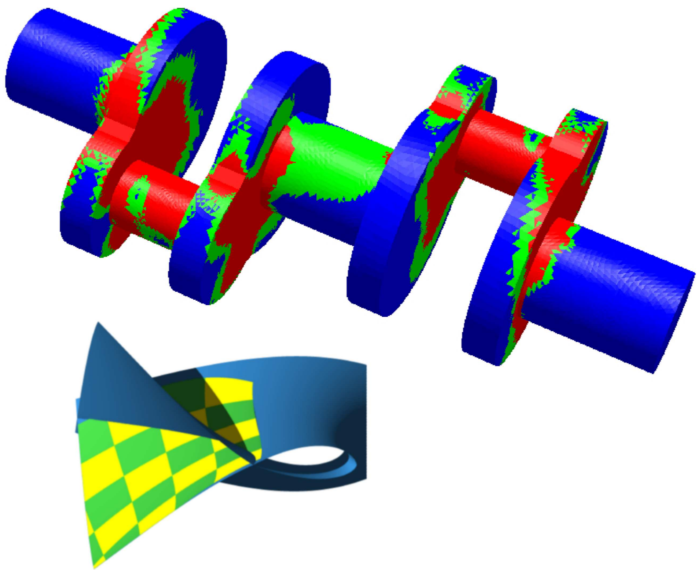
## Special Research Program (SFB) F 013

# Numerical and Symbolic Scientific Computing

## Annual Report 2006


**Johannes Kepler University Linz**
**A–4040 Linz, Austria**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# Special Research Program SFB F013

## “Numerical & Symbolic Scientific Computing”

**Speaker: Prof. Dr. P. Paule**

**Vice Speaker: Prof. Dr. H.W. Engl**

**Office: M. Schimpl**
**System Administration: M. Winkler**

This Annual Report gives a summary of SFB results achieved in 2006.

Also in its ninth year of funding, the overall scientific goal of the SFB is the design, verification, implementation, and analysis of numerical, symbolic, and geometrical 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. This includes so-called field problems, usually described by partial differential equations (PDEs), and algebraic problems, e.g., involving constraints in algebraic formulation.

Concerning the fine structure of the *Scientific Concept* and of the *Long Term Goals* of the SFB, we permanently have made adaptations in order to focus more properly on our overall objective. These adjustments have been driven by the advice and the suggestions of the referees, by our experience made during the SFB work, but also by the changing requirements in the international research community.

By supplementary measures, like joint internal seminars between numerical and symbolic groups or target-oriented structure of the SFB status seminars, the coherence between the numerical and symbolic groups has been further improved.

Also in the ninth year of SFB funding, the scientific results obtained within the SFB by the participating institutes gave rise to various activities concerning knowledge and technology transfer to the industry, especially, in Upper Austria. For more details see the sections describing the scientific progress achieved within the subprojects of the SFB.

The following institutes of the Johannes Kepler University (JKU) of Linz are currently involved in the subprojects of the SFB:

- Institute of Applied Geometry,
- Institute of Computational Mathematics,
- Institute of Industrial Mathematics,
- Institute of Symbolic Computation (RISC).

Another participating institution is the Johann Radon Institute for Computational and Applied Mathematics (RICAM) of the Austrian Academy of Sciences (ÖAW).

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

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

or contact our office.

Linz, August 2007 Peter Paule

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# F 1301: Scientific Part of the Service Project

**Prof. Dr. P. Paule**
**Prof. Dr. J. Schöberl, Dr. V. Levandovskyy**
**DI V. Pillwein, MSc. F. Stan**

In the third funding period of the SFB the major objectives of the scientific part of subproject F1301 are: (i) the development of computer algebra tools (e.g., for symbolic integration and summation of special functions) in connection with high order finite element methods; (ii) the development of (non–commutative) Gröbner bases software that can be exploited by other subprojects. In all these areas significant progress has been achieved which is documented by 9 publications.

## 1 High Order Finite Elements

**Inner shape functions using integrated Jacobi polynomials.** Two major objectives in the design of high order basis functions are to obtain a sparse structure and a small condition number of the resulting system matrix. In [1] and [2] S. Beuchler and V. Pillwein propose families of interior bubbles for triangles and tetrahedra that lead to a sparse system matrix in the case of a polygonally bounded domain and a constant coefficient function. For the case of a curved domain or a non constant coefficient function efficient preconditioners are derived.

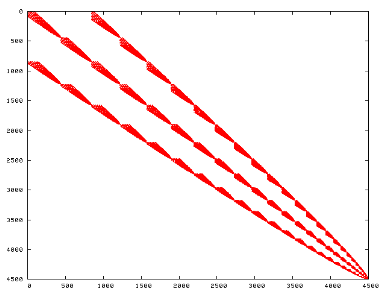

Figure 1: Nonzero pattern of the system matrix for polynomial degree 32, $a = b = 0$, tetrahedral case

The basis functions are constructed using a tensor product structure of Jacobi polynomials. The main result is the nonzero pattern of the stiffness matrix, and thereby also the number of nonzero entries, which can be given explicitely. In the case of tetrahedral elements the definition of the shape functions depends on two parameters $a, b$ with $0 \le a \le 4,\ a \le b \le 6$. In dependence of $a$ and $b$ we have,

$$\begin{aligned} &K_{i,j,k;l,m,n} = 0 \Leftrightarrow |i-l| \notin \{0,2\}, \\ \text{or} \quad &|i-l+j-m| > 3+a, \\ \text{or} \quad &|i-l+j-m+k-n| > 2+b. \end{aligned}$$

The optimal choice of parameters with respect to sparsity *and* condition number of the system matrix is $a = b = 0$, see Figures 1 and 2, respectively. This result was proven by explicitely computing the matrix entries in an algorithmic manner with a Mathematica implementation. This proof would not have been feasible without the application of computer algebra software. In the course of building the algorithm, several relations between Jacobi polynomials with different parameters were needed that can also be generated and proven using symbolic summation algorithms [19], [7].

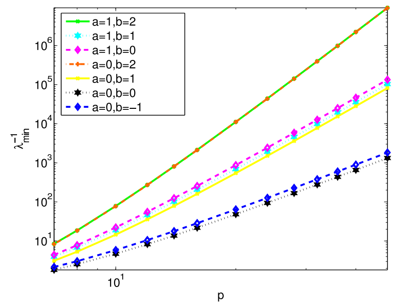


Figure 2: Inverse of minimal eigenvalue, tetrahedral case, for different choices of $a, b$

**Smoothing operator.** When working on a convergence proof for a certain finite element scheme J. Schöberl defined a smoothing operator as a weighted sum over Legendre polynomials. He was lead to conjecture that the inequality

$$\sum_{j=0}^{n} (4j+1)(2n-2j+1) P_{2j}(0) P_{2j}(x) \ge 0$$

holds for $x \in [-1, 1],\ n \ge 0$. This inequality is used to show $L^1$ boundedness of the smoothing operator's kernel.

Recently V. Pillwein [15] was able to reformulate this inequality with the assistance of the symbolic summation package `SumCracker` [7]. This rewriting lead to a computer algebra based proof of the non-negativity as well as an extension of the conjectured inequality to Gegenbauer polynomials $C_n^{\lambda}(x)$ for $\lambda \in [0, 1]$.

# 2 Special Functions and Poisson Integrals

Computer algebra tools, developed in SFB work, played a prominent role in solving special function problems arising in finite element methods; see the previous section. Of course, these tools are ready to be applied also to other areas of mathematical analysis.

Using classical analytic methods, E. Symeonidis [17] derived explicit expressions for the Poisson kernels of geodesic balls in higher dimensional spheres and real hyperbolic spaces. As a consequence, he was able to solve the Dirichlet problem for the projective space explicitly. As a by-product of his work, Symeonidis obtained indirect proofs of two new and non-trivial special function identities involving Gegenbauer polynomials $C_k^\lambda(x)$. The first identity holds for $|x| < 1$, $|t| < 1$ and integer $n > 2$, and reads as follows,

$$\sum_{k\geq 0} \frac{\binom{k+n-2}{k}}{\binom{k+\frac{n}{2}-2}{k}} t^k {}_2F_1\left(\begin{matrix} k, 1-\frac{n}{2} \\ k+\frac{n}{2} \end{matrix}; t^2\right) C_k^{\frac{n-2}{2}}(x) = \left(\frac{1-t^2}{1-2tx+t^2}\right)^{n-1};$$

the second one is of slightly more complicated form. The question for a direct proof, despite being posed to a wider audience (e.g. [14]), has been settled only recently by F. Stan in her SFB work [16]. One of the essential ingredients of Stan's proof is the RISC package *MultiSum* [19].

# 3 Applications of Gröbner Bases

## 3.1 Implementations of Gröbner Bases

In the algebraic treatment of systems of equations, involving linear operators (like partial differentiation, partial difference and so on), the choice of coefficients in equations leads us to different algebraic structures. For the case of constant (scalar) coefficients, the underlying system algebra is commutative. If the coefficients are polynomial in the variables of the system, we obtain a non–commutative $G$–algebra. Numerous algorithms, based on Gröbner bases for these two cases, are implemented in the specialized Computer Algebra System SINGULAR ([6]). The system is freely available for the non–commercial use and, moreover, is widely known for its performance. In 2004, the SINGULAR team was awarded with the Richard D. Jenks Memorial Prize for Excellence in Software Engineering for Computer Algebra. The non–commutative subsystem SINGULAR:PLURAL ([5]) handles the algebras, arising from systems with polynomial coefficients, including algebras with additional polynomial identities. For example, the algebra of linear differential operators with polynomial coefficients in trigonometric functions is realized as a factor algebra of a non–commutative algebra as follows. Let $A$ be the algebra, generated by $\{sin, cos, \partial\}$ over $\mathbb{K}$ subject to relations $\partial \cdot sin = sin \cdot \partial + cos$, $\partial \cdot cos = cos \cdot \partial - sin$ and $sin \cdot cos = cos \cdot sin$. Then, we consider the two–sided ideal $T = \langle sin^2 + cos^2 - 1\rangle \subset A$, compute its two–sided Gröbner basis (which is just $\{sin^2 + cos^2 - 1\}$ in this case) and pass to the factor algebra $A/T$.

**Extension of Gröbner Bases to Ore Localizations.** In order to treat the case where the coefficients of the system are rational functions in the variables, we employ the notion of an *Ore localization.* We extend the Gröbner bases theory to the Ore–localized $G$–algebras (not restricting ourselves to the case of so-called *Ore algebras* ([3], [4]). We show that among the criteria for discarding the critical pairs the most useful one, namely the *chain criterion*, generalizes completely to the localized case while the generalization of the *product criterion* (which is very natural for the commutative case) does not bring sufficient improvements. We started to implement Gröbner bases algorithms in the framework of SINGULAR. One of the most important and complicated tasks is to provide really efficient algorithms and their implementation for the complicated arithmetics over rings of quotients of non–commutative domains. At the time being we use a compromise approach via syzygies. The implementation is available as a combination of enhancements in the kernel of SINGULAR and a SINGULAR library `ratgb.lib` [9].

**Intercommunication packages.** With the help of recent intercommunication packages, the fast and functionally rich implementation of algorithms, relying on Gröbner bases, in SINGULAR is available to the general purpose systems, like MAPLE and MATHEMATICA.

The user–friendly and easy–to–use package, allowing MATHEMATICA to exchange data and to call numerous functions of SINGULAR externally, has been developed by Manuel Kauers (F1305) and Viktor Levandovskyy (F1301). This package [8] is available for free download.

## 3.2 Symbolic Generation and Stability Analysis of Finite Difference Schemes

For the linear PDE's with constant coefficients, the process of generating finite difference schemes may be performed symbolically, with the help of Gröbner bases for submodules of free modules over a commutative polynomial ring. We propose a more efficient method, than the one proposed in [18]. Moreover, it turned out, that using the computer–algebraic approach of *elimination of module components*, the same ideas carry over to the case of linear PDE's with polynomial and rational coefficients as well as to systems of linear PDE's.

Our method can be applied, in particular, for higher spatial dimensions without significant loss of performance. The input data consist of equations and corresponding approximation rules for the partial derivatives, written in terms of polynomials in partial difference operators like $T_x$, where $T_x \bullet u(x_j, t_n) = u(x_{j+1}, t_n)$ for discrete indices $j, n$.

For the equation $u_{tt} - \lambda^2 u_{xx} = 0$ with some initial conditions, we apply the 2nd order central approximations for both $x$ and $t$ in the vector operator form, e. g. $(-\triangle x^2 \cdot T_x,\ (1-T_x)^2) \bullet (u_{xx}, u)^T = 0$. With this symbolic data we form a submodule of a free module, involving partial difference operators. By using Gröbner bases, we eliminate certain module components from a given module and obtain a submodule, corresponding to the operators, which depend only on $u$ and not on its derivatives.

We denote $d := \lambda \triangle t / \triangle h$, and obtain the scheme, written in terms of operators,

$$d^2 T_x^2 T_t - T_x T_t^2 + (-2d^2 + 2) T_x T_t - T_x + d^2 T_t = 0.$$

Using specially developed visualization tools (e. g. the Singular library `discretize.lib`), in a semi–automatic way we are able to present the scheme above in the more convenient nodal form, namely as

$$(u_{j+1}^{n+2} - 2u_{j+1}^{n+1} + u_{j+1}^{n}) = \lambda^2 \frac{\triangle t^2}{\triangle h^2} \cdot (u_{j+2}^{n+1} - 2u_{j+1}^{n+1} + u_{j}^{n+1}).$$

In our work we discovered the *semi–factorized* form of the difference scheme. It is much more compact than the nodal form and more informative than the polynomial operator form above. For example, the semi–factorized form of the scheme above is $T_x(T_t - 1)^2 - d^2 \cdot (T_x - 1)^2 T_y = 0$. The usefulness of a semi–factorized form increases while working in higher–dimensional situation. For example, applying the same approximations as above for the 1+3D equation $u_{tt} - \lambda^2(u_{xx} + u_{yy} + u_{zz}) = 0$, both operator form and the nodal form are hardly readable, while the semi–factorized form is $T_x T_y T_z (T_t - 1)^2 - d_x^2 \cdot (T_x - 1)^2 T_y T_z T_t - d_y^2 \cdot T_x (T_y - 1)^2 T_z T_t - d_z^2 \cdot T_x T_y (T_z - 1)^2 T_t = 0$.

With these methods we are able to generate all the classical linear schemes (as it has been noted in [18]) as well as more complicated schemes, including the schemes with parametric switches.

Using the efficient implementation of Gröbner bases, the schemes for 1–dimensional in time and 1,2,3–dimensional in space equations can be computed in a few seconds.

