Special Research Program (SFB) F 013

Numerical and Symbolic Scientific Computing

Annual Report 2005

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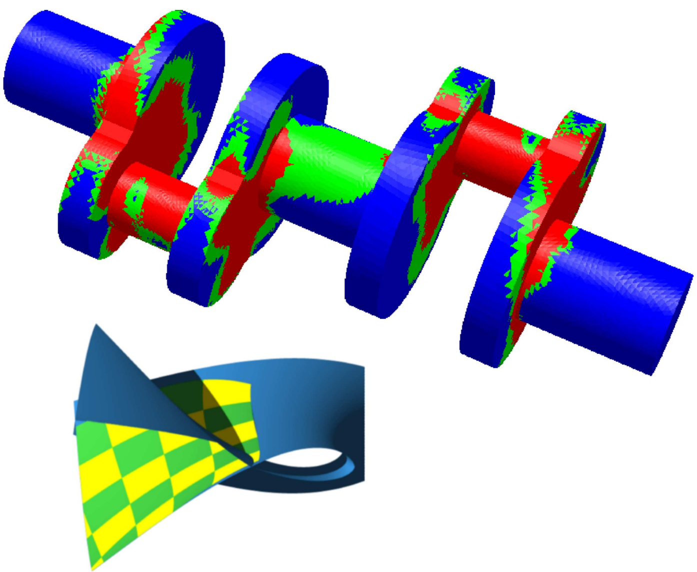

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Special Research Program SFB F013

"Numerical & Symbolic Scientific Computing"

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This Annual Report gives a summary of SFB results achieved in 2005.

Also in its eighth 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.

As pointed out in the Annual Report 2004, 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.

To achieve the goal of a *proper combination of numerical and symbolic scientific computing*, again strong emphasis has been put on supplementary measures, like joint internal seminars between numerical and symbolic groups or a new target-oriented structure of the SFB status seminars. This way the coherence between the numerical and symbolic groups has been further improved. A whole network of concrete links between numerics, symbolics, and geometry has been established and expanded.

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. The highlights are the foundation of the Software Competence Center Hagenberg and the Industrial Mathematics Competence Center in 1999. For more details see the sections describing the scientific progress achieved within the subprojects of the SFB.

On the academic level, the efforts of the institutes participating in the SFB to combine numerical-symbolic scientific computing with applied mathematics led to the foundation of the Johann Radon Institute for Computational and Applied Mathematics (RICAM) by the Austrian Academy of Sciences as a Center of Excellence in Applied Mathematics. Outstanding internationally recognized activities under the lead of RICAM have been organized:

- Special Semester on Computational Mechanics
- Special Semester on Gröbner Bases and Related Methods

The following institutes of the University 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.

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

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

or contact our office.

Linz, July 2006 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, Mag. B. Zimmermann

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.

1 High Order Finite Elements

Basis functions minimizing the condition number. In [1] the construction of basis functions minimizing the iteration number is described. The resulting shape functions φ_i are compositions of certain orthogonal polynomials involving integration and linear combinations. Using his symbolic summation package `Sigma` [11] C. Schneider derived recurrence relations allowing an efficient computation of the functions φ_i.

Inner shape functions using integrated Jacobi polynomials. In [2] shape functions for triangular p-FEM are described which are constructed using products of specific Jacobi polynomials $P_n^{(\alpha,\beta)}$. The parameters α, β are chosen to obtain a sparse system matrix in the case of a constant coefficient function and a polygonally bounded domain. For the case of a curved domain or a non constant coefficient function an efficient preconditioner is derived.

The idea of this design was carried over to tetrahedral finite elements. To obtain the correct parameters α, β in the definition of the basis functions and especially to prove the sparsity of the system matrix, the assistance of computer algebra software was needed. With a Mathematica program we proved the nonzero pattern of the interior block of the system matrix, i.e.,

$$K_{i,j,k,l,m,n} \neq 0 \quad \Leftrightarrow \quad |i-l| \in \{0,2\},$$
$$|i-l+j-m| \leq 4 \text{ and } |i-l+j-m+n-k| \leq 4.$$

Currently we are investigating the numerical properties of these basis functions as well as the construction of an efficient preconditioner for the system matrix.

