, vol. 75 of *NATO Science Series: II, Mathematics, Physics and Chemistry*. Kluwer Academic Publishers, Dordrecht, 2002, ch. 4, pp. 103–154. Anne Bourlioux and Martin J. Gander (eds.).

[20] Haase, G., Langer, U., Lindner, E., and Mühlhuber, W. Optimal sizing of industrial structural mechanics problems using automatic differentiation. In *Proceedings of "Automatic Differentiation 2000: From Simulation to Optimization* (2002), G. Corliss, C. Faure, A. Griewank, L. Hascoet, and U. Naumann, Eds., Springer, pp. 181–188.

[21] Hemmecke, R. Continuously Parameterized Symmetries and Buchberger's Algorithm. *J. of Symbolic Computaion 33*, 1 (2002), 43–55.

[22] Hemmecke, R. An efficient method for finding a simplifier in an involutive basis computation (extended abstract). In *Proceedings of the Workshop on Under- and Overdetermined Systems of Algebraic or Differential Equations, March 18-19, 2002, Karlsruhe, Germany* (Mar. 2002), J. Calmet, M. Hausdorf, and W. M. Seiler, Eds., Institut für Algorithmen und Kognitive Systeme, Universität Karlsruhe, pp. 87–95. Local proceedings.

[23] Hofer, M., Lerch, R., Finger, N., Kovacs, G., Schöberl, J., Zaglmayr, S., and Langer, U. Finite element calculation of wave propagation and excitation in periodic piezoelectric systems. In *Proceedings to Fifth World Congress on Computational Mechanics (WCCM V)* (2002).

[24] H.W. Engl, P. K. The influence of the equation type on iterative parameter identification problems which are elliptic or hyperbolic in the parameter. *European Journal on Applied Mathematics* (2002). accepted.

[25] H.W. Engl, P. K. Parameter identification in industrial problems via iterative regularization methods. *submitted* (2002).

[26] H.W.Engl. Identification of parameters in polymer crystallization, semiconductor models and elasticity via iterative regularization methods. *submitted* (2002).

[27] H.W.Engl, P. K. Identification of a temperature dependent heat conductivity by tikhonov regurlaization. *J. of Inverse and Ill-Posed Problems 10 10* (2002), 67–90.

[28] Kaltenbacher, B. V-cycle convergence of some multigrid methods for ill-posed problems. *Mathematics of Computation* (2002). to appear.

[29] Kaltenbacher, B., Kaltenbacher, M., and S.Reitzinger. Identification of nonlinear $b-h$ curves based on magnetic field computations and multigrid methods for ill-posed problems. *European Journal of Applied Mathematics* (2002). to appear.

[30] Kaltenbacher, B., Neubauer, A., and Ramm, A. Convergence rates of the continuous regularized gauss-newton method. *J. Inv. Ill-Posed Problems 10* (2002), 261–280.

[31] Kaltenbacher, B., and Schicho, J. A multi-grid method with a priori and a posteriori level choice for the regularization of nonlinear ill-posed problems. *Numerische Mathematik* (2002).

[32] Kaltenbacher, B., and Schöberl, J. A saddle point variational formulation for

projection-regularized parameter identification. *Numerische Mathematik* (2002).

[33] Kovacs, J., Kusper, G., Lovas, R., and Schreiner, W. Integrating temporal assertions into a parallel debugger. In *Lecture Notes in Computer Science* (Aug. 2002), Springer. Euro-Par 2002, 8th International Euro-Par Conference, Paderborn, Germany.

[34] Kügler, P. Identification of a temperature dependent heatconductivity from single boundary measurements. *SIAM Journal on Numerical Analysis* (2002). submitted.

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

[36] Kutsia, T. Pattern unification with sequence variables and flexible arity symbols. In *Proceedings of the Workshop on Unification in Non-Classical Logics* (Malaga, Spain, July 2002), M. Ojeda-Asiego, Ed., vol. volume 66 of *Electronic Notes on Theoretical Computer Science*, Elsevier Science.

[37] Kutsia, T. Theorem proving with sequence variables and flexible arity. In *Logic in Programming, Artificial Intelligence and Reasoning. Proceedings of the 9th International Conference LPAR'02* (Tbilisi, Georgia, October 14-18 2002), M. Baaz and A. Voronkov, Eds., vol. 2514 of *Lecture Notes in Artificial Intelligence*, Springer Verlag, pp. 278–291. ISBN 3-540-00010-0.