**Von Neumann Stability Analysis.** The investigation of von Neumann stability of a given finite difference scheme can be done by symbolic methods. Moreover, for (un-)conditionally stable schemes we can perform the dispersion analysis. For both applications, the system Singular is used for polynomial computations, mappings and the translation of the output to the nodal form, standardly used in the literature on finite difference schemes. Mathematica is used for computing the Cylindrical Algebraic Decomposition, arising in the final stage of both stability and dispersion analysis.

Let us continue with the example above. We use the *stability morphism* between the rings $R = \mathbb{K}(d)[T_x, T_t]$ and $S = \mathbb{K}(d)[i, sin, cos, g]/\langle sin^2 + cos^2 - 1, i^2 + 1\rangle$, sending $T_x \mapsto sin + i \cdot cos$, $T_t \mapsto g$. Here, $sin = \sin(\alpha), cos = \cos(\alpha)$ and $\alpha = \beta \triangle x$ for some $\beta$.

After the purely algebraic simplification in the ring $S$, we obtain the stability polynomial in one variable $g^2 + 2bg + 1 = 0$, where $b := -1 + 2d^2 \sin^2(\alpha/2)$. A scheme, given by a polynomial in one variable is *von Neumann stable*, if the modulus of every root is at most 1. In our example, the stability polynomial has roots $b \pm \sqrt{b^2 - 1}$. If $b^2 > 1$, the absolute value of one of the roots is bigger than one. If $b^2 \leq 1$, the modulus of both roots is equal to 1. Moreover, $b^2 \leq 1 \Leftrightarrow d \leq 1$. Hence, the investigated scheme is conditionally stable with the condition for the Courant number $d = \lambda \triangle t / \triangle h \ \leq 1$.

We are going to apply the developed methods for finite difference schemes in cases of higher spatial dimensions, for systems of multidimensional equations, for two–step schemes like Lax–Wendroff etc.

Consider a difference scheme for an initial–boundary value problem. Assume the problem is bounded in each spatial variable. It is known, that the von Neumann condition for the difference scheme, considered as a difference scheme for an initial value problem, is a necessary condition for stability. However, when a problem is solvable by standard finite Fourier series, the von Neumann condition is both a necessary and sufficient condition; otherwise, one should consider generalized basis functions (e.g. non–standard Fourier modes). It seems that we can support the search for non–standard Fourier modes with symbolic methods.

For systems of PDE's, the von Neumann condition, in general, is only a necessary condition for stability. For equations with non–constant coefficients there is no established theory of von Neumann analysis. Applying the method of frozen coefficients and doing then the von Neumann analysis for the constant coefficients gives only very a rough picture. It is better to use so called energy methods, which have to be investigated. These and other results will appear in [10].

### 3.3 Control Theory

Given a module $M$ over an algebra $A$, we can present $M$ as a sum $M = T + F$, where $T$ is a torsion submodule of $M$ and $F$ a torsion–free submodule respectively. In Control Theory, there is a correspondence between this presentation and the decomposition of a system into a controllable part (torsion–free submodule) and an autonomous part (torsion submodule). For systems of equations, involving linear operators, the torsion submodule can be described and computed by using the tools of homological algebra ([4]), which in turn depend heavily (both algorithmically and in the implementation) on Gröbner bases.

The methods of algebraic analysis, applied to the problems of Control Theory, have been implemented ([11, 13]) in the library `control.lib` for the system Singular for the case of constant coefficients. The development of the generalization to the case of variable coefficients is in progress. It relies on the implementation of Gröbner bases in the system Singular:Plural ([5]) and on the library for non–commutative homological algebra.

**Genericity of Parameters** In systems containing parameters, it often happens that some structural properties, like controllability or autonomy, hold only for the *generic* case, that is for almost all values of parameters. It means, that there might exist such values of parameters that e.g. a generically controllable system, specialized at these values, becomes non–controllable. We provide an algorithmic way to detect such and similar phenomena, which we call the *genericity violation*. The results for 1–dimensional systems appeared in [12], while very recently [13] we gave a complete recipe to obtain all such obstructions to genericity. This includes the computation of transformation matrices between the original set of generators and its Gröbner basis as well as solving systems of equations and inequations. We successfully apply our methods and obtain, in particular, a complete solution of a problem posed many years ago.

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# F 1302: THEOREMA: Proving, Solving, and Computing in the Theory of Hilbert Spaces

**Prof. Dr. T. Jebelean, Prof. Dr. B. Buchberger**

**Dr. W. Windsteiger, Dr. T. Kutsia,**
**Dr. M. Rosenkranz, Dr. M. Giese,**
**Dr. F. Piroi,**

**DI A. Craciun, DI N. Popov,**
**DI L. Kovacs, DI G. Regensburger,**
**DI C. Rosenkranz, DI R. Vajda**

The main emphasis of the research in this subproject is on building up case studies of significant size in the main areas of interest of the SFB project: functional analysis, Groebner Bases, and basic algorithmic domains. In the course of development of these case studies we also aim to improve the functionality of our system: added proving–computing–solving power, increased usability and interaction with other projects and systems, capabilities for building-up and management of mathematical knowledge, analysis and synthesis of algorithms, etc.

The main directions of research in the reporting period have been: *theory exploration and proving in special domains*, *algorithm analysis*, and *advanced proving techniques*.

## 1 Theory Exploration and Proving in Special Domains

Our group continued to implement the scheme-based exploration of theories which are typically used in the development of mathematics and computing. In particular, in [3], we investigated in detail the aspects of building-up in a systematic manner the theory of natural numbers, which is a prerequisite for all algebraic theories (like e. g. the theory of polynomials) as well as for the elementary and advanced theories used in numerical analysis.

Moreover, we continued to develop special proving techniques for basic domains which are used in Mathematical theories: the domain of sets and the domain of real numbers.

The work described in [13] concentrates on some fundamental aspects of the design and the implementation of an automated prover for Zermelo-Fraenkel set theory within the Theorema system. The method applies the *Prove-Compute-Solve*–paradigm as its major strategy for generating proofs in a natural style for statements involving constructs from set theory.

In [1], we approach reasoning in number theory for a quite nontrivial problem (the Mordell-Weil Theorem), as we design specific inference rules and strategies for proving in number domains.

The work presented in [12] extends the capabilities of the previously developed S-decomposition method for proving in elementary analysis, by adding the usage of algebraic algorithms (in particular the Cylindrical Algebraic Decomposition) for the automatic discovery of witnesses for existentially quantified variables. This prover was used for part of the examples developed in the CreaComp project for computed aided learning.

## 2 Algorithm Analysis

An essential aspect of program analysis (in particular of program verification) is the generation of invariants for imperative loops – which is a problem closely related to the generation of preconditions and postconditions for recursive functions in functional programming. In [5], [4] we present an algorithm for finding valid polynomial relations (i. e. invariants) among program variables for imperative loops. The algorithm is implemented in the verification environment for imperative programs (using Hoare logic). We use techniques from (polynomial) algebra and combinatorics, namely Groebner Bases, variable elimination, algebraic dependencies and symbolic summation (the Gosper algorithm, handling geometric series, C-finite solving). These methods are demonstrated on several examples which have been treated completely automatically by our implementation.

This approach is further developed in [6], where we also present the relation between the problem of invariant generation in imperative programming and the problem of verification of functional programs.

The problem of verification of functional programs is approached in a specific manner in [10], [11], where we show the completeness of the method developed earlier. The specific features of this method, which are crucial for the automation of verification and proving, are, on one hand, the presence in the verification conditions of constants (functions, predicates) which belong exclusively to the theory of the domain treated by the program, and on the other hand, the usage of algebraic techniques for the discovery of the preconditions and postconditions of the auxiliary (recursive) function.

# 3 Advanced Proving Techniques

A crucial aspect of using automated reasoning both for exploring mathematical theories as well as for algorithm analysis and algorithm synthesis is the efficiency of the automatic proving engines. Our research continued to address the problem of developing new methods and strategies for automated reasoning in predicate logic and in equational logic (in particular in equational logic with sequence variables, which was pioneered in the Theorema system).

In [2] we present an adaptation of the technique of saturation up to redundancy, as introduced by Bachmair and Ganzinger, to tableau and sequent calculi for classical first-order logic. This technique can be used to easily show the completeness of optimized calculi that contain destructive rules e.g. for simplification, rewriting with equalities, etc., which is not easily done with a standard Hintikka-style completeness proof. The notions are first introduced for Smullyan-style ground tableaux, and then extended to constrained formula free-variable tableaux.

The work presented in [8] develops an algorithm for constraint solving over hedges and contexts built over individual, sequence, function, and context variables and flexible arity symbols, where the admissible bindings of sequence variables and context variables can be constrained to languages represented by regular hedge or regular context expressions. We identify sufficient syntactic restrictions that enable to solve such constraints by matching techniques, and describe a solving algorithm that is sound and complete. This approach is further developed in [7], where we describe a framework for solving equational and membership constraints for terms built over individual, sequence, function, and context variables and flexible arity symbols. Each membership constraint couples a variable with a regular expression on terms or contexts. There can be several membership constraints with the same constrained variable, and expressions may contain variables themselves. A membership constraint is satisfied if an instance of the constrained variable belongs to the language generated by the corresponding instance of the regular expression. We identify sufficient syntactic restrictions that allow us to use matching techniques for solving such constraints, describe a complete algorithm, and discuss applications.

Furthermore in [9], we describe the foundations of a system for rule-based programming which integrates two powerful mechanisms: (1) matching with context variables, sequence variables, and regular constraints for their matching values; and (2) strategic programming with labeled rules. The system is called rhoLog, and is built on top of the pattern matching and rule-based programming capabilities of Mathematica.

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# F 1303: Proving and Solving over the Reals

**Prof. Dr. J. Schicho**
**Dr T. Beck, DI B. Moore, Dr J. Pílniková**

In 2007, two quite successfull PhD theses have been defended. The thesis of Dr J. Pílniková [8] contains the development of a new method for solving certain types of Diophantine equations, based on Lie algebras. This method was used for solving the last unresolved cases in the problem of parametrizing rational surfaces over $\mathbb{Q}$. The thesis of Dr. T. Beck contains not only sparse versions of algorithms for curve parametrization, but the rudiments of an algorithm for surface parametrizations which – according to first experiments – is expected to be much faster than existing methods.

## 1 Sparse Methods for Plane Curves

Another algorithm for rational parametrization of curves has been adapted to sparse polynomials (see [2, 3]). Toric techniques can take advantage of the sparsity of the given polynomial equation of the curve. This is particularily useful in the parametrization problem because here the non-toric approach leads to complicated singularities at infinity in the case of sparse input equations. In the toric approach, this is avoided by "taking another infinity", i.e. by completing the curve not in the projective plane but in a certain toric variety, which is determined by the Newton polygon of the polynomial equation.

## 2 Formal Resolutions

Every algebraic variety over a field of characteristic zero has a resolution of singularities. However, the algorithms for computing such a resolution (due to Villamayor, Bierstone/Milman, and others) are extremely complicated and lead to large outputs. This is unfortunate because there are potential applications that could well use resolutions, for instance adjoint computation, genus computation, parametrization of algebraic surface.

We developed the concept of formal resolutions, which basically gives information about the divisors in some resolution [1]. We also implemented a computation of formal resolutions in Magma. In the examples we tried, computing formal resolutions is much cheaper than computing resolutions. For many potential applications, for instance for those mentioned above, formal resolutions actually suffice.

## 3 The Lie Algebra Method for Diophantine Problems

For finding rational points on a Del Pezzo surface of degree 9, we have developed a method based on Lie algebras [4]. The idea is compute the Lie algebra of the symmetry group of the surface and then construct an isomorphism of the Lie algebra and some well-known Lie algebra. We could adapt the method also to Del Pezzo surfaces of degree 8 [5] and of degree 6 [6].

## 4 Splitting Central Simple Algebras

Central simple algebras appear in various diophantine problems, for instance in the problem of finding points on a Severi-Brauer variety. It is often necessary to decide whether a given central simle algebra is isomorphic to a matrix algebra. This can be done by local methods. However, these local methods do not give an explicit isomorphism to a matrix algebra. For degree 3 algebras, this problem was solved in [4]. In [9], we also gave an algorithm for the degree 4 case.

## 5 The Casas-Alvero Conjecture

In a field of characteristic zero, it is clear that the $d$-th power of a linear polynomial has a non-trivial common factor with each of its first $d-1$ derivatives. The converse has been conjectured by Casas-Alvero. The conjecture was proved for $d \leq 8$ with the help of computer algebra using Gröbner bases computation. Together with H.-C. von Bothmer, O. Labs, and C. van de Woestijne, we proved the conjecture for $d$ being a prime power and for twice a prime power. Hence the lowest possible degree for which the conjecture is still open is now 12, followed by 15 and 20.

This cooperation grew out of a joint discussion that started during the special semester on Gröbner bases held at RICAM in the first half of 2006. The discovery of the results was aided by experimental calculations in Singular, Magma, Macaulay2 and Maple. The final proof does not contain computer algebra; it is based on reduction techniques modulo primes.

## 6 Topology meets Algebra

In a group $G$, a function $f : G \to G$ is called polynomial iff it can be written as a product of constants, the argument, and the inverse of the argument. (In general signatures, a function from a structure is called polynomial iff it can be expressed by the available function symbols and constants.) Together with pointwise multiplication and functional decomposition, the set of all polynomial functions forms a near ring, and it is of interest to study this structure for various groups.

For the group $G = \mathrm{GL}(2, \mathbb{R})$, algebraic techniques do not suffice to decide the question whether transposition is a polynomial. We could answer this question negatively by topological methods, in a cooperation with G. Landsmann and P. Mayr from the University of Linz [7].

## 7 Balancing Parallel Robots

Together with C. Gosselin from Naval University, Quebec, Canada, we studied the problem of devising a robot manipulator that does not exert forces (static balancing) or torques (dynamic balancing) to the base during its moves (see Figure 3). This is relavant for robotics applications in optics and in aeronautics.

For the easiest parallel manipulator, the planar four-bar linkage, generic solutions have been known since 1965, and Gosselin detected a new solution. Using methods of toric geometry, we could now give a complete description of all solutions.