A Mathematica FEM package. In order to have a platform for numerical–symbolic interaction V. Pillwein developed the Mathematica package `Fem2D`.
Within this program the RISC symbolic summation package (including `Sigma`, `MultiSum`, ...) can be invoked directly.

Orthogonal polynomials, which are widely used in the design of fe-basis functions, can be represented in different ways such as using their recursive description or hypergeometric sum representation. In a symbolic framework one can exploit this variety and study the benefits of different representations.

In the example described above, carefully chosen Jacobi polynomials were used in the construction of new shape functions. The Mathematica FEM package allows to generalize this idea to a systematic application of CA in the designing process. In `Fem2D` it is possible to implement families of basis functions leaving some parameters unknown, which are later specified according to desired numerical properties.

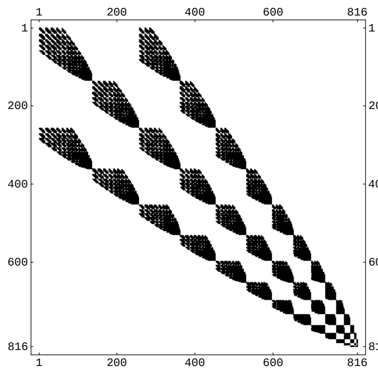

Figure 1: Nonzero pattern of the system matrix

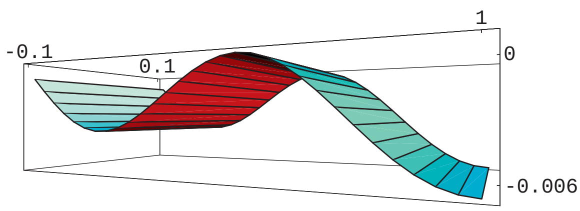

Figure 2: Elastic beam (solution by `Fem2D`)

2 Symbolic Integration of Special Functions

The particular need within F1301 for a symbolic integration algorithm that can do definite integrals arising in connection with high order finite element methods such as

$$\int_{-1}^{1} (x-1)^{d-1} (P_i^{(d-2,-1)})'(x) (P_j^{(d-2,-1)})'(x)\, dx \quad (1)$$

involving Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ led B. Zimmermann to a new symbolic algorithm for doing definite integrals of a large class of special functions that depend on a discrete parameter.

A function is called *elementary* if it is obtained by composing exponentials, logarithms, algebraic functions, and field operations. Risch gave a complete algorithm for the symbolic integration of elementary functions. Given an elementary function f, it decides if an elementary function g exists such that $f = g'$. If such a g exists, it returns it. Note that Risch's algorithm does not apply to integrals such as (1) for two reasons. First, the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ appearing in (1) are not elementary (when n is undetermined); in fact, most of the classical special functions from mathematical physics are not elementary. Second, Risch's algorithm is restricted to *in*definite integration problems, while (1) is definite.

A recent algorithm that applies to a wide class of non-elementary special functions is Manuel Bronstein's *Poor Man's Integrator* [3]. It is a variant of Risch–Norman's parallel integration method, based on a new structure theorem of Manuel Bronstein.

Within the frame of F1301, B. Zimmermann extended Bronstein's Poor Man's Integrator to definite integration problems where the integrand depends on a discrete parameter n. Given such an integrand $f(x;n)$ and a natural number r, his algorithm looks for coefficients $c_0(n), c_1(n), \ldots, c_r(n)$ and a function $g(x;n)$ such that

$$c_0(n)f(x;n) + \cdots + c_r(n)f(x;n+r) = g'(x;n);$$

this relation implies the linear recurrence

$$c_0(n)s(n) + \cdots + c_r(n)s(n+r) = g(b;n) - g(a;n)$$

for the definite integral $s(n) := \int_a^b f(x;n)dx$ under consideration.

Zimmermann's extension of the Poor Man's Integrator is inspired by Doron Zeilberger's extension of Gosper's algorithm for hypergeometric summation (Zeilberger's algorithm). The same method was used by C. Schneider [11] in his extension of Karr's summation algorithm to definite summation. In all three cases, the key is to observe that the underlying algorithm has the special property that it can be applied to an input $f(x;n) := c_0(n)f_0(x;n) + \cdots + c_r(n)f_r(x;n)$, where $c_0(n), \ldots, c_r(n)$ are initially undetermined coefficients and $f_0(x;n), \ldots, f_r(x;n)$ are given. These coefficients show up as additional variables in the linear equation system which the underlying algorithm solves. That way, the underlying algorithm determines them, in addition to determining a suitable $g(x;n)$ such that $f(x;n) = g'(x;n)$. To find recurrences for integrals, one uses this with $f_i(x;n) := f(x;n+i)$ for $i = 0, \ldots, r$.