[38] Kutsia, T. Unification with sequence variables andflexible arity symbols and its extension with pattern-terms. In *Artificial Intelligence, Automated Reasoning and Symbolic Computation. Proceedings of Joint AICS'2002 - Calculemus'2002 conference* (Marseille, France, July 2002), B. B. J. Calmet, O. Caprotti, L. Henocque, and V. Sorge, Eds., vol. volume 2385 of *Lecture Notes in Artificial Intelligence*, Springer Verlag, pp. 290–304. ISBN 3-540-43865-3.

[39] Landsmann, G. Implicitization of algebraic varieties. In *Proceedings of the SCI2002, Vol. 11* (July 2002), N. Callaos, Ed.

[40] Langer, U., Reitzinger, S., and Schicho, J. Symbolic methods for the element precondition technique. In *Proc. SNSC Hagenberg 2001* (2002), U. Langer and F. Winkler, Eds., Springer.

[41] Lyons, R., Paule, P., and Riese, A. A computer proof of a series evaluation in terms of harmonic numbers. *Appl. Algebra Engrg. Comm. Comput. 13* (2002), 327–333.

[42] M.Burger. Growth and impingement in polymer melts. In *Free Boundary Problems* (2002). Submitted.

[43] M.Burger, Engl, H., J.Haslinger, and U.Bodenhofer. Regularized data-driven construction of fuzzy controllers. *J. Inverse & Ill-posed Problems*, 10 (2002), 319–344.

[44] P. Kügler, A. L. Mean value iterations for nonlinearelliptic cauchy problems. *Numerische Mathematik* (2002). submitted.

[45] Pérez-Díaz, S., Schicho, J., and Sendra, J. R. Properness and inversion of rational parametrizations of surfaces. *AAECC 13* (2002), 29–51.

[46] Piroi, F. Focus windows: A tool for automated provers. In *Sybolic and Numeric Algorithms for Scientific Computing. Proceeding of SYNASC'02 International Worksop.* (Timisoara, Romania, October 2002), D. Petcu, V. Negru, D. Zaharie, and T. Jebelean, Eds. ISBN 973-585-785-5.

[47] Piroi, F., and Buchberger, B. Focus windows: A new technique for proof presentation. In *Proceedings of the 8th Rhine Workshop on Computer Algebra.* (Mannheim, Germany, March 2002), H. Kredel and W. M. Seiler, Eds., University of Mannheim, Germany.

[48] Piroi, F., and Buchberger, B. Focus windows: A new technique for proof presentation. In *Artificial Intelligence, Automated Reasoning and Symbolic Computation. Proceedings of Joint AICS'2002 - Calculemus'2002 Conference.* (Marseille, France, July 2002), J. Calmet, B. Benhamou, O. Caprotti, L. Henocque, and V. Sorge, Eds., vol. 2385 of *Lecture Notes in Artificial Intelligence*, Springer Verlag, pp. 290–304. ISBN 3-540-43865-3.

[49] R. Chapko, P. K. On the landweber method for aninverse parabolic boundary value problem. *Journal of Computational and Applied Mathematics* (2002). submitted.

[50] Ratschan, S. Approximate quantified constraint solving by cylindrical box decomposition. *Reliable Computing 8*, 1 (2002), 21–42.

[51] Ratschan, S. Quantified constraints under perturbation. *Journal of Symbolic Computation 33*, 4 (2002), 493–505.

[52] Ratschan, S. Search heuristics for box decomposition methods. *Journal of Global Optimization 24*, 1 (2002), 51–60.

[53] REITZINGER, . S., AND SCHÖBERL, J. Algebraic multigrid for edge elements. *Numerical Linear Algebra with Applications 9*, 3 (2002), 223–238.

[54] REITZINGER, S., AND SCHOEBERL, J. An algebraic multigrid method for finite element discretizations with edge elements. *Numerical Linear Algebra with Applications 9*, 3 (2002), 223–238.

[55] ROBU, J. Systematic exploration of geometric configurations using mathematica. In *Analele Universitatii Timisoara* (Timisoara, Romania, 2002), vol. XXXIX of *Seria Matematica-Informatica*, pp. 209–216.