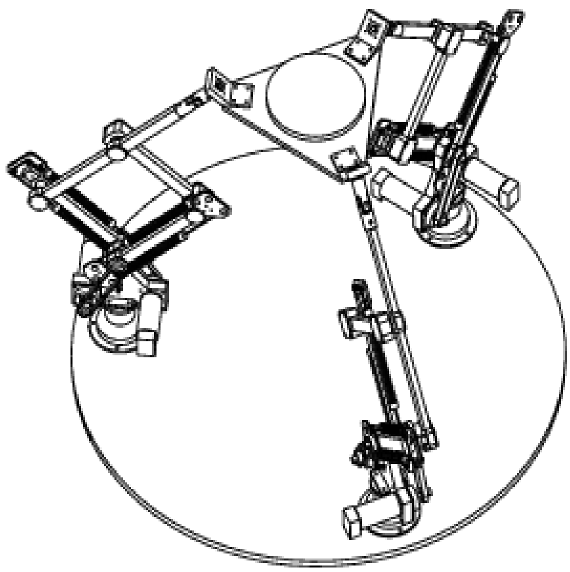

Figure 3: balancing parallel robot

## 8 Quadratic Bezier Clipping

Together with B. Juettler, a new geometric method based on the Bezier clipping approach has been developed to compute the intersections of two plane algebraic curves on a given domain. Part of the family of interval reduction approaches, it iteratively computes increasingly accurate domains in which the roots lie, until a certain accuracy is reached.

The new method has several advantages: it find all real solutions, it is numerically stable due to the use of Bernstein-Bezier basis and it could be extended to an interval computation approach, thus giving a bound on the numerical error of the solutions.

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# F 1304: Symbolic Differential Computation

Prof. Dr. F. Winkler
Dr. H. Gu, Dr. E. Kartashova
DI E. Shemyakova

This report covers the period from January 2006 until December 2006. During this period we have investigated factorization of linear partial differential operators, invariants for linear partial differential operators, differential characteristic sets, symbolic-numerical methods for polynomial equation solving, differential equations in mathematical physics, and computer algebra in general.

## 1 Factorization of Linear Partial Differential Operators

In the previous year our group has started to work on algorithms for factoring LPDOs. In their seminal paper Grigoriev and Schwarz have shown how this factorization problem can be reduced to the solution of algebraic and often linear equations over the field of coefficients. This algorithm has been investigated further by Kartashova in [5] and [14]. Shemyakova and Winkler have considered situations in which the factorization algorithm fails to produce factors [17], [18]. These conditions of failure (obstacles) form an interesting algebraic structure and can be used to measure how far an operator is from a factorizable one.

## 2 Invariants for linear partials differential operators

The work on factorization leads in a natural way to invariants for LPDOs under certain (gauge) transformations. Kartashova has presented a hierarchy of invariants for bivariate LPDOs in [6]. In [16] Shemyakova and Winkler have sketched how a full system of invariants can be determined for low order (order 3) operators. Such a full system has been derived rigorously by Shemyakova in [15].

## 3 Differential characteristic sets

Differential characteristic sets have been introduced by Ritt as a tool in differential elimination theory. They allow to find elements of lowest order or depending only on certain partial derivations in ideals of LPDOs. Aistleitner has received a scholarship for some months in 2004 to work on a diploma thesis for implementing differential characteristic sets in a generic way. He has completed his diploma thesis in December 2005 [1] and finished his diploma studies early in 2006. Parts of his diploma thesis have been presented at the Rhine Workshop on Computer Algebra [2].

## 4 Symbolic-numerical methods for polynomial equation solving

Gu has cooperated within the SFB (M. Burger) [3] and also outside the SFB (H. Herrmann (Institut f. Theoretische Physik, TU Berlin) [4]. In these cooperations Gu could demonstrate successfully his symbolic-numerical solutions method for polynomial equation solving.

## 5 Differential equations in mathematical physics

E. Kartashova has worked on the analysis of differential equations arising in theoretical physics. Her work is mainly directed towards laminated wave turbulance and resonances amoung gravity waves [7] [11] [8] [12] [13] [10] [9].

## 6 Computer algebra

In a previous phase of the SFB Winkler has worked on symbolic computation problems of algebraic curves. A paper concerning this work has finally been published [19]. Winkler has discussed these methods also in invited talks at Aristotle University in Thessaloniki [22] and at the Erwin Schrödinger Institute in Wien [24].

Winkler has worked on problems of differential elimination theory, in particular on a Gröbner basis algorithm for rings of linear partial differential operators [20] [21].

A general discussion of problems in computer algebra was given in [23].

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# F 1305: Proving and Solving in Special Function Domains

**Prof. Dr. P. Paule**
**Dr. M. Kauers, Dr. C. Schneider**
**DI C. Koutschan, Mag. B. Zimmermann**

The scientific output achieved in 2006 by the SFB project group F1305 is documented in the form of 33 publications: 22 articles were (or will be soon) published in journals and 4 in conference proceedings; 7 technical reports have been produced.

## 1 Identities

Schneider's summation algorithms implemented in the summation package Sigma [32] were the basis for solving various non-trivial multi-sum problems. E.g., it is shown that a quadruple sum expression evaluates to zeta-functions [28, 33], or identities were proven in the context of Padé approximation [6, 7] and supercongruences [26]. In particular, it is demonstrated that the derivation of the key recurrences in Apery's proof (the irrationality of $\zeta(3)$) becomes trivial [29] by using Schneider's algorithms. Moreover, a proof of an identity [32, Section 10.2] in the Handbook of Mathematical Functions (Abramowitz/Stegun) was produced whose original proof has been lost; several other such identities are proven in joint work of the F1305-group. In cooperation with C. Schneider, B. Zimmermann and S. Gerhold (former member of F1305), the asymptotic behavior of one-dimensional Schelling population models could be derived [8]. Moreover, P. Paule and C. Schneider generalized identities arising in the field of statistics [27]. Besides this, in cooperation with J. Schöberl and V. Pillwein (see F1301), recurrences were computed that can speed up the computations in Finite Element Methods [5]. As worked out in [30], it is remarkable that symbolic summation tools, in particular telescoping and creative telescoping, allow to prove algebraic independence of certain classes of sums; for instance the harmonic numbers $\{H_n^{(i)} | i \geq 1\}$ with $H_n^{(i)} = \sum_{k=1}^{n} \frac{1}{k^i}$ are algebraically independent.

Besides refined difference field theory [31] various generalizations of summation algorithms have been accomplished. Due to Schneider's and Kauers' cooperation it is now possible to treat also generic (unspecified) sequences [21, 20] and radical sequences [22], like $\sqrt{n}$, within given summation problems.

Using different techniques, M. Kauers's developed new algorithms [17] that can discover and prove sum identities involving, e.g., Stirling numbers. His work on algorithms and software for the class of "admissible sequences", which he studied in his thesis, has lead to a couple of new extensions. His implementation of these algorithms [13, 14] in form of the Mathematica package SumCracker is able to prove and to discover identities which were previously considered out of scope of symbolic computation. Examples include properties of Somos sequences, nested C-finite expressions, orthogonal polynomials, continued fractions, etc. Some of these computations exceed the capabilities of Mathematica's Gröbner basis engine, which is used by default inside SumCracker. Therefore, V. Levandovsky (F1301) and Kauers have implemented an interface linking Mathematica and Singular [18], a special purpose CAS allowing fast Gröbner basis computations.

In a cooperation of Kauers and Zimmermann, an algorithm for determining the algebraic relations among C-finite sequences was found [23]. This algorithm solves an important subproblem arising in symbolic summation of special sequences; e.g. concerning identities like in [11]. In another article [12], Kauers gives an algorithm for solving another important subproblem arising in symbolic summation, namely the problem of deciding shift-equivalence of P-finite sequences.

## 2 Inequalities

In 2005, Gerhold and Kauers have proposed a procedure for automatically proving inequalities among expressions that are defined via recurrence equations. With this procedure it is possible to verify a large number of inequalities appearing in the literature by applying a computer procedure. This was an unexpected success in view of the fact that special function inequalities have generally been viewed as inaccessible to symbolic computation. A remarkable example is the computer proof of Turán's inequality for Legendre polynomials [9], of which a new refinement [1] has been derived. A conjectured inequality which arose in the numerical work of J. Schöberl (F1319) has been explored with these new methods; see [10]. Moreover, a long-standing log-concavity conjecture related to the closed form of a certain quartic integral could be proven with our computer algebra methods; see [19]. Furthermore, the article [15] concerns automated proofs of positivity of the Taylor coefficients in the expansion of multivariate rational functions. An overview of these activities is given in [16].

# 3 Other aspects

C. Koutschan completed his work on the inverse Schützenberger methodology which is based on Soittola's Theorem (concerning the $\mathbb{N}$-rationality of formal power series); see [25]. The $\mathbb{N}$-rationality test can be performed by his Maple package RLangGFun. C. Koutschan started to cooperate with H. Hauser, Innsbruck, in order to illuminate the properties of the generating function of linear multivariate recurrences. Result: The reformulation of such a recurrence as a division with remainder leads to a better understanding of the corresponding generating function. The results are submitted for publication [24].

The longterm collaboration between the principal investigator and G. Andrews (Penn State) on partition analysis was continued and has led to significant progress [2, 3, 4]. Within F1305, the Mathematica package Omega was developped; it provides an algorithmic version of MacMahon's Omega calculus. More than a century ago MacMahon had invented this calculus in order to prove a conjecture about the form of the generating function for plane partition. However, at that time the conjecture remained open because of the immense computational complexity required by his method. Now, with the availability of both computers and sophisticated computer algebra software, MacMahon's dream has come true [2] and [4].

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# F 1306: Nonlinear 3D Mechanical Problems

**Prof. Dr. U. Langer, Prof. Dr. J. Schöberl**
**DI. P. G. Gruber, DI. J. Kienesberger**
**Dr. J. Valdman, Dr. S. Beuchler**

The development of adaptive multilevel methods for nonlinear 3D mechanical problems is the topic of this project. The main focus in the past year was to enhance the already existing fast and robust solvers for 2D and 3D elastoplastic problems.

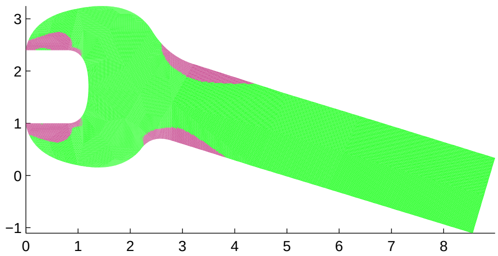


Figure 4: A screw wrench when pressed down: The plot shows elastic *(green)* and plastic *(pink)* zones.

Elastoplastic materials are modeled by the decomposition of the strain into an elastic and a plastic part; the equilibrium of forces and the linear dependence of the stresses on the strains are then inherited elastic laws. The term describing the plastic strain is zero if the forces acting on the body are small enough such that the material behaves only elastically.

If the stresses in the considered body exceed a certain threshold, the plastic strains become nonzero. Figure 4 shows a screw wrench under heavy load, such that plastic deformations take place. The time evolution of the plastic strain is described by the Prandtl-Reuß normality law. After time discretization, the modeling process in each time step yields a minimization problem in two variables, namely the displacement $u$ and the plastic strain $p$. One has to find $u$ and $p$, such that the identity

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

is satisfied under some additional incompressibility constraint. The objective $f$ is smooth in the displacement, but non-smooth in the plastic strain. The central issue for the development of efficient solvers is to overcome this non-smoothness.

The first class of algorithms is based on the regularization of the objective, where the modulus is smoothed such that the proximate objective $f_\epsilon$ is twice differentiable. These techniques were studied by J. Kienesberger and are summarized in her PhD thesis [6].

A major progress was achieved by finding, that due to a theorem of J. J. Moreau in the scope of convex analysis, one can avoid to regularize the original functional $f$. Notice, that the formula for minimizing $f(u,p)$ with respect to the plastic strain $p$ for a given displacement $u$ is already known explicitly, i. e., we know a function $\tilde{p}(u)$, such that there holds

$$F(u) := f(u,\tilde{p}(u)) = \inf_q f(u,q)\,.$$

Thus, there remains to solve a minimization problem with respect to only one variable, $F(u) \to \min$. The theorem of Moreau says, that due to the certain structure of $f(u,p)$, the functional $F(u)$ is Fréchet differentiable and strictly convex. Moreover, the explicit form of the derivative is provided also. Hence, it suffices to find $u$ such that the first derivative of $F$ vanishes. This approach was first discussed in the master thesis [2] of P. G. Gruber.

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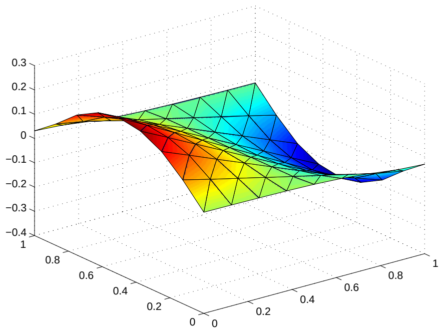
| 1-2 | 2.559e-03 | 9.493e-04 | 2.478e-04 | 9.472e-05 |
| 2-3 | 5.274e-05 | 3.859e-05 | 8.815e-06 | 2.776e-06 |
| 3-4 | 1.814e-08 | 1.250e-07 | 1.147e-09 | 1.357e-08 |
| 4-5 | 5.741e-15 | 1.337e-13 | 3.872e-15 | 1.388e-14 |
| res: | | | | |
| 0 | 7.471e+02 | 5.410e+02 | 3.423e+02 | 1.977e+02 |
| 1 | 2.619e+01 | 1.186e+01 | 3.144e+00 | 1.237e+00 |
| 2 | 5.991e-01 | 3.939e-01 | 1.207e-01 | 3.793e-02 |
| 3 | 2.209e-04 | 1.711e-03 | 1.234e-05 | 1.862e-04 |
| 4 | 7.575e-11 | 1.756e-09 | 1.687e-10 | 3.653e-10 |
| 5 | 4.131e-11 | 8.289e-11 | 1.698e-10 | 3.437e-10 |
| sec: | 15 | 54 | 227 | 1081 |

Table 1: This table outlines the convergence of the Newton-like method. In horizontal direction, the refinement of the starting mesh takes place, where the degrees of freedom (`dof`) are growing roughly by a factor 4. In the last line (`sec`) the computational time is displayed in seconds. The two blocks in between the first and the last line report on the convergence behavior. The first block (`dis`) displays the distance of two consecutive Newton iterates $|u_{j+1} - u_j|$ measured in the $H^1$ semi norm, the second block (`res`) shows the $l_2$ values of the residual, i. e., the right hand side of Newton's method.

The second derivative of $F$ does not exist. As a remedy, the concept of slanting functions, introduced by X. Chen, Z. Nashed, and L. Qi, allows for the application of a Newton-like method. In [3], P. G. Gruber and J. Valdman prove the local super-linear convergence of the resulting solver in the spatial discretized case (see Table 1), and formulate sufficient regularity conditions, which would guarantee superlinear convergence in the nondiscretized case also.