The new algorithm works in a field of of rational functions $F = K(X_{u+1}, \ldots, X_{u+v})$ where $K = k(X_1, \ldots, X_u)$ with k a field. F is endowed with a shift σ and a derivation D, which commute with each other, and such that the field of constants of D is K and that k is in the field of constants of σ. Each indeterminate X_i corresponds to some term which possibly involves n and x, the shift σ corresponds to the shift $n \mapsto n+1$, and the derivation D corresponds to the partial derivative $\frac{\partial}{\partial x}$. For any P-finite function $f(x;n)$ one can construct such a suitable field F which models the field of functions generated by all the shift-derivatives of $f(x;n)$. Given $f_1, \ldots, f_r$ in F, the new algorithm returns a basis for the K-vector space of all $(c_1, \ldots, c_r, g) \in K \times F'$ such that $c_1 f_1 + \cdots + c_r f_r = g$ and F' is an elementary extension of the differential field (F, D). As the algorithm is based on Bronstein's heuristic Poor Man's Integrator, it may, in rare occasions, return a basis for a proper subspace of this K-vector space.

So far, the best computer algebra methods for definite symbolic integration of special functions were based on elimination in Ore Algebras by Gröbner basis methods (e.g. [4])). These methods are restricted to P-finite integrands, and they are known to terminate for the class of holonomic integrands, which form a subclass of the class of P-finite integrands. While Zimmermann's extension also handles any P-finite integrand and terminates on holonomic input, it can handle a wider class of inputs. The class of inputs which it can handle is closed under composition – unlike the class of P-finite functions. It contains certain non-P-finite functions such as the tangent function and Lambert's W function.

The new algorithm is not yet published; it will appear in a forthcoming Ph.D. thesis [13].

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 coefficient domain 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 (e.g. [8]). Numerous algorithms, based on Gröbner bases for these two cases, are implemented in the specialized Computer Algebra System SINGULAR [7]. 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 [6] 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. Let A be the algebra generated by $\{sin, cos, \partial\}$ over $\mathbb{K}$ subject to the 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, where the further computations will take place.

Generalization of Gröbner Bases. In order to treat the case of rational functions in the variables as the coefficient domain, we employ the notion of an *Ore localization.* Our aims are to extend the Gröbner bases theory to the Ore–localized G–algebras, not restricting ourselves to the case of so-called *Ore algebras* ([4], [5]), to investigate the criteria for discarding the critical pairs and to implement efficiently Gröbner bases and related algorithms (involving advanced ones as in e.g. [8]) in the framework of Singular. One of the most important tasks is to provide powerful algorithms and their efficient implementation for the complicated arithmetics over rings of quotients of non–commutative domains.

Intercommunication packages. With the help of recent packages, the fast and functionally rich implementation of algorithms, relying on Gröbner bases in Singular, became available to the general purpose systems. The package, allowing Mathematica to exchange data and to call Singular externally, is being developed by Manuel Kauers, F1305.

3.2 Symbolic Generation and Stability Analysis of Finite Difference Schemes

For the linear PDEs 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 [12]. Our method can be applied, in particular, for *higher spatial dimensions* without significant loss of performance. It can be shown that applying several symbolic approaches we are able to reproduce all the classical finite difference schemes. 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. a 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

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

With our methods we are able to generate all the classical linear schemes (as it has been noted in [12]) as well as more complicated schemes, including the schemes with parametric switches.

Using the efficient implementation of Gröbner bases, these 1–dimensional examples both in time and space can be computed in seconds.

Von Neumann Stability Analysis. Also, 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 special (nodal) form, 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.

In the example above, we employ the *stability morphism* from the ring $R = \mathbb{K}(d)[T_x, T_t]$, sending $T_t \mapsto g$ and $T_x \mapsto sin + i \cdot cos$ to the ring $S = \mathbb{K}(d)[i, sin, cos, g] / \ / \langle sin^2 + cos^2 - 1, i^2 + 1 \rangle$. Here, $sin = \sin(\alpha), cos = \cos(\alpha)$ and $\alpha = \beta \triangle x$ for some β. 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.