[56] SCHICHO, J. Simplification of surface parametrizations. In *Proc. ISSAC 2002* (2002), ACM Press, pp. 229–237.

[57] SCHINNERL, M., SCHÖBERL, J., KALTENBACHER, M., AND LERCH, R. Multigrid methods for the 3d simulation of nonlinear magneto-mechanical systems. *IEEE Transactions Magnetics 38*, 3 (2002), 1497–1511.

[58] SCHREINER, W. A Java Toolkit for Teaching Distributed Algorithms. In *ITiCSE 2002, 7th Annual Conference on Innovation and Technology in Computer Science Education* (June 2002), ACM Press.

[59] SCHREINER, W., MITTERMAIER, C., AND BOSA., K. Distributed Maple: Parallel computer algebra in networked environments. *Journal of Symbolic Computation* (2002).

[60] SHALABY, M., JÜTTLER, B., AND SCHICHO, J. Spline implicitization for planar curves. In *Curve and Surface Fitting. St. Malo 2002* (2002), Nashboro Press.

[61] SHALABY, M., JÜTTLER, B., AND SCHICHO, J. $c1$ spline implicitization of planar curves. In *Proceedings of ADG 2002* (2003).

[62] V.CAPASSO, A.MICHELETTI, AND M.BURGER. Densities of n-facets of incomplete johnson-mehl tessellations generated by inhomogeneous birth-and-growth processes. *submitted* (2002).

[63] V.CAPASSO, M.BURGER, A.MICHELETTI, D.MORALE, AND C.SALANI. Mathematical models for polymer crystallization processes. In *Mathematical Modelling for Polymer Industry* (2002), V. Capasso, Ed., Springer. To appear.

[64] V.CAPASSO, M.BURGER, A.MICHELETTI, D.MORALE, AND C.SALANI. Mathematical models for polymer crystallization processes. In *Mathematical modelling for polymer industry* (Berlin, Heidelberg, 2002), V. Capasso, Ed., Springer.

[65] WINKLER, F. Advances in Algebraic Geometric Computation. In *Proc. International Conf. on Algebra and Its Applications (ICAA'2002), Bangkok, Thailand* (March 2002), pp. 107–120. ISBN 970-13-2182-1.

3 Conference Talks

[1] BODNÁR, G. Testing the normal crossing property of hypersurfaces. talk on ADG 2002, RISC, Johannes Kepler University, Linz, Austria, 2002.

[2] BODNÁR, G. Unification of blowing up sequences. talk on EACA 2002, University of Valladolid, Spain, 2002.

[3] BODNÁR, G., AND SCHICHO, J. An algorithm for resolution of singularities in characteristic zero. talk on GAMM 2002, University of Augsburg, Germany, 2002.

[4] BUCHBERGER, B. Formal exploration management for hilbert space theory. Talk at the SFB Status Seminar, April 2002, Strobl, Austria, April 2002.

[5] CARUSO, F. A library for polynomial arithmetic. Contributed talk at Workshop on Applications of Commutative Algebra, Catania, Italy, April 2002.

[6] CRACIUN, A. The sequence provers in theorema. Joint AISC'02 - Calculemus '02 conference, Marseille, France, July 1-5, 2002; Appears in: Seki-Report Series Nr. SR-02-04, Calculemus 2002, Work in Progress Papers, Universitaet des Saarlandes, July 2002.

[7] EGGER, H. The inverse problem of option pricing. Conference on Computational Methods for Inverse Problems, Strobl, 2002.

[8] EGGER, H. The inverse problem of option pricing. ECMI 2002, Riga, 2002.

[9] HAASE, G. Modeling and computation of sea surface heights in complex domains. Int. Workshopon Numerical Mathematics at the SZE of Györ, Hungary., May 2002.

[10] HAASE, G. Optimal sizing and shape optimization in structural mechanics. Int. Conf. on Industrial Mathematics at IIT Bombay, India., December 2002.

[11] H.W.ENGL. Alan tayler lecture: Identification of parameters in polymer crystallization, semiconductor models and elasticity via iterative regularization methods. ECMI Conference, Riga, September 2002.

[12] H.W.Engl. Identification of parameters in polymer crystallization, semiconductor models and elasticity via iterative regulariaztion methods. June 2002.