J. Valdman, in cooperation with C. Carstensen and A. Orlando (both HU Berlin), established an adaptive finite element algorithm for the solution of elastoplastic problems. Such algorithm yields an energy reduction and, up to higher order terms, the $R-$linear convergence of the stresses with respect to the number of loops. Applications include several plasticity models: linear isotropic-kinematic hardening, linear kinematic hardening, and multi-surface plasticity as a model for nonlinear hardening laws. The work led to a journal publication, see [1].

A. Hofinger from Project F1308 and J. Valdman also concentrated on fast calculation techniques for the two-yield elastoplastic problem, which is a locally defined, convex but non-smooth minimization problem for the unknown plastic-strain increment matrices $p_1$ and $p_2$. Their results were summarized in a technical report [4] and were also accepted for a journal publication, see [5].



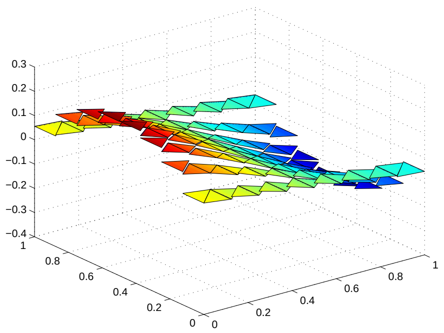


Figure 5: Flux function (its x-component) using nodal *(top)* and Raviart-Thomas *(bottom)* elements.

J. Valdman continued the cooperation with S. Repin (St. Petersburg) on reliable error estimates for scalar problems. Their research on estimates for scalar problems with the nonlinearity on the boundary was documented in a joint technical report [7].

Another issue being studied is the computational efficiency of so called "functional estimates". Let us consider the boundary value problem

$$-\triangle u = f \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \partial\Omega.$$

Then, one can find a norm estimate of the form

$$||\nabla(u - v)||_0 \leq ||\nabla v - y^*||_0 + C_\Omega||\text{div} y^* + f||_0$$

which is valid for all $y^* \in H(\Omega, \text{div})$ and for all $v \in H_0^1$. The constant $C_\Omega$ is known from Friedrich's inequality and can be computed independently. The interpretation of this formula is that any "flux" function $y^*$ provides us with a guaranteed upper bound for the energy error of the computed solution $v$. The right term in the inequality can be minimized in a way, the upper bound becomes the smallest possible. The pictures presented in Figure 5 demonstrate possible "fluxes" using nodal continuous and normal component continuous (Raviart-Thomas) elements.

Such minimization leads to a linear system of equations as a part of the global nonlinear minimization process. J. Valdman explored these linear systems and applied a multigrid based solver in order to obtain the optimal convergence.

The joint work will be extended to problems of elasticity with so-called friction boundary conditions and to elastoplasticity as well.

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# F 1308: Computational Inverse Problems and Applications


Prof. Dr. H. W. Engl, Prof. Dr. M. Burger

Dr. H. Egger, Dr. B. Hackl, Dr. L. He,
Dr. A. Hofinger, Dr. S. Kindermann,
Dr. H. K. Pikkarainen, Dr. M. Sini,
DI M. T. Wolfram
Dr. P. Kügler (Basic Staff)


## 1 Bayesian Approach to Inverse Problems

The research on stochastic inverse problems in the Project F1308 has been continued in 2006, following previous studies ([9, 15]). The main idea there was to extend the deterministic regularization theory for linear and nonlinear inverse problems to a stochastic setting using stochastic metrics such as the Ky-Fan metric and the Prokhorov metric.

This framework has now been used to develop a convergence theory for linear and nonlinear inverse problems using the Bayesian approach. Contrary to the deterministic or frequentist viewpoint, in Bayesian theory the solution to an inverse problem is not an unknown function but a probability distribution – the so-called posterior distribution – on the space of unknowns. The posterior distribution is constructed from the model, the given noise distribution and the prior distribution using Bayes' rule. The prior distribution represents information on the unknown thought to be available prior to the measurements. From the posterior distribution, one constructs estimates of the unknown solution using point estimators (e.g., the MAP-estimator or the conditional mean estimator).

As the solution of the inverse problems is then a probability distribution, the classical convergence theory in Hilbert spaces cannot be applied, but stochastic metrics have to be used. In [18, 19] a convergence theory for the Bayesian setup was developed using the Ky-Fan metric and the Prokhorov metric; so far, this was only possible for finite-dimensional linear problems with Gaussian assumptions. Nevertheless, it should be noted that these are the first quantitative convergence results for the Bayesian approach to inverse problems. As a main condition, the variance in the prior distribution has to be related to the noise-level in order to guarantee convergence. With this convergence theory, it is also possible to obtain confidence interval estimates for the MAP-estimator.

Besides the Bayesian approach, the stochastic convergence theory of regularization ([9, 15]) has been further extended in [16, 14, 17]. As an application of this theory an ongoing project has been started with the aim of identifying the nucleation rate in a mesoscale crystal birth-and-growth model. This model involves stochasticity since the birth of a crystal is described by a random process. Of particular interest is the case when the process is influenced by external random variables (doubly stochasticity). In this case the inverse problem of identifying the kinetic parameters of the crystallization process leads to an inverse problem which stochasticity. The analysis and solution of this problem by regularization heavily relies on the stochastic convergence theory for Tikhonov regularization mentioned above. This is a collaboration of V. Capasso (University of Milan), H. W. Engl and S. Kindermann.

## 2 Image Processing

A well-known method in image processing is based on a minimization of the Rudin-Osher-Fatemi (ROF) functional. This functional has been used for tasks such as denoising, deblurring or impainting. Recently, several modifications of the classical ROF-method have been proposed and applied. One of the ideas was to replace the original minimization problem by an iterative method much in the spirit of iterative Tikhonov regularization, which led to the Bregman iteration algorithm. The original idea of Bregman iteration was analyzed in more detailed and generalized to other applications. Research on this topic has been carried out by M. Burger and L. He, who joined the SFB in July 2006. The Bregman iteration was extended to non-quadratic functionals in [11], and error estimates were proven in [6]. Moreover, viewing this iteration as a discrete version of an evolution equation, in the limit, the Bregman iteration tends to a so-called inverse scale space flow. The corresponding equations were investigated from a theoretical point of view in [3]. For their numerical computation, a new method was proposed and implemented by M. Burger in collaboration with G. Gilboa and S. Osher in [4].

Another generalization of the original ROF-model allows for anisotropy in the functional. This idea has been used for the classification of aerial images in [2].

## 3 Inverse Scattering

Inverse Scattering deals with the reconstruction of objects from measurements of the far-field pattern of (acoustic or electromagnetic) waves scattered by these objects. Research on such type of problem attracted attention within this project by the work of M. Sini, who joined the SFB in September 2006. The main focus in the project is the reconstruction of complex obstacles, i.e., simultaneously finding the shape of the obstacle as well as material properties of its surface (e.g. sound-hard or sound-soft or mixed) [24, 25]. If measurements for multiple incident waves are available, it is known that this information is enough to reconstruct both shape and surface properties from far-field measurements. Although several well-known numerical algorithms for the reconstruction of shapes (e.g. probing method, sampling method) are nowadays widely used, less is known for the complex obstacle case. In a recently started cooperation between M. Sini, L. He and S. Kindermann, the aim is to develop new algorithms which are able to find the properties of complex obstacles. The idea is to improve probing methods by combining them with level-set iterations and regularization in order to obtain a more precise reconstruction.

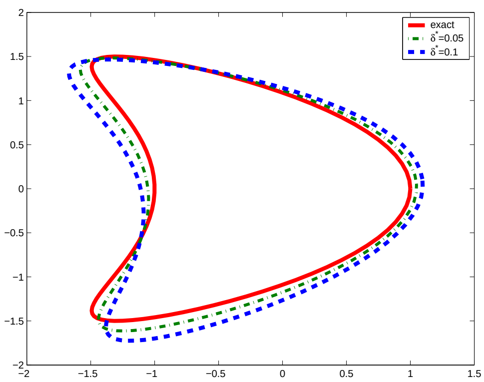


Figure 6: Inverse Scattering: Reconstructions of a shape by the probing method.

## 4 Level Sets

In the year 2006, the work on level set methods for geometric inverse problems has been continued. One of the new aspects was to further investigate the coupling between the level set methods and the topological derivative [12]. Such a coupled algorithm has been successfully applied to image segmentation in [13]. Furthermore, continuing previous work, theoretical questions for the level set method in linear elasticity have been studied. The problem of finding inclusions from measurements of boundary displacements was considered, and stability estimates for the level set method were proven in [1]. In 2006, B. Hackl finished his PhD-thesis [10], which investigated the use of second order derivative information to improve algorithms based on topological derivatives.

Related to the work on anisotropy in image processing, a similar level set evolution including anisotropy has been proposed and investigated in [5].

An alternative to the level set method for interface problems has been developed in [23]. The procedure there is not based on evolution equations, but on minimizing Tikhonov functionals combined with thresholding.

## 5 Regularization

Several contributions were made to the theory of regularization of ill-posed problems. H. Egger, who left the SFB in March 2006, continued his work on preconditioning of iterative regularizations. The improvement of preconditioning on the conjugate gradient iteration for ill-posed problems was analyzed in [8]. Furthermore, Newton-type method were accelerated by using advanced iterative methods for solving the Newton equations [7].

In [21], a new regularization method was proposed based on the idea of dynamic programming.

## 6 Cooperations

In a cooperation with SFB project F1306, an improvement of the numerical calculations for a two-yield problem in elastoplasticity was made [20]. This new algorithm could significantly reduce the number of total iterations needed to compute a solution to a certain accuracy.

The cooperation with the RICAM finance group on the identification of parameters in option price models was continued. In previous work by Egger and Engl, Tikhonov regularization was successfully applied to volatility identification in Black-Scholes type models. A similar methodology was used to compute a local speed function in a Levy model which is a generalization of the Black-Scholes model. In [22], it was shown that Tikhonov regularization yields a stable method and convergence rates were shown. A numerical procedure to find the unknown parameters in this model from observed data was developed.

## 7 Personnel Development

B. Hackl finished his PhD in September 2006 and left the SFB. A. Hofinger finished his PhD in April 2006 and also left the SFB. H. Egger left the SFB for a research position at the University of Aachen. M. Burger accepted a position as Professor for Applied Mathematics at the Westfälische Wilhelms Universität Münster in October 2006. M. T. Wolfram joined the research group of M. Burger at the University of Münster.

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# F 1309: Multilevel Solvers for Large Scale Discretized Optimization Problems

**Prof. Dr. U. Langer, Prof. Dr. H. W. Engl, Prof. Dr. W. Zulehner, Dr. E. Lindner, Dr. R. Stainko, C. Pechstein, R. Simon**

## 1 PDE-Constrained Optimization Problems

During the last year, we focussed our work on efficient solution techniques of large-scale systems of optimization problems with constraints described by a partial differential equation (PDE) or by a system of PDEs. There are basically two approaches for such problems. Under proper conditions, the constraining PDE, mostly called the state equation, can be eliminated and formally hidden in the objective functional. In comparison to this classical nested formulation, there exists the simultaneous formulation, where the state equation is treated as constraint. Using this approach, one can solve the optimization problem by solving the corresponding system of optimality conditions, the Karush-Kuhn-Tucker (KKT) system. This leads to large scale symmetric, but indefinite systems of the form

$$\begin{pmatrix} A & B^T \\ B & -C \end{pmatrix} \begin{pmatrix} x \\ p \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}, \qquad (1)$$

which are solved by iterative methods.

In particular, we considered elliptic optimal control problems. In such problems the primal unknown $x$ consists of two parts: the state $y$ and the control $u$. The problem is to find $x = (y, u)$ that minimizes a given cost functional subject to a constraint, the so-called state equation, which, for each control $u$, is an elliptic boundary value problem in $y$. It is typical for such problems that the cost functional contains an extra regularization parameter.

## 2 Multigrid Methods for KKT

In principle, there are two different approaches to take advantage of the multigrid idea. One way is to use an outer iteration, typically a preconditioned Richardson method (possibly accelerated by a Krylov subspace method), applied to the discretized problem. The preconditioners of KKT systems usually rely on efficient solvers or preconditioners for the underlying PDEs and on the construction of a good preconditioner for the corresponding Schur complement. Multigrid techniques (as an inner iteration) can be used for (some or all of) these components. For control problems with elliptic state equations and distributed control, J. Schöberl and W. Zulehner proposed a special indefinite preconditioner for the KKT system which leads to convergence rates of the preconditioned conjugate gradient method that are not only independent of the mesh size but also independent of the regularization parameter, see [4].

The other way is to use multigrid methods directly applied to the KKT system as an outer iteration based on appropriate smoothers (as a sort of inner iteration). For PDE-constrained optimization problems this approach is also known as one-shot multigrid strategy. One of the most important ingredient of such a multigrid method is an appropriate smoother.

One class of smoothers are point smoothers, where the variables are grouped pointwise (with respect to the nodes of the underlying mesh) and one or several sweeps of point-block Jacobi or point-block Gauß-Seidel iterations are performed, see [1].

A natural extension are patch smoothers: The computational domain is divided into small patches, see Figure 7.

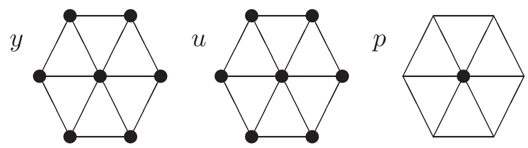


Figure 7: local patch

One iteration step of the smoothing process consists of solving local saddle point problems on each patch one-by-one either in a Jacobi-type or Gauß-Seidel-type manner. This results in an additive or multiplicative Schwarz-type smoother. The general construction and the analysis of patch smoothers for mixed problems was discussed in [3], where a particular patch smoother was proposed for the Stokes problem. A straight forward application of this construction to KKT systems for elliptic control problems fails, since an essential feature exploited in the multigrid convergence analysis of the Stokes problem was the positivity of (1,1)-block everywhere, whereas in optimal control problems the (1,1)-block is usually positive only on the kernel of the (2,1)-block. We successfully extended the construction to KKT systems arising in optimal control problems, see [5], using an augmentation technique for the approximation of the (1,1)-block in the smoothing step to ensure the positivity everywhere. Table 2 contains the (averaged) convergence rates for different numbers of smoothing steps. The numerical results show the typical multigrid behavior, namely the level-independence of the convergence rate and the improvement of the rates with an increasing number of smoothing steps.

| | | smoothing steps | | |
|---|---|---|---|---|
| level | $n_h + m_h$ | 5+5 | 7+7 | 10+10 |
| 5 | 3 267 | 0.668 | 0.538 | 0.411 |
| 6 | 12 675 | 0.679 | 0.578 | 0.455 |
| 7 | 49 923 | 0.685 | 0.587 | 0.467 |
| 8 | 198 147 | 0.685 | 0.588 | 0.469 |
| 9 | 789 507 | 0.685 | 0.589 | 0.469 |

Table 2: Convergence rates for the additive Schwarz smoother

The multigrid convergence analysis for KKT systems of PDE-constrained optimization problems is not as developed as for elliptic PDEs. One line of argument exploits the fact that the reduced KKT system (by eliminating the control) is a compact perturbation of an elliptic problem. This guarantees the convergence of the multigrid method if the coarse grid is fine enough. A second strategy is based on a Fourier analysis, which covers only the case of uniform meshes with special boundary conditions. Both strategies applied to optimal control problems can be found in [1].