A very important direction of further research (discussed with Prof. W. Zulehner, F1306) is to elaborate the conditions for boundary value problems, for which von Neumann stability (which can be checked by symbolic methods as we have sketched above) implies the numerical stability.

3.3 Control Theory

Algebraic Analysis. Given a module M over an algebra A, we can present it as a sum $T + F$, where T is a torsion submodule of M and F a torsion–free submodule. 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 with the help of homological algebra [5], 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 for the case of constant coefficients [9] in the library `control.lib` for the system SINGULAR [7]. 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 [6] 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, 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 appear in [10], while in the future we concentrate on the general situation.

References

[1] A. BECIROVIC, P. PAULE, V. PILLWEIN, A. RIESE, C. SCHNEIDER, AND J. SCHÖBERL. Hypergeometric Summation Methods for High Order Finite Elements. Tech. Rep. 2006-8, SFB F013, J. Kepler University Linz, 2006.

[2] BEUCHLER, S., AND SCHÖBERL, J. New shape functions for triangular p-FEM using integrated Jacobi polynomials. *Num. Mathematik* (2006). to appear.

[3] BRONSTEIN, M. *Symbolic Integration I (Transcendental Functions)*, 2nd ed. Springer, 2005.

[4] CHYZAK, F. AND SALVY, B. Non–commutative Elimination in Ore Algebras Proves Multivariate Identities. *J. Symbolic Computation 26*, 2 (1998), 187–227.

[5] CHYZAK, F., QUADRAT, A. AND ROBERTZ, D. Linear control systems over Ore algebras. Effective algorithms for the computation of parametrizations. In *Proc. TDS'03* (2003), INRIA.

[6] GREUEL, G.-M., LEVANDOVSKYY, V., AND SCHÖNEMANN H. PLURAL, a SINGULAR 3.0 Subsystem for Computations with Non–commutative Polynomial Algebras. University of Kaiserslautern, 2005.

[7] GREUEL, G.-M., PFISTER G., AND SCHÖNEMANN H. SINGULAR 3.0. A Computer Algebra System for Polynomial Computations. Centre for Computer Algebra, University of Kaiserslautern, 2005. Available from `http://www.singular.uni-kl.de`.

[8] LEVANDOVSKYY, V. Intersection of Ideals with Non-commutative Subalgebras. Tech. Rep. 2006-14, SFB F013, J. Kepler University Linz, 2006.

[9] LEVANDOVSKYY, V. AND ZERZ, E. Computer algebraic methods for the structural analysis of linear control systems. *PAMM 5* (2005), 717–718.

[10] 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.

[11] SCHNEIDER, C. A new Sigma approach to multi-summation. *Advances in Applied Math. 34*, 4 (2005), 740–767.

[12] V. P. GERDT, Y. A. BLINKOV, AND V. V. MOZZHILKIN. Gröbner Bases and Generation of Difference Schemes for Partial Differential Equations. *SIGMA 2* (2006), 051.

[13] ZIMMERMANN, B. *Symbolic Definite Integration and Summation of Special Functions.* PhD thesis, RISC, J. Kepler University Linz, 2006. In preparation.

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

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1 Proving, Solving, and Computing in the Theory of Hilbert Spaces

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.

As detailed in the project proposal, the two main directions of research are: *management of mathematical knowledge* and *equational reasoning*.

Mathematical Knowledge Management. We continued our activity for building up case studies in the areas of: functional analysis, Groebner bases, and basic algorithmic domains. In parallel, we are developing the concepts and the tools necessary for defining and supporting theory exploration and use in the frame of specific applications (algorithm synthesis, proving, program verification).

An overview of the capabilities of our system which have been recently developed and of the design goals for the next future are given in [8] and in [4, 1]. The fact that our research group is in the very center of the international activity in the area of mathematical theory exploration is revealed by the great success of the "Special Semester on Groebner Bases and Related Methods", which was organized by Prof. Buchberger and Prof. Engel at RICAM and RISC and was attended by some of the most important researchers in the field of symbolic computation.