[13] H.W.Engl. Identification of parameters in polymer crystallization, semiconductor models and elasticity via iterative regulariaztion methods. Conference "Inverse and Ill-Posed Problems", Russian Academy of Science, Novosibirsk, August 2002.

[14] H.W.Engl. Iterative methods for nonlinear inverse problems. SIAM Annual Meeting, Philadelphia, USA, July 2002.

[15] Jebelean, T. Theorema: A system for the working mathematician. International Symposium "35 years of Automath" Edinburgh, Scotland, 10 - 13 Aug. 2002, August 2002.

[16] Jebelean, T. Theorema: A system for the working mathematician. software demonstration. ISSAC'02 (International Symposium for Symbolic and Algebraic Computation, Lille, France, July 2002). The abstract of the talk and the software demo are published electronically on the CD-ROM accompanying the proceedings (ACM Press, ISBN 1-58113-582-3)., July 2002.

[17] Jebelean, T. Using hyper-inferences for natural style proving in predicate logic. SFB workshop Strobl, April 2002, April 2002.

[18] Kaltenbacher, B. Regularization of parameter estimation by adaptive discretization using refinement and coarsening indicators. SFB Konferenz Computational Methods for Inverse Problems, Strobl, 26.-30.August 2002, august 2002.

[19] Kienesberger, J. A multigrid preconditioned solver for elastoplastic problems. SFB-Conference on "Computational Methods for Inverse Problems", August 2002.

[20] Kienesberger, J. A multigrid preconditioned solver for elastoplastic type problems. Chemnitz FEM Symposium, September 2002.

[21] Kindermann, S. Algorithms for ill-posed problems with discontinous solutions: The moving grid method and hamilton-jacobi equations. SFB Status Seminar in Strobl, April 2002.

[22] Kindermann, S. Regularization by hamilton-jacobi type equation. Conference on Computational Methods for Inverse Problems, Strobl, August 2002.

[23] Kügler, P. An iterative regularization method for an inverse problem in the manufacture of car windshields. SIAM2002, 2002.

[24] Kügler, P. A parameter identification problem ofmixed type related to the manufacture of car windshields. ECMI2002, 2002.

[25] Kügler, P. The sagging process for the manufacture of car windshields as an inverse problem of mixed type. GlassDays2002, 2002.

[26] Kusper, G. Investigation of binary representations of sat, especially 2-literal representation. Conference of PhD Students in Computer Science, Szeged, Hungary, July 1-4, 2002, July 2002.

[27] Kusper, G. Solving the resolution-free sat problem by hyper-unit propagation in linear time. Fifth International Symposium on the Theory and Applications of Satisfiability Testing, Cincinnati, Ohio, USA, May 6-9, 2002, May 2002.

[28] Kutsia, T. Groebner bases approach towards formula simplification in operator theory. Talk at the SFB Status Seminar, April 2002, Strobl, Austria, April 2002.

[29] Kutsia, T. Unification with sequence variables and flexible arity symbols. Talk at the SFB Status Seminar, April 2002, Strobl, Austria, April 2002.

[30] Langer, U. Boundary element tearing and interconnecting methods. Talk on the Oberwolfach Conference on "New Trends in Boundary Elements", Oberwolfach, Germany (joint talk with O. Steinbach), December 2002.

[31] Langer, U. Multigrid methods for magnetomechanical problems. Fifth World Congress on Computational Mechanics (WCCM V), Vienna, Austria, July 2002.

[32] M.Burger. A framework for the construction of level set methods for shape reconstruction and optimization. SFB-Conference "Computational Methods for Inverse Problems", Strobl, August 2002.

[33] M.Burger. A framework for the construction of level set methods for shape reconstruction and optimization. Geometrically based motions, Reunion Conference, Lake Arrowhead, USA, September 2002.

[34] M.Burger. Growth and impingement in polymer melts. Invited talk at the Minisymposium "Free Boundary Problems in Polymers" at the Conference "Free Boundary Problems", Trento., June 2002.

[35] Nakagawa, K. Logicographic symbol. SFB Status Seminar Strobl, Austria, April 26, 2002, April 2002.

[36] Nakagawa, K. User-friendly features of mathematical software system theorema. Invited talk of the Computer Algebra Seminar at Kobe Univ., Japan, Feb. 5, 2002, February 2002.

[37] Nakagawa, K. User-friendly features of mathematical software system theorema. Invited talk at Kyusyu Univ., Japan, Feb. 12, 2002, February 2002.