A classical technique for analyzing the convergence of multigrid methods relies on two properties: the approximation property and the smoothing property. In [5] we were able to prove both properties, which led to a rigorous convergence analysis of the corresponding multigrid method.

## 3 Topology Optimization Problems

R. Stainko finished his PhD-thesis and graduated in April 2006. His work deals with mathematical methods for topology optimization problems. In particular, he considered two specific design - constraint combinations, namely the maximation of material stiffness at given mass and the minimization of mass while keeping a certain stiffness.

The first problem, also known as the minimal compliance problem, is solved by an adaptive multilevel approach. The resulting optimization problems on each level are solved by the method of moving asymptotes. For the efficient solution of the linear systems, raising from the finite element discretization of the PDEs, a multigrid method is applied.

In the treatment of the second combination, the main source of difficulties is a lack of constraint qualifications for the set of feasible designs, defined by local stress constraints. A reformulation of the constraints overcomes this problem. These are finally relaxed by a phase-field approach, which also regularizes the problem, see [2]. This relaxation scheme results in large scale optimization problems, which are finally solved by an interior-point method. Applying a multigrid method with a similar Schwarz smooting technique to the KKT system leads to an optimal solver, see [6]. A picture showing the optimal material distribution of benchmark beam w.r.t. local von Mises stress constraints can be found in Figure 8 (red indicates material, blue indicates air).

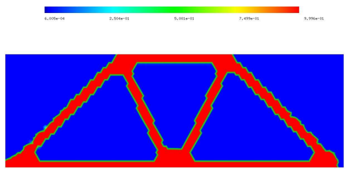

Figure 8: Optimal material distribution

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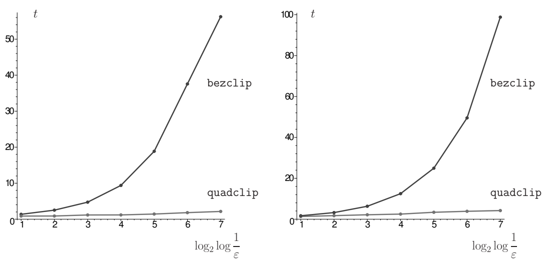
# F 1315: Numerical and Symbolic Techniques for Algebraic Spline Surfaces

Prof. Dr. J. Schicho, Prof. Dr. B. Jüttler
Dr. M. Aigner, Dr. M. Bartoň,
Dr. P. Chalmovianský, Dr. M. F. Shalaby
DI M. Kapl

The work in this subproject was devoted to several tasks.

## 1 Polynomial equations

We presented an algorithm which is able to compute all roots of a given univariate polynomial within a given interval. In each step, we used degree reduction to generate a strip bounded by two quadratic polynomials which encloses the graph of the polynomial within the interval of interest. The new interval(s) containing the root(s) is (are) obtained by intersecting this strip with the abscissa axis. In the case of single roots, the sequence of the lengths of the intervals converging towards the root has the convergence rate 3. For double roots, the convergence rate is still superlinear ($\frac{3}{2}$). We showed that the new technique (algorithm `quadclip`) compares favorably with the classical technique of Bézier clipping (algorithm `bezclip`). An example can be seen in Figure 9. For future work we will focus on the extension of the technique to the multivariate case. [2]




$n = 4$ $n = 8$

Figure 9: Computing time $t$ in $10^{-5}s$ vs. accuracy for a polynomial of degree $n$ in the case of double roots.

## 2 Approximate implicitization

We compared several methods for approximate implicitization by polynomials and by piecewise polynomials. We investigated both quantitative criteria (such as computing time, memory use, and the error of the approximation) and qualitative criteria. As demonstrated by the results, piecewise approximate implicitization was able to handle surfaces arising in industrial applications. Figure 10 shows that the two goals of reproducing singularities and avoiding unwanted branches are often in conflict with each other. Further research will focus on the important issue of avoiding unwanted branches and additional singularities. [9]

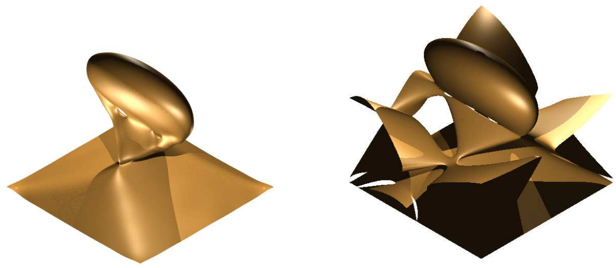


Figure 10: Reproducing singularities vs. avoiding unwanted branches.

## 3 Robustness of implicitization

We considered the following problem: given a curve in parametric form, compute the implicit representation of another one that approximates the parametric curve on a certain domain of interest. We studied this problem from the numerical point of view: what happens with the output curve if the input curve is slightly changed? It was shown that for any approximate parameterization of the given curve, the curve obtained by an approximate implicitization with a given precision is contained within a certain perturbation region. [1]

## 4 $B$-$H$ curves

$B$-$H$–curves are used for modeling ferromagnetic materials in connection with electromagnetic field computations. Starting from real–life measurement data, we have presented an approximation technique which is based on the use of spline functions and a data–dependent smoothing functional. It preserves physical properties, such as monotonicity, and is robust with respect to noise in the measurements. [7]

## 5 Weighted spline wavelets

Our work was focused on finding a wavelet representation of implicitly defined spline curves for which the region of interest - the curve - is preserved better than for existing uniform wavelets. For this purpose we have constructed the so called weighted spline wavelets. Weighted spline wavelets are wavelets that are adapted to the region of interest by means of a weighted inner product. Figure 11 shows an example of a weighted wavelet construction. Furthermore we constructed lazy wavelets for periodic $B$-splines of degree $d > 1$. Lazy wavelets are wavelets with poor approximation properties but with simple analysis and synthesis filters. For future work we will use the concept of weighted wavelets to construct semiorthogonal weighted wavelets, i.e. semiorthogonal wavelets with respect to a weighted inner product. [5, 6]

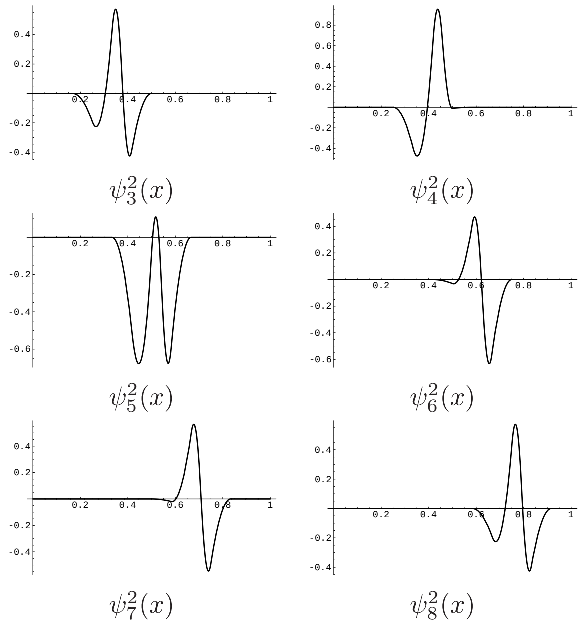



Figure 11: Example of weighted wavelets $\psi_i^2$ for 1-periodic uniform $B$-splines of degree 2.

# 6 Other activities

The work in this subproject led to numerous further activities which can be found in [3, 4, 8, 10].

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# F1322: Computer Algebra for Pure and Applied Functional Analysis

**Prof. Dr. B. Buchberger, Prof. Dr. H.W. Engl**

**Dr. M. Rosenkranz, Dr. G. Regensburger**

Project F1322 deals with the symbolic computation aspects of operators that typically occur in analysis (e.g. differential, integral, and boundary operators). Their algebraic features are captured by noncommutative polynomial identities describing interactions between certain basic operators. For this purpose, the TH∃OREM∀ system [1, 21] provides a generic language and a flexible framework (see Project F1302) for dealing with various polynomial notions [12], both in an inferential and computational setting; in particular, Gröbner bases methods can be applied.

In 2006, we have extended and generalized the concept/methodology of boundary problems in two major directions—one in differential rings and algebras, the other in (infinite-dimensional) vector spaces. Research on generalized solutions for nonlinear first-order ordinary boundary problems has been focused on interpolation methods in max-plus algebras. In our work on parametrized wavelets, we have studied various new applications. In the first half of the year, we have been engaged in the Special Semester on Gröbner Bases and Related Methods.

## 1 Boundary Problems in Differential Algebra

The classical setting of two-point boundary problems [10, 13] has been formulated in a completely abstract setting that refers to a wide class of differential algebras [18]. Besides the usual two-point boundary conditions, it allows arbitrary Stieltjes boundary conditions for building up regular boundary problems. Setting up a multiplication that mirrors the composition of Greens operators, the resulting monoid structure is analyzed: Any factorization of the underlying linear differential operator can be lifted (algorithmically!) to a decomposition of boundary problems. See [11, 15, 14, 17] for details.

## 2 Abstract Approach to Boundary Problems

In the more abstract approach of [9], the theory does not rely on any notion of differentiation, defining a boundary problem as an arbitrary linear endomorphism on a vector space together with an orthogonally closed subspace of its dual. Despite its generality, this approach allows to develop a significant portion of the algebraic theory of boundary problems: Regularity, multiplication and factorization can be defined in such a way that it subsumes many important classes of boundary problems—the classical two-point setting as well as linear systems of ODEs and linear PDEs.

## 3 Parametrized Wavelets

In our work on symbolic computation and wavelets, we focused on applications of parametrized wavelets [6]. For example, we constructed more regular wavelets than the Daubechies wavelets, see the figure below. Moreover, we discussed the construction of the least asymmetric orthonormal wavelets and the existences of rational filter coefficients, see [7, 8] for further details.

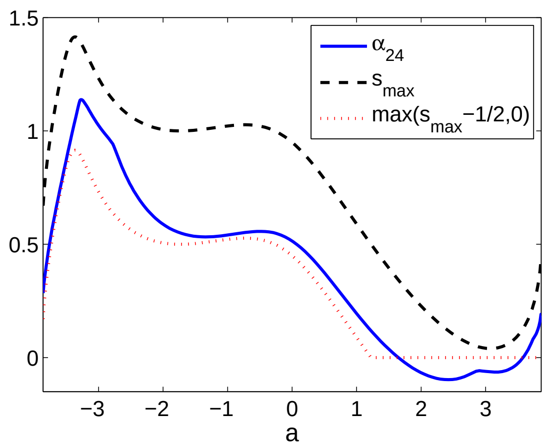


Figure 12: Lower bound for Hölder exponent $\alpha_{\max}$ for scaling functions with six filter coefficients depending on one parameter, with $\alpha_{\max} \in [s_{\max} - 1/2, s_{\max}]$ where $s_{\max}$ denotes the Sobolev exponent.

## 4 Max-plus Interpolation

We continued our research on generalized solutions of nonlinear first-order ordinary boundary problems and the max-plus algebra, where the addition is replaced by the maximum and the multiplication by the sum; see [3, 4, 5]. This work started from a suggestion by Martin Burger at the SFB-Statusseminar 2005. The implementation of the method for constructing generalized solutions via max-plus interpolation for the computer algebra system Maple was revised and a publication is in preparation.

## 5 Gröbner Bases Special Semester

In the spring and summer of 2006, the Radon Institute for Computational and Applied Mathematics (RICAM), in close cooperation with the Research Institute for Symbolic Computation (RISC), organized the Special Semester on Gröbner Bases and Related Methods. Directed by Bruno Buchberger (RISC) and Heinz W. Engl (RICAM) the special semester offered a program of specialized workshops, in particular "D2: Gröbner Bases in Symbolic Analysis" and "D3: Gröbner Bases in Control Theory and Signal Processing"; see [7, 16, 20]. Markus Rosenkranz has chaired—with Dongming Wang and Viktor Levandovskyy—the D2 workshop. A proceedings volume [2] for D3 are edited by Hyungju Park (Korea Institute for Advanced Study) and Georg Regensburger, a proceedings [19] for D2 by Markus Rosenkranz and Dongming Wang (School of Science, Beihang University, Beijing, China).

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# SFB F013: Numerical and Symbolic Scientific Computing

## Coherence within the SFB

### Cooperation between F1301, F1305 and F1306

***Summation and Finite Elements.*** The cooperation between F1301 and F1306 by using symbolic summation algorithms from F1305 has been successfully continued.

V. Pillwein and M. Kauers worked on applications of M. Kauers' symbolic summation package `SumCracker` on problems arising in the context of high order finite element method. `SumCracker` was used to generate relations between Jacobi polynomials that entered in the construction of triangular and tetrahedral interior shape functions. Another field of application was finding closed form expressions for sums arising in the definition of a smoothing operator that was used in the convergence proof of a certain finite element scheme.

***New shape functions for triangles and tetrahedra.***
S. Beuchler from F1306 and V. Pillwein continued their investigation on high order basis functions for the second order boundary value problem $-\nabla(A(x, y)\nabla u) = f$. They extended previous results to the definition of families of interior shape functions for both two and three dimensional case on triangular respectively tetrahedral meshes.

***Special Function Inequalities in Convergence Proofs of Numerical Methods.*** J. Schöberl from F1301 has conjectured an inequality for a sum of Legendre polynomials. Gerhold, Kauers and Schöberl were able to provide a partial proof of this inequality. Recently V. Pillwein, using tools from F1305, was able to provide a complete proof.

### Cooperation between F1302 and F1301

In the context of our case study on Gröbner domains, we are extending and improving both the knowledge base implemented in *Theorema*, as well as the concepts and tools for mathematical knowledge management in order to be able to use them in the context of the applications developed in the frame of the project F1301, namely the verification and synthesis of generic algorithms for Gröbner Bases.

### Cooperation between F1302, F1305, and F1303

We expanded the use of combinatorial and algebraic techniques for the generation of loop invariants and recursion invariants, as well as for the simplification of the verification conditions. By using such techniques we are able to solve verification problems which are beyond the power of currently used methods (e.g. model checking). Moreover, by using advanced algebraic algorithms (like e. g. Cylindrical Algebraic Decomposition), we improved the capabilities of the Theorema prover for elementary analysis.