Several case studies have been implemented which deal with basic algorithmic domains: polynomial domains (for Groebner Bases) [6, 5], proving irrationality of the square root [32], verification of programs over number domains [26]. In the context of this latter and particularly important application, we continued to develop specific techniques for combining automated reasoning and program verification with advanced algebraic methods: combinatorics, Groebner Based, Cylindrical Algebraic Decomposition, and others [14, 15, 10, 13, 29]. This research activity constitutes an important link between the project 1302 and other projects of the SFB.

A major and novel application of mathematical theory exploration is algorithm synthesis. This topic has been actively promoted by our research group and lead to important advacements in the area: [7, 2, 3, 11].

As a preparation for building up case studies in functional analysis, we implemented special provers as well as sample theories for elementary analysis, which are also used in the context of e-learning (the CreaComp project) [16, 28, 31, 30, 12].

The case studies in the area of functional analysis are developed in close cooperation with the subproject F 1322, and are based a novel approach to solving differential equations using symbolic techniques. The activity in presented in more detail in the respective section of this report.

The usage of our system for the purpose of theory exploration was enhanced by studying and implementing novel features for the orgnization and presentation of mathematical knowledge [24, 27].

The proving power of *Theorema* was increased by studying and implementing new methods for predicate logic proving in typed theories [9] as well as propositional proving [17].

The improvement of our system from the point of view of its usability was furher pursued by implementing advanced interactive features [25].

Equational Reasoning. An unique and novel feature of the *Theorema* system is the use of sequence variables. The syntax, semantics, and the concrete implementation of this feature have been further developed [19].

Our researchers developed and implemented very powerful techniques for matching and rewriting [22, 23].

As a particular and important application of these techniques we studied the possibility of using them in the context of internet technologies [18, 21, 20].

References

[1] Buchberger, B. A View on the Future of Symbolic Computation, July 25-27 2005. Invited talk at ISSAC 2005 (International Symposium on Symbolic and Algebraic Computation), Bejing.

[2] Buchberger, B. Algorithmic Algorithm Invention in the Theorema Project, May 16-18 2005. Invited talk at Conference on Algorithms and Information Theory, University of Vaasa, Finland.

[3] Buchberger, B. Algorithmic Algorithm Synthesis: Case Study Gröbner Bases, March 12 2005. Invited talk at East Coast Computer Algebra Day, University of Ohio, Ashland, USA.

[4] Buchberger, B. Formal Mathematical Theory Exploration in Theorema (4 lectures), August 3-13 2005. Invited talk at Summer School on Theoretical Computer Science, Marktoberdorf.

[5] Buchberger, B. From Gröbner Bases to Automated Theorem Proving and Back, July 9-22 2005. 3 lectures. Invited talk at Summer School on Gröbner Bases and Applications, Zanjan, Iran.

[6] Buchberger, B. Introduction to Gröbner Bases, May 16-18 2005. Invited talk at Introduction to Gröbner Bases, University of Vaasa, Finland.

[7] Buchberger, B. Lazy Thinking: A New Method for Algorithm Synthesis., September 26-30 2005. Invited colloquium talk at Workshop Algebraic and Numeric Algorithms and Computer-Assisted Proofs. Research Center Schloss Dagstuhl, Germany.

[8] Buchberger, B., Craciun, A., Jebelean, T., Kovacs, L., Kutsia, T., Nakagawa, K., Piroi, F., Popov, N., Robu, J., Rosenkranz, M., and Windsteiger, W. Theorema: Towards Computer-Aided Mathematical Theory Exploration. *Journal of Applied Logic* (2005), –. To appear.

[9] Giese, M. A calculus for type predicates and type coercion. In *Automated Reasoning with Analytic Tableaux and Related Methods, Tableaux 2005* (2005), B. Beckert, Ed., vol. 3702 of *LNAI*, Springer, pp. 123–137.

[10] Jebelean, T. Using Computer Algebra for Automated Reasoning in the Theorema System, December 15 2005. Invited talk at Seventh Asian Symposium on Computer Mathematics (ASCM 2005).

[11] Jebelean, T., and Szakacs, L. Functional-Based Synthesis of Systolic Online Multipliers. In *SYNASC-05 (International Symposium on Symbolic and Numeric Scientific Computing)* (2005), D. Zaharie, D. Petcu, V. Negru, T. Jebelean, G. Ciobanu, A. Cicortas, A. Abraham, and M. Paprzycki, Eds., IEEE Computer Society, pp. 267–275.