[38] Nakagawa, K. User-friendly features of mathematical software system theorema. Invited talk at Fujitsu Laboratories LTD., Japan, Mar. 11,2002, March 2002.

[39] Nakagawa, K. Variable shape logicographic symbols. In Symposium in Honor of Bruno Buchberger's 60th Birthday, Logic, Mathematics and Computer Science: Interactions (LMCS 2002), Schloss Hagenberg, Austria, RISC. October 20-22, 2002, October 2002.

[40] Neubauer, A. Estimation of discontinuous solutions of ill-posed problems by regularization for surface representations: numerical realization via moving grids. Int. Conference on Inverse Problems, Hongkong, January 2002.

[41] Paule, P. Symbolic summation: Algorithms and missed opportunities. Invited talk at “Special Functions in the Digital Age”, Minneapolis, Minnesota, July 2002.

[42] Piroi, F. Focus windows. talk at the sfb status seminar. SFB Status Seminar Strobl, Austria, April 26, 2002, April 2002.

[43] Piroi, F., and Jebelean, T. Interactive proving in theorema. Ninth Workshop on Automated Reasoning, AISB'02. 3-5 April, 2002, Imperial College of Science, Technology and Medicine, University of London. England. Appears in: Collected Abstracts, Toby Walsh editor., April 2002.

[44] Riese, A. Computer proofs of hypergeometric summation identities and partition analysis. Invited talk at “Special Functions in the Digital Age”, Minneapolis, Minnesota, July 2002.

[45] Riese, A. Randomization speeds up hypergeometric summation. Contributed talk at “SFB Workshop”, Strobl, Austria, April 2002.

[46] Robu, J. Geometry theorem proving in the frame of theorema project. 4th International Workshop on Automated Deduction in Geometry (ADG 2002), RISC, Sept. 4-6, 2002, Linz, September 2002.

[47] Rosenkranz, M. A groebner bases approach towards solving linear bvp. SFB Status Seminar Strobl, Austria, April 26, 2002, April 2002.

[48] Rosenkranz, M., Buchberger, B., and Engl, H. W. Computing the moore-penrose-inverse by groebner bases. Conference on Computational Methods for Inverse Problems Strobl, Austria, August 27, 2002, August 2002.

[49] Rosenkranz, M., Buchberger, B., and Engl, H. W. Solving linear boundary value problems via non-commutative groebner bases. Fourth International SYNASC Workshop Timisoara, Romania, October 9-12, 2002, October 2002.

[50] Rosenkranz, M., and Engl, H. W. Solving linear boundary value problems via non-commutative groebner bases. Symposium in Honor of Bruno Buchberger's 60th Birthday, Logic, Mathematics and Computer Science: Interactions (LMCS'2002) Hagenberg, Austria, October 20-22, 2002, October 2002.

[51] Schneider, C. How one can play with sums. Contributed talk at the 8th Rhine Workshop on Computer Algebra, Germany, Mannheim, March 2002.

[52] Schneider, C. Sigma: A summation package for discovering and proving. Invited talk at the IMA Summer Program on “Special Functions in the Digital Age”, Minnesota, Minneapolis, July 2002.

[53] Schöberl, J. Algebraic multigrid methods for h(div) and h(curl). Workshop on Linear Algebra, Neuchatel, CH, Nov 2002.

[54] Schöberl, J. Anisotropic mesh generation with netgen. in Minisymposium by. J. Häuser and J. Schöberl, March 2002.

[55] Schöberl, J. Automatic mesh generation with netgen. Chemnitzer FE Symposium, Sep 2002.

[56] Schöberl, J. Commuting interpolation operators. Foundations of Comp. Mechanics, IMA Minnesota, Aug 2002.

[57] Schöberl, J. Multigrid methods in elasticity. Fifth World Congress on Computational Mechanics, Vienna (WCCM V), July 2002.

[58] Schöberl, J. Simulation of a power transformer by multigrid methods. Scientific Computing in Electrical Engineering (SCEE), June 2002.

[59] Shalaby, M., Jüttler, B., and Schicho, J. Spline implicitization of planar curves. talk on Geometrie-Tagung 2002, Stift Vorau, Austria, 2002.