### Cooperation between F1302, F1322, and F1308

As emphasized in the previous reports, project F1322 was born by a nontrivial cooperation between projects F1302 and F1308. This cooperation deepened in the reporting period. The initial bridge carrying the cooperation between the symbolic world of F1302 with the numerical-analytic one of F1308 was the systematic exploitation of the equational properties of certain operators in Hilbert spaces; the crucial tool for realizing solution algorithms was the generalized Moore-Penrose theory for Hilbert spaces (using oblique projectors for the nullspace and range of the operators to be inverted). Currently we extended this approach into two major directions: one in differential rings and algebras, the other in (infinite-dimensional) vector spaces. Research on generalized solutions for nonlinear first order ordinary boundary problems has been focused on interpolation methods in max-plus algebras. In our work on parametrized wavelets, we have studied various new applications. In the first half of the year, we have been engaged in the Special Semester on Gröbner Bases and Related Methods. (for more details see the section about F1322).

### Cooperation between F1303 and F1315

Together with B. Jüttler we developed a new geometric method based on the Bezier clipping approach in order to compute the intersections of two plane algebraic curves on a given domain.

### Cooperation between F1304 and F1308

H. Gu has cooperated with M. Burger (F1308) for symbolic and numeric computation of geometric problems.

### Cooperation between F1306 and F1308

A. Hofinger from Project F1308 and J. Valdman concentrated on fast calculation techniques for the two-yield elastoplastic problem, which is a locally defined, convex but non-smooth minimization problem for the unknown plastic-strain increment matrices $p_1$ and $p_2$. They summarized they results in the technical report which has also been accepted for a publication in Computing.

**Cooperation between F1315 and others**

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. We continued the cooperation between M. Barton and J. Valdman about robust methods for solving systems of polynomial equations.

**Cooperation between F1322, F1302, and F1308**

Project F1322 was created from a symbiosis between Projects F1302 and F1308. It benefits from bringing together the symbolic expertise from F1302 with the functional analysis know-how from F1308. The crucial link is that certain operators that are relevant in the abstract treatment of functional analysis can be modeled by noncommutative polynomials, which can be manipulated efficiently by Gröbner bases methods. In particular, the solving engine for linear two-point boundary value problems—which is continually extended to cover more problem types—is implemented in the TH∃OREM∀ system of F1302. The leading theme of inverse problems in F1308 provides an ample field of studying operator problems relevant in practical applications. In particular, stability issues are crucial for combining the new factorization methods for boundary problems with numerical and hybrid solvers: A given well-posed problem should be factored in a such a way (if possible) that both lower order problems are still well-posed.

**Cooperation between F1322 and F1303**

With Josef Schicho (F1303) we discussed how one can prove identities in Witt rings using Gröbner bases. Moreover, we showed that the isomorphism connecting the equivalent quadratic forms corresponding to an identity can be computed by tracing the Gröbner basis computation. The results where presented during the Special Semester on Gröbner Bases.

# SFB F013: Numerical and Symbolic Scientific Computing

## National and International Cooperations

# 1 Cooperations

**RWTH Aachen (Germany)**

The cooperation of Dr. V. Levandovskyy with Prof. E. Zerz on constructive methods of algebraic analysis has been continued. In the articles [1], [2] we have studied, developed and implemented the algorithms for commutative and non–commutative structures arising in connection with Control Theory. The article [3] provides a complete set of algorithms for the algebraic and contol–theoretic analysis of systems of equations involving constant parameters. Moreover, in this article the implementation is described and as an important example of performance we provide the first *complete* solution to the "two pendula, mounted on a cart" problem, stated e.g. in the book of Poldermann and Willems.

F1309 started a cooperation with Dr. V. Levandovskyy, discussing the possibility to develop a symbolic tool for the local mode analysis, which would be useful in contructing appropriate smoothers for a multigrid method. The goal is to determine the influence of damping parameters on the smoothing property.

Prof. W. Zulehner together with Prof. J. Schöberl constructed a symmetric indefinite preconditioner for saddle point problems. This joint work led to a journal publication in SIAM J. Matrix Anal. Appl.

**TU Cottbus (Germany)**

Together with Prof. M. Fröhner and Prof. B. Martin, the development of theoretical tools and the implementation of them were continued by Dr. V. Levandovskyy, concerning the symbolic generation and symbolic analysis of finite difference schemes for linear PDEs and systems of linear PDEs. Among other, we work on the symbolic von Neumann stability analysis as well as the dispersion analysis [4].

**University of Seville and University of Zaragoza (Spain)**

The SINGULAR library for computations with algebraic $D$–modules `dmod.lib` [5] has been released as the result of a joint work of Dr. V. Levandovskyy and J. Morales (Zaragoza). The tools, implemented in the library are of interest for F1304 and F1305. Together with Prof. F. Castro (Seville) we continue investigating algorithms for local algebraic and analytic settings in $D$–module theory. With the help of the library `dmod.lib` we are able to answer for the first time several hard computational problems in $D$–module theory.

**Center for Applied Mathematics and Theoretical Physics, University of Maribor (Slovenia)**

V. Romanovski from Maribor together with Dr. V. Levandovskyy developed and applied new methods, based on algebraic geometry, for studying the problem of bifurcations of limit cycles from a center or a focus of polynomial differential system (a system of ODEs). The problem of cyclicity of a center or a focus is also known as *the local 16th Hilbert problem* and it is still open. The novel methods, combining theoretical approach from algebraic geometry with the computational methods of computer algebra, allowed us to give a unified algorithm for solving the cyclicity problem for several concrete cases [6, 7].

**The project CreaComp**

This project, ended in December 2006, had a volume of 72 man-months and resulted in the construction of and contents development for a novel e-learning platform for mathematics, covering theory exploration, construction of mathematical models, and automatic reasoning (proving). The project was funded by the JKU Linz and was pursued by the Theorema group at RISC (Prof. Bruno Buchberger) in cooperation with the Department of Algebra, JKU (Prof. Guenther Pilz), the Fuzzy Logic Lab. Linz, JKU (Prof. Peter Klement). The new platform builds-up on the capabilities of the mathematical assistant Theorema from our group, and on the e-learning system MeetMATH developed in cooperation by the Department of Algebra and by the Fuzzy Logic Laboratory, and implements some of the newest concepts in e-learning, like constructive and exploratory learning. For implementing such concepts it was crucial to use the natural style and natural language proving capabilities of Theorema, because the lessons are modifiable by the user - in contrast to fixed-content classical text-books used for read-only based learning.

**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. The results of this research are to be applied in concrete industrial environments inside software companies in Romania and Austria.

**Blocked Lectures at Timisoara and Cluj (Romania)**

T. Jebelean (F1302) gave blocked lectures (8 hours) on automated reasoning techniques and their implementation in Theorema at the Universities of Cluj (May 2006) and Timisoara (Dec 2006).

**RICAM**

Together with H.-C. von Bothmer, O. Labs, and C. van de Woestijne, we proved some cases of the Casas-Alvero conjecture. The cooperation was during the special semester on Gröbner bases held at RICAM in the first half of 2006.

The cooperation with the RICAM finance group on inverse problems in option pricing models was continued. A parameter identification problem in a Levy-model for option pricing was approached by Tikhonov regularization [21].

Like other parts of the SFB, project F1322 is conducted over the Radon Institute for Applied and Computational Mathematics (RICAM). The interdisciplinary environment of this institution provides an additional incentive to cross-group (in particular symbolic-numerical) cooperations.

**University of Linz**

Together with G. Landsmann and P. Mayr , we could answer the question whether transposition of matrices in $G = \mathrm{GL}(2, \mathbb{R})$ is a polynomial function in the sense of universal algebra. The answer requires a combination of algebraic and topological methods, there is no purely algebraic proof known.

**Naval University, Quebec, Canada**

Together with C. Gosselin from Naval University, Quebec, Canada we studied the problem of devising a robot manipulator that does not exert forces (static balancing) or torques (dynamic balancing) to the base during its moves. This is relavant for robotics applications in optics and in aeronautics.

**Joint work with Dr. H. Herrmann, Inst. f. Theor.Physik, TU Berlin**

Gu has continued the cooperation with Dr. H. Herrmann, a theoretic physicist from TU Berlin on heat conduction problems. Herrmann has visited our research group for 1 week in March. A joint paper has been published [8].

**Cooperation with Dr. F. Schwarz, Fraunhofer Gesellschaft, Bonn**

We have been in contact with Dr. Fritz Schwarz concerning the factorization of differential operators. Schwarz has visited our research group in May, and we have agreed on future close cooperation.

**Cooperation with Prof. Lv́ov, Weizmann Institute, Israel**

Kartaschova has visited the Weizmann Institute and Prof. Victor Lv́ov has visited our research group in October. The publication [9] is a result of this cooperation.

**INRIA Paris**

The long term cooperation with Prof. Paule's group is continued. For 2008, a long term visit (6 months) of M. Kauers (F1305) to the INRIA group is currently being planned.

**DESY, Zeuthen**

As it turns out, Schneider's new summation algorithms (F1305) can be applied successfully to evaluate Feynman integrals that arise in the field of perturbative quantum field theory. A follow up project in cooperation with Deutsches Elektronen Synchrotron (DESY) in Zeuthen, Germany, is in preparation where we plan to extend our algorithms in order to evaluate Feynman integrals that could not be handled so far.

**International university cooperations of F1305**

Several joint articles have been published/accepted in cooperation with Helmut Prodinger (University of Stellenbosch, South Africa) [10, 11], with George E. Andrews (The Pennsylvania State University) [12, 13, 14, 15], and with R. Pemantle (University of Pennsylvania) [16].

**Petersburg Department of Steklov Institute of Mathematics**

Prof. S. Repin and Dr. Jan Valdman finished their work on reliable error estimates for the scalar nonlinear problem. The cooperation was described in a RICAM report and is also submitted for a journal publication.

**University of California, Los Angeles**

Several cooperations in the field of image processing and level set methods have been continued with the research group of S. Osher at the University of California, Los Angeles. This concerns, for instance, work on inverse scale space [17, 18], Bregman iteration [19], and level set and topological derivative methods [20]. Also L. He, who did her PhD at the UCLA joined the project in July 20006.

**VSB-Technical University Ostrava (Czech Republic)**

The cooperation of R. Simon with Prof. Z. Dostál and Dr. D. Lukáš (former SFB member, F1309) concerning the construction of optimal solution techniques for optimality systems using multigrid methods has been continued. Additonally Dr. J. Kraus and Dr. D. Lukáš worked together on algebraic multigrid methods for shape optimization problems.

**International Conferences**

Prof. U. Langer organized together with Prof. E.W. Sachs (University of Trier (Germany), Virginia Tech (USA)) a minisymposium on the "GAMM-SIAM Conference on Applied Linear Algebra" in Düsseldorf. The aim was to bring together scientists working on preconditioning techniques in PDE-constrained optimization.

On the "6th International Congress on Industrial and Applied Mathematics", Zurich, a minisymposium was organized by Prof. W. Zulehner and Prof. A. Wathen (Oxford, UK). The subject was the iterative solution of saddle point problems, which arise in PDE-constrained optimization.

**Austrian Research network on Industrial Geometry**

In the frame of the Austrian research network on Industrial Geometry (FSP S92), B. Jüttler cooperated with the group of O. Scherzer (University Innsbruck) and F. Aurenhammer / O. Aichholzer (Graz University of Technology).

**Presentation of F1315 at Universities**

B. Jüttler visited the University of Hongkong (Prof. Wenping Wang), the Seoul National University (Prof. Myung-Soo Kim) and the Munich University of Technology (Prof. Bernd Simeon) and gave presentations related to on–going research. in the SFB.

**Gröbner Bases Special Semester**

As explained in the project description of F1322, Markus Rosenkranz has co-chaired the D2 workshop and edits a proceedings volume with Dongming Wang (School of Science, Beihang University, Beijing, China); Georg Regensburger edits a proceedings volume for D3 with Hyungju Park (Korea Institute for Advanced Study).

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## 2 Guests

**Dr. Ibolya Szilagyi:** University of Eger Hungary, Feb. 1–3, 2006, Joint scientific research and talk

**Prof. Herwig Hauser:** University of Innsbruck Austria, Feb. 7–9, 2006, Talk: "Blowing up of flat varieties", Participation on the workshop

**Prof. Petr Lisonek:** Simon Fraser University Canada, Feb. 12–13, 2006, Scientific Cooperation about "Quasi-Polynomials and Partition Analysis" and Talk: "Combinatorial families enumerated by quasi-polynomials"

**Prof. Gert Almkvist:** Lund University Sweden, March 20, 2006, Talk: "Linear and Quadratic Recursions, Harmonic Sum Identities"

**Prof. Martin P. Bendsøe:** Technical University of Denmark, March 22–23, 2006, Rigorosum Stainko, Talk: "Topology optimization – Status and Trends"

**Dr. Christiaan Van De Woestijne:** Mathematical Institute The Netherlands, April 24, 2006, Talk: "Deterministic equation solving over finite fields"

**Prof. Volker Strehl:** Erlangen-Nürnberg University Germany, April 28–30, 2006, Joint scientific research and talk

**Prof. Doron Zeilberger:** Rutergs University USA, May 4–5, 2006, Joint scientific research and talk

**Dr. Klaus Gärtner:** WIAS Berlin Germany, May 23–24, 2006, Talk: "Parallel LU-decomposition techniques for sparse matrices, present status of PARDISO"

**Prof. Helmut Prodinger:** Stellenbosch University South Africa, July 13–16, 2006, Talk: "Old and new results about approximate counting, digital search trees, and skip lists"

**Prof. Ulrich Kohlenbach:** TU Darmstadt Germany, October 18–20, 2006, Talk: " Effective Uniform Bounds from Ineffective Proofs in Nonlinear Analysis and Geodesic Geometry"

**Dr. Willem A. De Graaf:** Dep. of Mathematics Trento Italy, October 12–15, 2006, Cooperation with J. Schicho and J. Pilnikova, Topic: Lie Algebra and diophantic equations

**Prof. Bill Chen:** Nankai University China, October 22–25, 2006, Joint scientific Cooperation and talk

**Prof. Dr. Christian Wieners:** University of Karlsruhe Germany, December 4–7, 2006, Talk: "SQP methods for incremental plasticity"

**Dr. Hans-Christian Graf Von Bothmer:** University of Hannover Germany, March 6–10, 2006, Cooperation (with O. Labs and J. Schicho): The method of solving large algebraic systems of equations through prime experiments should be tested on interesting case studies.