[12] Kovacs, L. Using Combinatorial and Algebraic Techniques for Automatic Generation of Loop Invariants. Tech. Rep. 05-16, RISC Report Series, University of Linz, Austria, 2005.

[13] Kovacs, L., and Jebelean, T. An Algorithm for Automated Generation of Invariants for Loops with Conditionals. In *Proceedings of the Computer-Aided Verification on Information Systems Workshop (CAVIS05), 7th International Symposium on Symbolic and Numeric Algorithms for Scientific Computing (SYNASC05)* (September 25-28 2005), D. P. et al, Ed., pp. 16–19. to appear in IEEE journal.

[14] Kovacs, L., Jebelean, T., and Kovacs, A. Practical Aspects of Algebraic Invariant Generation for Loops with Conditionals. In *Bulletins for Applied and Computer Mathematics, Pannonian Applied Mathematical Meetings, PC-147/148* (Balatonalmadi, Hungary, 26-29 May 2005), F. F. et al, Ed., Technical University of Budapest, PAMM-Centre, pp. —-.

[15] Kovacs, L., Popov, N., and Jebelean, T. A Verification Environment for Imperative and Functional Programs in the Theorema System, 18-19 November 2005. Satellite of 2nd Balkan Conference in Informatics, 17-19 November, Ohrid. Contributed talk at 2nd South-East European Workshop on Formal Methods (SEEFM05), "Practical dimensions: Challenges in the business world", Ohrid, FYR of Macedonia.

[16] Kovacs, L., Popov, N., and Jebelean, T. Verification Environment in Theorema. *Annals of Mathematics, Computing and Teleinformatics (AMCT) 1*, 2 (2005), 27–34.

[17] Kusper, G. Solving the Resolution-Free SAT Problem by Hyper-Unit Propagation in Linear Time. *Annals of Mathematics and Artificial Intelligence 43*, 1-4 (2005), 129–136.

[18] Kutsia, T. Context Sequence Matching for XML. In *Proceedings of the 1th International Workshop on Automated Specification and Verification of Web Sites (WWV'05)* (Valencia, Spain, March 14–15 2005), M. Alpuente, S. Escobar, and M. Falaschi, Eds., pp. 103–119. (Final version to appear in Elsevier ENTCS).

[19] Kutsia, T., and Buchberger, B. Predicate Logic with Sequence Variables and Sequence Function Symbols. Tech. Rep. 05-17, RISC Report Series, University of Linz, Austria, 2005.

[20] Kutsia, T., and Marin, M. Can Context Sequence Matching be Used for Querying XML? In *Proceedings of the 19th International Workshop on Unification (UNIF'05)* (2005), L. Vigneron, Ed., pp. 77–92.

[21] Kutsia, T., and Marin, M. Can Context Sequence Matching Be Used for XML Querying?, April 22 2005. Contributed talk at the 19th International Workshop on Unification (UNIF'05), Nara, Japan.

[22] Kutsia, T., and Marin, M. Matching with Regular Constraints. In *Logic for Programming, Artificial Intelligence, and Reasoning. Proceedings of the 12th International Conference LPAR'05* (2005), G. Sutcliffe and A. Voronkov, Eds., vol. 3835 of *Lecture Notes in Artificial Intelligence*, Springer Verlag, pp. 215–229.

[23] Kutsia, T., and Marin, M. Matching with Regular Constraints. Tech. Rep. 05-05, RISC Report Series, University of Linz, Austria, 2005.

[24] Piroi, F., and Buchberger, B. Label Management in Theorema. In *Informal proceedings of the 4th International Conference on Mathematical Knowledge Management* (July 2005), M. Kohlhase, Ed., pp. –. Bremen, Germany.

[25] Piroi, F., and Kutsia, T. The Theorema Environment for Interactive Proof Development. In *Logic for Programming, Artificial Intelligence, and Reasoning. Proceedings of the 12th International Conference, LPAR'05* (2005), G. Sutcliffe and A. Voronkov, Eds., vol. 3835 of *Lecture Notes in Artificial Intelligence*, Springer Verlag, pp. 261–275.

[26] Popov, N. Verification of Simple Recursive Programs in Theorema: Completeness of the Method. Tech. Rep. 05-06, RISC Report Series, University of Linz, Austria, June 2005.