[60] Windsteiger, W. An automated prover for set theory in theorema. Calculemus'02, Marseille,

France, June 3-5, 2002; Appears in: Seki Report Nr.SR-02-04, Work in Progress Papers at the 10th Symposium on the Integration of Symbolic Computation and Mechanized Reasoning, June 2002.

[61] Windsteiger, W. An automated prover for zermelo-fraenkel set theory in theorema. Symposium in Honor of Bruno Buchberger's 60th Birthday, Logic, Mathematics and Computer Science: Interactions (LMCS'2002) RISC-Linz, Castle of Hagenberg, Austria, October 20-22, 2002. Appers in RISC-report nr. 02-60, October 2002.

[62] Winkler, F. Advances in Algebraic Geometric Computation. International Conf. on Algebra and Its Applications (ICAA'2002), Bangkok, Thailand, March 2002.

[63] Zimmermann, B. Structure set computation in hypergeometric summation. Contributed talk at Eighth International Conference on Applications of Computer Algebra, Volos, Greece, June 2002.

[64] Zimmermann, B. Wavelets and Gröbner bases: How to reduce the number of variables by a factor of two. Contributed talk at GAMM 2002, Augsburg, Germany, March 2002.

4 SFB Reports

2002

02–1 Reitzinger, S., Schreiber, U., van Rienen, U. : *Algebraic Multigrid for Complex Symmetric Matrices: Numerical Studies.* January, 2002. Eds.: U. Langer, A. Neubauer

02–2 Engl, H. W.: *Identification of Parameters in Polymer Crystallization, Semiconductor Models and Elasticity via Iterative Regularization Methods* January, 2002. Eds.: U. Langer, B. Jüttler

02–3 Langer, U. Reitzinger, S. Schicho, J.: *Symbolic Methods for the Element Preconditioning Technique* January, 2002. Eds.: W. Engl, F. Winkler

02–4 Paule, P.: *Wavelets with Scale Dependent Properties* January, 2002. Eds.: J. Schicho, F. Winkler

02–5 Haase, G. Reitzinger, S.: *Algebraic Multigrid Methods for Linear Systems with Multiple Right-Hand Sides* March, 2002. Eds.: W. Engl, U. Langer

02–6 Kutsia, T.: *Unification in a Free Theory with Sequence Variables and Flexible Arity Symbols and its Extensions* March, 2002. Eds.: B. Buchberger, P. Paule

02–7 Lyons, R. Paule, P. Riese, A.: *A Computer Proof of a Series Evaluation in Terms of Harmonic Numbers* April, 2002. Eds.: J. Schicho, F. Winkler

02–8 Burger, M.: *Growth Fronts of First-Order Hamilton-Jacobi Equations* May, 2002. Eds.: B. Jüttler, W. Engl

02–9 Sohn, Kyung-Ah. Jüttler, B. Kim, Myung-Soo.: *Computing the Distance Between Two Surfaces via Line Geometry* June, 2002. Eds.: J. Schicho, E. Lindner

02–10 Kindermann, S. Neubauer, A.: *Parameter Identification by Regularization for Surface Representation via the Moving Grid Approach* July, 2002. Eds.: B. Jüttler, J. Schicho

02–11 Burger, M., Haslinger, J., Bodenhofer, U., Engl, H.W.: *Regularized data-driven construction of fuzzy controllers* July, 2002. Eds.: B. Jüttler, B. Buchberger

02–12 Burger, M.: *A Framework for the Construction of Level Set Methods for Shape Optimization and Reconstruction* September, 2002. Eds.: H.W. Engl, J. Schicho

02–13 Apel, J., Hemmecke, R.: *Detecting Unnecessary Reductions in an Involutive Basis Computation* October, 2002. Eds.: F. Winkler, J. Schicho

02–14 Schicho, J.: *Simplification of Surface Parametrizations* November, 2002. Eds.: P. Paule, F. Winkler

02–15 Schicho, J.: *An Inequality for Lattice Polygons* November, 2002. Eds.: P. Paule, F. Winkler

02–16 Schicho, J., Pau, P.: *Computation and Validation of Root Clusters for Univariate Polynomials* November, 2002. Eds.: P. Paule, F. Winkler

02–17 Schicho, J.: *Simplification of Surface Parametrizations A Lattice Polygon Approach* November, 2002. Eds.: P. Paule, F. Winkler