**Dr. Heiko Hermann:** Technical University Berlin Germany, March 4–11, 2006, Cooperation on the topic of mathematical physics.

**Dr. Bjorn Fredrik Nielsen:** SIMULA Research Labs Oslo Norway, April 24–28, 2006, Cooperation about Level Set Methods; Talk: "Computational issues in heart modelling"

**Mr. Simon Huffeteau:** Ecole Polytechnique France, April 24–July 23, 2006, Cooperation about image processing; Level Set Methods

**DI Adrian Craciun:** Institute E-Austria Timisoara Romania, April 26–May 2, 2006, Cooperation in Theorema-Project

**Prof. Olaf Steinbach:** Technical University Graz Germany, July 3–7, 2006, Invited Speaker at the Conference "DD17 - 17th International Conference on Domain Decomposition Methods"

**Prof. Mark Ainsworth:** Strathclyde University United Kingdom, July 3–7, 2006, Invited Speaker at the Conference "DD17 - 17th International Conference on Domain Decomposition Methods"

**Prof. Günter Leugering:** University of Erlangen Germany, July 3–7, 2006, Invited Speaker at the Conference "DD17 - 17th International Conference on Domain Decomposition Methods"

**Prof. Mark Adams:** Columbia University USA, July 3–7, 2006, Invited Speaker at the Conference "DD17 - 17th International Conference on Domain Decomposition Methods"

**Prof. Zoran Andjelic:** University of Baden Germany, July 3–7, 2006, Invited Speaker at the Conference "DD17 - 17th International Conference on Domain Decomposition Methods"

**Prof. Yuri Kuznetsov:** University of Houston USA, July 3–7, 2006, Invited Speaker at the Conference "DD17 - 17th International Conference on Domain Decomposition Methods"

**Prof. Dr. Rene Pinnau:** TU Kaiserslautern Germany, August 21–25, 2006, Talk: "Mathematische Herausforderungen bei der Optimalsteuerung von strahlungsdominanten Prozessen" Cooperation at the topic Optimization of semiconductor components.

**Prof. Victor L'Vov:** Weizmann Institut of Science Israel, Oct. 27–Nov. 5, 2006, Finishing of a joint paper: "Climate variability" and talk about achieved results.

# SFB F013: Numerical and Symbolic Scientific Computing

## Statistical Appendix

## 1 Monographs, PhD Theses, Diploma Theses


[1] Gruber, P. G. Solution of elastoplastic problems based on the moreau-yosida theorem. Master's thesis, Institut für numerische Mathematik, Johannes Kepler Universität Linz, 2006.

[2] Hackl, B. *Shape Variations, Level Set and Phase-field Methods for Perimeter Regularized Geometric Inverse Problems.* PhD thesis, JK University Linz, September 2006.

[3] Hofinger, A. *Ill-posed problems: Extending the deterministic theory to a stochastic setup.* PhD thesis, Universitaet Linz, 2006. ISBN: 3854990197.

[4] Kienesberger, J. *Efficient Solution Algorithms for Elastoplastic Problems.* PhD thesis, Johannes Kepler University Linz, 2006.

[5] Stainko, R. *Advanced Multilevel Techniques to Topology Optimization.* PhD thesis, J. Kepler University Linz, SFB F013, February 2006.


## 2 Publications (appeared in 2006)


[1] Ameur, H. B., Burger, M., and Hackl, B. Cavity identification in linear elasticity and thermoelasticity. *Mathematical Methods in the Applied Sciences* (2006). accepted.

[2] Andrews, G. E., Knopfmacher, A., and Zimmermann, B. On the number of distinct multinomial coefficients. *Journal of Number Theory 118*, 1 (May 2006), 15–30.

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

[4] Becirovic, A., Paule, P., Pillwein, V., Riese, A., Schneider, C., and Schöberl, J. Hypergeometric summation algorithms for high order finite elements. *Computing 78*, 3 (2006), 235–249. Preliminary version available.

[5] Buchberger, B., and Rosenkranz, M. Theorema: Towards computer-aided mathematical theory exploration. *Journal of Applied Logic 4*, 4 (December 2006), 359–652. ISSN 1570-8683.

[6] Burger, M. Surface diffusion including free adatoms. *Comm. Math. Sci. 4* (2006), 1–51.

[7] Burger, M., and Kaltenbacher, B. Regularizing Newton-Kaczmarz methods for nonlinear ill-posed problems. *SIAM J. Numer. Anal. 44* (2006), 153–182.

[8] Driver, K., Prodinger, H., Schneider, C., and Weideman, A. Padé Approximations to the Logarithm II: Identities, Recurrences, and Symbolic Computation. *Ramanujan Journal 11*, 2 (April 2006), 139–158. Preliminary version online.

[9] Driver, K., Prodinger, H., Schneider, C., and Weideman, A. Padé Approximations to the Logarithm III: Alternative Methods and Additional Results. *Ramanujan Journal 12*, 3 (2006), 299–314. Preliminary version online.

[10] Egger, H. Semiiterative regularization in hilbert scales. *SIAM J. Numer. Anal. 44* (2006), 66–81.

[11] Egger, H., Hein, T., and Hofmann, B. On decoupling of volatility smile and term structure in inverse option pricing. *Inverse Problems 22* (2006), 1247–1259.

[12] Gerhold, S., and Kauers, M. A computer proof of turan's inequality. *Journal of Inequalities in Pure and Applied Mathematics 7*, 2 (May 2006), 1–4. Article 42.

[13] Giese, M. Saturation up to redundancy for tableau and sequent calculi. In *Logic for Programming, Artificial Intelligence, and Reasoning, 13th Intl. Conf., LPAR 2006, Phnom Penh, Cambodia* (2006), M. Hermann and

A. Voronkov, Eds., vol. 4246 of *LNCS*, pp. 182–196.

[14] Giese, M. Superposition-based equality handling for analytic tableaux. *Journal of Automated Reasoning 38*, 1-3 (December 2006), 127–153. Appeared online 2 December 2006, in print April 2007.

[15] Haase, G., Lindner, E., Mühlhuber, W., and Rathberger, C. Optimal sizing and shape optimization in structural mechanics. In *Industrial Mathematics* (2006), M. C. J. et al, Ed., Narosa Publishing House, New Delhi, India, pp. 221 — 240.

[16] Hofinger, A. Nonlinear function approximation: Computing smooth solutions with an adaptive greedy algorithm. *Journal of Approximation Theory* (2006). http://dx.doi.org/10.1016/j.jat.2006.03.016.

[17] Jebelean, T., Kovacs, L., and Popov, N. Experimental program verification in the theorema system. *STTT* (2006). in press.

[18] Kauers, M. Shift equivalence of p-finite sequences. *The Electronic Journal of Combinatorics 13*, 1 (2006), 1–16. R100.

[19] Kauers, M. Sumcracker – a package for manipulating symbolic sums and related objects. *Journal of Symbolic Computation 41*, 9 (2006), 1039–1057.

[20] Kauers, M., and Paule, P. A computer proof of moll's log-concavity conjecture. *Proceedings of the AMS* (2006). to appear.

[21] Kauers, M., and Schneider, C. Indefinite summation with unspecified summands. *Discrete Math. 306*, 17 (2006), 2073–2083. Preliminary version online.

[22] Kienesberger, J., and Valdman, J. An efficient solution algorithm for elastoplasticity and its first implementation towards uniform h- and p- mesh refinements. In *Numerical Mathematics and Advanced Applications: Enumath 2005* (2006), A. B. de Castro, D. Gomez, P. Quintela, and P. Salgado, Eds.

[23] Langer, U., and Pechstein, C. Coupled finite and boundary element tearing and interconnecting solvers for nonlinear potential problems. *Journal of Applied Mathematics and Mechanics (ZAMM)* (2006). accepted for publication.

[24] Levandovskyy, V. and Zerz, E. Algebraic systems theory and computer algebraic methods for some classes of linear control systems. In *Proc. MTNS'06* (2006). to appear.

[25] P. Paule and V. Pillwein and C. Schneider and S. Schöberl. Hypergeometric Summation Techniques for High Order Finite Elements. *PAMM 6* (2006).

[26] Pechstein, C., and Jüttler, B. Monotonicity-preserving interproximation of B-H-curves. *J. Comp. Appl. Math. 196/1* (2006), 45–57.

[27] Pikkarainen, H. State estimation approach to nonstationary inverse problems: discretization error and filtering problem. *Inverse Problems 22*, 1 (2006), 365–379.

[28] Sampoli, M. L., Peternell, M., and Jüttler, B. Rational surfaces with linear normals and their convolutions with rational surfaces. *Computer Aided Geometric Design 23*, 2 (2006), 179–192.

[29] Shemyakova, E., and Winkler, F. Obstacle to factorization of LPDOs. In *Proc. Transgressive Computing 2006, Granada, Spain* (April 2006), J.-G. Dumas, Ed., pp. 435–441.

[30] Stainko, R. An adaptive multilevel approach to the minimal compliance problem in topology optimization. *Communications in Numerical Methods in Engineering 22* (2006), 109–118.

[31] Stainko, R., and Burger, M. A one shot approach to topology optimization with local stress constraints. In *IUATM Symposium on Topology Design Optimization of Structures, Machines and Materials* (2006), M. P. Bendsoe, N. Olhoff, and O. Sigmund, Eds., vol. 137 of *Solid Mechanics and its Applications*, IUTAM, Springer, pp. 181–184.

[32] Stainko, R., and Burger, M. Phase–field relaxation of topology optimization with local stress constraints. *SIAM Journal on Control and Optimization 45*, 4 (2006), 1447–1466.

[33] Szilágyi, I., Jüttler, B., and Schicho, J. Local parametrization of cubic surfaces. *J. Symbolic Comput. 41*, 1 (2006), 30–48.

[34] Windsteiger, W. An automated prover for zermelo-fraenkel set theory in theorema. *JSC 41*, 3-4 (2006), 435–470.

[35] Windsteiger, W., Buchberger, B., and Rosenkranz, M. *The Seventeen Provers of the World (ed. Freek Wiedijk).* LNAI 3600. Springer, Berlin Heidelberg New York, 2006, pp. 96–107 Theorema. ISBN 3-540-30704-4.

[36] Windsteiger, W., Buchberger, B., and Rosenkranz, M. *Theorema*, vol. 3600 of *LNAI*. Springer Berlin Heidelberg New York, 2006, pp. 96–107.

## 3 Talks at Conferences, Universities and other Institutions


[1] Barton, M. Bézier clipping via degree reduction. Workshop on Algebraic Spline Curves and Surfaces, Eger, Hungary, May 17-18 2006.

[2] Barton, M. Bézier clipping via degree reduction. Sixth International Conference on Curves and Surfaces, Avignon, France, June 29-July 5 2006.

[3] Beck, T. Computational Formal Desingularization of Surfaces in $P^3_C$. Magma 2006, Berlin, Germany, 30.07.06–02.08.06, 2006.

[4] Beck, T. An economic model for hypersurfaces. Workshop on Resolution of Algebraic Varieties, Kaiserhaus, 2006.

[5] Beck, T., and Schicho, J. Analytic Resolution of Surfaces. WSCA 06 (Poster), Barcelona, Spain, February 2006.

[6] Beck, T., and Schicho, J. Parametrization of Algebraic Curves Defined by Sparse Equations. 10th RWCA, Basel, Switzerland, March 2006.

[7] Buchberger, B. Automated mathematical theory exploration: How far can we go? Invited colloquium talk at DERI, Innsbruck, December 2006.

[8] Buchberger, B. Automated synthesis of a gröbner bases algorithm. Talk at Workshop "Formal Gröbnerr Bases Theory", March 6 2006.

[9] Buchberger, B. Die zukunft der algorithmischen mathematik: Kann mathematische forschung automatisiert werden? Invited colloquium talk at OCG, OVE, Graz, November 2006.

[10] Buchberger, B. Formal mathematics: A key to the future. Invited talk at "Engineering and Life Sciences", Avignon, France, June 2006.

[11] Buchberger, B. Mathematical theory exploration. Invited talk at IJCAR, Seattle, USA, August 2006.

[12] Buchberger, B. Mathematical theory exploration: Case study groebner bases. Invited talk at SYNASC 2006, Timisoara, September 2006.

[13] Buchberger, B. Symbolic computation: Current trends. Talk at Max Planck Institute for Physics, München, January 31 2006.

[14] Buchberger, B. Symbolic computation: Self-application of algorithmic mathematics. Invited talk at MAP 06 (Mathematics, Algorithms, Proofs), Mathematical Research Center, Castro-Urdiales, Spain, Jan 9-13, 2006, January 10 2006.

[15] Buchberger, B. Symbolic computation: Some thoughts about the future. Invited talk at LL2006 (Loops and Legs in Quantum Physics), Eisenach, Germany, April 2006.

[16] Egger, H. Acceleration of iterative methods for inverse problems. Intern. Conf. on "Inverse Problems and Simulation", Fethiye, May 2006.

[17] Egger, H. Preconditioning iterative regularization methods. Intern. GAMM/SIAM Conf. on "Applied Linear Algebra", Düsseldorf, July 2006.

[18] Engl, H. Hot stuff: From iron and steel making via inverse problems to finance. ICIAM Board Meeting, Shanghai, China, May 2006.

[19] Engl, H. Hot stuff: From ironmaking furnaces via inverse problems to mathematical finance. Universitaet Goettingen, April 2006.

[20] Engl, H. Iterative methods for the regularization of nonlinear inverse problems. Colloquium There is nothing more practical than a good theory, Fraunhofer-Institut Kaiserslautern, September 2006.

[21] Engl, H. Iterative regularization methods for nonlinear inverse problems for partial differential equations. TX Joint Mathematics Meetings, Texas, USA, January 2006.

[22] Engl, H. Mathematical Modelling and Numerical Simulation: From Iron and Steel Making via Inverse Problems to Finance. invited talk at the University of Tokyo, October 2006.

[23] Engl, H. Mathematics and industry a relation for mutual benefit: The austrian experience. Workshop in Applied Mathematics, Experiences and Visions for Industrial Mathematics in Europe, Bedlewo, Polen, April 2006.

[24] Engl, H. Mathematics and industry a relationship for mutual benefit. 10. Internationale Tagung ueber Schulmathematik, Wien: Mathematik die Schluesseltechnologie in Industrie und Wirtschaft, February 2006.

[25] Engl, H. Regularization of nonlinear inverse problems: Convergence analysis, new challenges. 3rd International Conference on Inverse Problems, Sapporo, Japan, July 2006.

[26] Engl, H. Regularization of nonlinear inverse problems: Convergence analysis, new challenges. Wichita State University, August 2006.

[27] Engl, H. Regularization of Nonlinear Inverse Problems: Mathematics, Industrial Application Fields, New Challenges. invited talk at the University of Tokyo, October 2006.