02–18 Korneev, V., Xanthis, L., Anoufriev, I.: *Hierarchical and Lagrange hp discretizations and fast domain decomposition solvers for them* November, 2002. Eds.: U. Langer, E. Lindner

02–19 Schneider, C.: *Solving Parameterized Linear Difference Equations in $\Pi\Sigma$-Fields* November, 2002. Eds.: P. Paule, F. Winkler

02–20 Schneider, C.: *A Collection of Denominator Bounds To Solve Parameterized Linear Difference Equations in $\Pi\Sigma$-Fields* November, 2002. Eds.: P. Paule, F. Winkler

02–21 Schneider, C.: *Degree Bounds to Find Polynomial Solutions of Parameterized Linear Difference Equations in* $\Pi\Sigma$*-Fields* November, 2002. Eds.: P. Paule, F. Winkler

02–22 Schneider, C.: *A Unique Representation of Solutions of Parameterized Linear Difference Equations in* $\Pi\Sigma$*-Fields* November, 2002. Eds.: P. Paule, F. Winkler

02–23 Jüttler, B., Schicho, J., Shalaby, M.: *Spline Implicitization of Planar Curves* November, 2002. Eds.: P. Paule, F. Winkler

02–24 Gu, H.: *Graphical Generating of Minimal Surfaces Subject to the Plateau Problems* November, 2002. Eds.: J. Schicho, F. Winkler

02–25 Ahlgren, S., Paule, P., Schneider, C.: *Computer Proofs of a New Family of Harmonic Number Identities* November, 2002. Eds.: P. Paule, J. Schicho

02–26 Winkler, F., Athale, M.: *Abstracts Booklet of the Fourth International Workshop on Automated Deduction in Geometry (ADG'02)* September, 2002. Eds.: F. Winkler, J. Schicho

02–27 Rosenkranz, M., Engl, H.W.: *Solving Linear Boundary Value Problems via Non-Commutative Gröbner Bases* December, 2002. Eds.: J. Schicho, T. Jebelean

02–28 Landsmann, G.: *Implicitization of Algebraic Varieties* December, 2002. Eds.: F. Winkler, J. Schicho

02–29 Burger, M., Pinnau, R.: *Fast Optimal Design of Semiconductor Devices* December, 2002. Eds.: H.W. Engl, U.Langer

02–30 Reitzinger, S., Kaltenbacher, B., Kaltenbacher, M.: *A Note on the Approximation of* $B-H$ *Curves for Nonlinear Magnetic Field Computations* December, 2002. Eds.: H.W. Engl, U.Langer

02–31 Craciun, A., Buchberger, B.: *Proving the Correctness of the Merge-Sort Algorithm with Theorema* December, 2002. Eds.: J. Schicho, T. Jebelean

02–32 Piroi, F., Buchberger, B.: *Focus Window: A New Technique for Proof Presentation* December, 2002. Eds.: J. Schicho, T. Jebelean

02–33 Piroi, F.: *Focus Window: A Tool for Automated Provers* December, 2002. Eds.: J. Schicho, T. Jebelean

02–34 Paule, P., Prodinger, H.: *Fountains, Histograms, and* q*-Identities* December, 2002. Eds.: J. Schicho, F. Winkler

02–35 Nakagawa, K.: *Variable Shape Logicographic Symbols* December, 2002. Eds.: J. Schicho, T. Jebelean

02–36 Kutsia, T.: *Theorem Proving with Sequence Variables and Flexible Arity Symbols* December, 2002. Eds.: J. Schicho, T. Jebelean

02–37 Kutsia, T.: *Pattern Unification with Sequence Variables and Flexible Arity Symbols* December, 2002. Eds.: J. Schicho, T. Jebelean

02–38 Windsteiger, W.: *An Automated Prover for Set Theory in Theorema* December, 2002. Eds.: J. Schicho, T. Jebelean

02–39 Windsteiger, W.: *An Automated Prover for Zermelo-Fraenkel Set Theory in Theorema* December, 2002. Eds.: J. Schicho, T. Jebelean

02–40 Kusper, G.: *Solving the SAT Problem by Hyper-Unit Propagation* December, 2002. Eds.: J. Schicho, T. Jebelean

02–41 Langer, U., Steinbach, O.: *Boundary Element Tearing and Interconnecting Methods* December, 2002. Eds.: B. Jüttler, W. Engl