[28] Gerhold, S. Special Functions: Applications of Computer Algebra in Stochastics. Invited colloquium talk at Vienna University of Technology, 10. January 2006.

[29] Giese, M. A logic with subtypes to talk about java objects. Invited colloquium talk at UCD Systems Research Group, Dublin, Ireland, August 2006.

[30] Giese, M. A logic with subtypes to talk about java objects. Invited talk at ESF Exploratory Workshop: Challenges in Java Program Verification, Nijmegen, The Netherlands, October 2006.

[31] Giese, M. Panelist at panel discussion, intl. workshop on implementation of logics, phnom penh, cambodia. November 2006.

[32] Giese, M. Practical reflection for formal mathematics in theorema,. Invited colloquium talk at SCORE Workshop on Proving and Solving, Aizu-Wakamatsu, Japan, 15.03.06 - 17.03.06, March 2006.

[33] Giese, M. Practical reflection for formal mathematics in theorema. Contributed talk at Workshop on Formal Gröbner Bases Theory, Linz, Austria, 06.03.06 - 10.03.06, March 2006.

[34] Kapl, M. Spline wavelets. Workshop on Algebraic Spline Curves and Surfaces, Eger, Hungary, May 17-18 2006.

[35] Kartashova, E. Weak turbulence – two-layers model. invited talk at the "Navier-Stokes and Turbulence Symposium", W.Pauli Institute, Univ. Wien, April 2006.

[36] Kartashova, E. What is important to know for modeling a wave turbulence. invited talk at the workshop "Waves in Shallow Environments (WISE-2006)", ISMAR, Venice, April 2006.

[37] Kauers, M. Application of unspecified sequences in symbolic summation. Contributed talk at ISSAC'06, 2006-07-12 2006.

[38] Kauers, M. Computer algebra proofs for combinatorial inequalities and identities. Contributed talk at MAP 2006, 2006-01-12 2006.

[39] Kauers, M. Computer proof of a longstanding conjectured inequality of moll. Contributed talk at SFB Cooperation Meeting, December 18 2006.

[40] Kauers, M. Proving and finding algebraic dependencies of combinatorial sequences. Invited talk at Special Semester on Groebner Bases and Related Methods, 08.05.2006 2006.

[41] Kauers, M. Symbolic computation for inequalities. Contributed talk at SFB Annual Status Meeting (Strobl), 2006-04-21 2006.

[42] Kutsia, T. Matching with regular constraints. Invited colloquium talk at Department of Computer Science, Graduate School of Systems and Information Engineering, University of Tsukuba, Japan, March 14 2006.

[43] Kutsia, T. Matching with regular constraints. Invited talk at SCORE Workshop on Proving and Solving, University of Aizu, Aizuwakamatsu, Japan, March 16 2006.

[44] Levandovskyy, V. Advances and Perspectives of the Non-commutative Computer Algebra. Invited talk at Noncommutative Algebra Conference (NCA) 2006, 5.09 2006.

[45] Levandovskyy, V. Applications of Groebner Bases in Non-commutative GR-algebras. Invited talk at Workshop D2 "Non-commutative Groebner Bases" of the Special Semester on Groebner Bases and Related Methods, 17.05. 2006.

[46] Levandovskyy, V. Constructive non-commutative algebra with computer algebra system Singular:Plural. Invited colloquium talk at Universitaet Kassel, 5.12 2006.

[47] Levandovskyy, V. Elimination in non–commutative $g$–algebras and applications to $d$–modules. Invited talk at Tenth Meeting on Computer Algebra and Applications (EACA) 2006, 8.09 2006.

[48] Levandovskyy, V. Genericity of Parameters in Control Theory. Invited talk at Workshop D3 "Groebner Bases in Control Theory and Signal Processing" of the Special Semester on Groebner Bases and Related Methods, 18.05. 2006.

[49] Levandovskyy, V. Intersection of ideals with non-commutative subalgebras. Invited talk at ISSAC 2006, 11.07 2006.

[50] Levandovskyy, V. Non-commutative Computations with SINGULAR. Invited talk at Workshop D1 "Groebner Bases Theory and Applications in Algebraic Geometry" of the Special Semester on Groebner Bases and Related Methods, 16.02. 2006.

[51] Levandovskyy, V. Non-commutative computer algebra and its applications with the computer algebra system Singular:Plural. Invited colloquium talk at RWTH Aachen, 13.12 2006.

[52] Levandovskyy, V. Non-commutative Groebner bases in SINGULAR. Invited talk at Workshop D1 "Groebner Bases Theory and Applications in Algebraic Geometry" of the Special Semester on Groebner Bases and Related Methods, 8.02. 2006.

[53] Levandovskyy, V. A symbolic approach to finite difference schemes and their von neumann stability. Contributed talk at SFB Status Seminar, Strobl, 21.04. 2006.

[54] Levandovskyy, V. Plural, a Non–commutative Extension of Singular: Past, Present and Future. Invited talk at International Congress on Mathematical Software (ICMS) 2006, 3.09. 2006.

[55] Levandovskyy, V. Singular:Plural. news from the non-commutative front. Invited colloquium talk at Universitaet Kaiserslautern, 7.12 2006.

[56] Moore, B. Polynomial equations solving in the context of parallel mechanisms. Workshop on Algebraic Geometry and Singularities, Obergurgl, Austria, September 2006.

[57] Moore, B. Robotics and sum of squares. Workshop on Algebraic Spline Curves and Surfaces, Eger, Hungary, May 2006.

[58] Paule, P. Computer algebra and the digital library of mathematical functions. Mathemtisches Kolloquium. Invited colloquium talk at University of Darmstadt, June 2006.

[59] Paule, P. Computer algebra, proving, and the digital library of mathematical functions. Contributed talk at MAP'06 conference, Castro Urdiales, Spain, January 2006.

[60] Paule, P. Computer Algebra, Proving, and the Digital Library of Mathematical Functions. Invited talk at the MAP'06 Conference, Castro Urdiales, Spain, 10. January 2006.

[61] Paule, P. The nist project and its relation to formal mathematics. Invited key-note lecture. Invited talk at Special Semester on Gröbner Bases and Related Methods, Linz, Austria, March 2006.

[62] Paule, P. Quartics, log-concavity and computer algebra. Dagstuhl Seminar No. 06271. Invited talk at Challenges in Symbolic Computation Software, 2-7 July 2006.

[63] Paule, P. Symbolic computation and the digital library of mathematical functions (dlmf). Colloquium, Theoretical Physics Group. Invited colloquium talk at DESY Zeuthen (near Berlin), September 2006.

[64] Pikkarainen, H. Bayesian approach to inverse problems. SFB Status Seminar, Strobl, Austria, April 2006.

[65] Pikkarainen, H. Convergence rates for the bayesian approach to linear inverse problems. Inverse Days 2006, Tampere, Finland, December 2006.

[66] Pikkarainen, H. Discretization error in dynamical inverse problems. The Third International Conference "Inverse Problems: Modeling and Simulation", Fethiye, Turkey, June 2006.

[67] Pikkarainen, H. State estimation approach to nonstationary inverse problems: discretization error and filtering problem. Inverse Problems in Applied Sciences, Sapporo, Japan, July 2006.

[68] Pillwein, V. Application of Computer Algebra Tools for Low Energy Basis Functions. 17th International Conference on Domain Decomposition Methods (DD17), St. Wolfgang/Strobl, Austria, 3.-7. July 2006.

[69] Pillwein, V. Applications of Computer Algebra Methods for High Order Finite Elements. International Conference on Multifield Problems, Universität Stuttgart, Germany, 4.-6. October 2006.

[70] Pillwein, V. Hypergeometric Summation Techniques for High Order Finite Elements. Contributed talk at GAMM Annual Meeting'06, Berlin, Germany, 29.March 2006.

[71] Pilnikova, J. Interations of geometry, algebra and number theory. Workshop on Algebraic Spline Curves and Surfaces, Eger, Hungary, May 2006.

[72] Pilnikova, J. On Lie Algebras arising from Schubert varieties. Department semiar, University of Trento, Italy, October 2006.

[73] Pilnikova, J. Schubert Calculus. Workshop on Algebraic Geometry and Singularities, Obergurgl, Austria, September 2006.

[74] Pilnikova, J. Splitting central simple algebras of degree 4. 4th Rhine Workshop on Computer Algebra, Basel, Switzerland, March 2006.

[75] Popov, N., and Jebelean, T. Algebraic methods in the verification of recursive programs. Contributed talk at SFB Statusseminar, Strobl, Austria, April, 20 2006.

[76] Popov, N., and Jebelean, T. Supporting functional program verification in theorema. Contributed talk at Calculemus, Genova, Italy, July 7 2006.

[77] Popov, N., and Jebelean, T. Using computer algebra techniques for the specification and verification of recursive programs. Contributed talk at ACA (Applications of Computer Algebra), Varna, Bulgaria, June 28 2006.

[78] Regensburger, G. Boundary value problems for nonlinear first-order odes - constructing generalised solutions via the max-plus algebra. Workshop on the Algebraic Theory of

Differential Equations, Edinburgh, Schotland, 07.08.06 - 11.08.06, August 2006.

[79] Regensburger, G. Max-plus linear algebra and nonlinear ordinary bvps. GAMM, Berlin, March 2006.

[80] Regensburger, G. Nonlinear first-order ordinary bvps via max-plus interpolation. SFB Status Seminar, Strobl, Austria, 20.04.06 - 22.04.06, April 2006.

[81] Regensburger, G. Parametrizing orthonormal wavelets by moments. Special Semester on Groebner Bases Workshop D3: Groebner Bases in Control Theory and Signal Processing, Linz, Austria, 18.05.06 - 19.05.06, May 2006.

[82] Repin, S., and Valdman, J. Functional a posteriori error estimates for problems with nonlinear boundary conditions. University Zuerich: Prof. Sauter, Prof. Chipot, April 2005.

[83] Repin, S., and Valdman, J. Functional a posteriori error estimates for problems with nonlinear boundary conditions. Tikhonov and Contemporary Mathematics, Moscow, June 2006.

[84] Rosenkranz, M. Algebraic methods for differential equations and boundary value problems. CNRS-NSF Symposium, Avignon, France, 26.06.06-30.06.06, June 2006.

[85] Rosenkranz, M. The lausch-noebauer functor: Polynomials in the old style. Theorema Seminar, Hagenberg, Austria, 27.11.06 - 27.11.06, November 2006.

[86] Rosenkranz, M. A novel treatment of linear two-point boundary value problems. GAMM, Berlin, March 2006.

[87] Rosenkranz, M. Symbolic computation with bvps. noncommutative polynomials + boundary calculus. Theorema seminar, Hagenberg, Austria, 16.10.06 - 16.10.06, October 2006.

[88] Rosenkranz, M. Symbolic computation with two-point boundary value problems. Workshop on the Algebraic Theory of Differential Equations, Edinburgh, United Kingdom, 07.08.06-11.08.06, August 2006.

[89] Rosenkranz, M. Using groebner bases for solving linear two-point boundary value problems. Special Semester for Groebner Bases / Workshop D2, Hagenberg, Austria, 08.05.06-17.05.06, May 2006.

[90] Rosenkranz, M., and Regensburger, G. Factorization and division in the realm of linear ordinary bvps. SFB Status Seminar, Strobl, Austria, 20.04.06-22.04.06, April 2006.

[91] Schicho, J. Algorithmic Resolution of Singularities. Special Gröbner Semester 2006, 2006.

[92] Schicho, J. Analysis of Plane Curve Singularities. Special Gröbner Semester 2006, 2006.

[93] Schicho, J. Construction of Rational Points on Rational Surfaces. Arithmetic and Algebraic Geometry, Clay Summer School, Göttingen 2006, 2006.

[94] Schicho, J. Linear Systems of Plane Curves. Algebraic Geometry and Geometric Modeling, Barcelona, Spain, September 2006.

[95] Schicho, J., and Harrison, M. Rational parametrizations for degree 6 Del Pezzo surfaces using lie algebras. International Symposium of Algorithmic and Algebraic computation, Genua, 2006.

[96] Schicho, J., and Regensburger, G. Groebner bases and identities in witt rings. Special Semester on Groebner Bases Workshop D2: Groebner Bases in Symbolic Analysis, Linz, Austria, 08.05.06 - 17.05.06, May 2006.

[97] Schneider, C. Sigma - a package for multisummation. Invited talk at Axiom Workshop 2006, RISC, Hagenberg, Austria, April 27 2006.

[98] Schneider, C. The summation package sigma simplifies harmonic sum expressions. Invited colloquium talk at DESY, Zeuthen, Germany, 21. September 2006.

[99] Schneider, C. Symbolic summation assists combinatorics. Invited talk at 56th Sém. Lothar. Combin., Ellwangen, Germany, April 9 - 12 2006.

[100] Shemyakova, E., and Winkler, F. Obstacles to factorization of linear partial differential operators into arbitrary number of factors. talk at the 12th Internat. Conf. on Applications of Computer Algebra (ACA-2006), Varna, Bulgaria, June 2006.

[101] Simon, R. Fast solution of KKT systems arising from a model control problem. GAMM-SIAM Conference on Applied Linear Algebra, Düsseldorf, July 2006.

[102] Windsteiger, W. Computer-supported proving in zf set theory with the theorema system. Invited colloquium talk at Carnegie Mellon University, Math Logic seminar, March 2 2006.

[103] Windsteiger, W. Introduction to the groebner bases method. Talk given in the frame of the seminar "Fast SAT Solvers and Practical Decision Procedures". Invited colloquium talk at Carnegie Mellon University, Computer Science Deptartment, April 28 2006.

[104] Windsteiger, W. Introduction to theorema: An example of a formal math system. Contributed talk at Special Semester on Groebner Bases: Workshop on Formal Groebner Bases Theory. RICAM, Linz, March 6 2006.

[105] Windsteiger, W. The theorema system. Invited colloquium talk at Carnegie Mellon University, Computer Science seminar, February 20 2006.

[106] Winkler, F. Gröbner bases in difference-differential modules. talk at the Internat. Symposium for Symbolic and Algebraic Computation (ISSAC 2006), Genova, Italy, July 2006.

[107] Winkler, F. Parametrization of algebraic curves. talk at the Dept. of Mathematics, Aristotle Univ. Thessaloniki, Greece, March 2006.

[108] Winkler, F. Selected topics in computer algebra. talk at the Dept. of Mathematics, Aristotle Univ. Thessaloniki, Greece, March 2006.

[109] Winkler, F. Symbolic parametrization of algebraic curves. invited talk at the Erwin Schrödinger Institute for Mathematical Physics (ESI), Univ. Wien, November 2006.

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