[27] Rosenkranz, C., and Piroi, F. Organizational Tools in Theorema, November 14-15 2005. Contributed talk at Theorema-Ultra-Omega Workshop.

[28] Saminger, S., Vajda, R., and Windsteiger, W. Using a Computer-Algebra System and a Theorem Prover to Stimulate Creativity in Learning Mathematics. *International Journal of Computers for Mathematical Learning* (2005), 0–0. Submitted.

[29] Vajda, R. Finding Witness Terms in ETRCF by Quantifier Elimination Techniques, November 14 2005. Contributed talk at Theorema-Ultra-Omega'05 Workshop.

[30] Windsteiger, W. CreaComp: Neue Möglichkeiten im e-learning für Mathematik, 22. April 2005. Invited colloquium talk at Research Net Upper Austria: Brennpunkt Forschung.

[31] Windsteiger, W. The CreaComp Project: Theorema for Computer-supported Teaching and Learning of Mathematics, November 14 2005. Contributed talk at Theorema-Ultra-Omega'05 Workshop.

[32] Windsteiger, W., Buchberger, B., and Rosenkranz, M. Theorema. In *The Seventeen Provers of the World*, F. Wiedijk, Ed., vol. 3600 of *LNAI*. Springer Berlin Heidelberg New York, 2006, pp. 96–107.

F 1303: Proving and Solving over the Reals

Prof. Dr. J. Schicho
DI T. Beck, DI J. Pílniková, DI I. Szilágyi

1 Sparse parametrization of plane curves

The known algorithms for parametrizing plane curves are robust but they neglect the "nice" properties the implicitly given curve has. If the plane curve is of high degree but its implicit equation contains only few monomials with nonzero coefficient, we say that this polynomial is sparse and we developed special algorithms for parametrizing such curve.

We used methods of toric geometry to construct a particularly nice birational model of such a curve. Namely the curve is embedded in a toric surface whose construction is guided by the shape of the Newton polygon of the defining equation and thus takes its sparsity into account. In [3] we showed how a parametrization algorithm can benefit from this special representation in terms of lower complexity.

2 Adjoint spaces

We developed and implemented an algorithm for computing the adjoint space of an algebraic surface, which was presented at [9]. The machinery of multivariate Puiseux series developed before (see [2]) was used to produce an "analytic resolution" of a given surface. We derived conditions for computing adjoint spaces from this data. Adjoint spaces are the central ingredient of Schicho's Parametrization algorithm for surfaces.

3 Parametric Degree

The degree of a parametric curve is also the degree of any of its parametrizations. For parametric surfaces, the situation is more complicated: for the same surface, there are parametrizations of different degree, even arbitrary large degree. The parametric degree is the degree of the smallest possible parametrization. This concept has its subtleties, for instance it depends on the choice of the field: for a fixed real algebraic surface, we may have a complex parametric degree and a real parametric degree. We discovered some relations to known numerical invariants (nefness value) that explain the relation between implicit and parametric degree, see [10].

4 Local parametrization

Several techniques for parametrizing a rational surface as a whole exist. In many applications, it is sufficient to parametrize only a small portion of the surface. We investigated such local parametrization in the case of nonsingular cubic surfaces. Together with B. Jüttler from subproject 1315 we gave several algorithms for constructing such local parametrizations that cover the surface exhaustively, see [13].

5 Stability of implicitization

Despite the fact that the implicitization problem for rational curves and surfaces makes sense when the input is only known up to a certain error level, and the fact that there are already several algorithms known for numerically solving this problem (see [4, 5, 8]), there was previously no investigation of the numerical stability of this problem and these algorithms.

In [12] we introduced a condition number measuring the stability of the implicitization algorithms, which depends on the numerical input and on some discrete information corresponding to the estimated degree of the unknown implicit equation, see [11].

Together with M. Aigner and B. Jüttler from subproject 1315 we also investigated the geometrical consequences of numerical instability in the implicitization process, see [1].

6 Exact solution over the rationals

The problem if finding rational solutions for systems of algebraic equations is, in general, tremendously difficult; it is not even known whether existence of a solution is decidable or not. Therefore in order to obtain any results one has to restrict to a specific class of varieties. In the previous year we developed a method for finding all rational points on Del Pezzo surfaces of degree 9, which are anticanonically embedded Severi-Brauer surfaces, see [7]. The idea is to compute the Lie algebra of the group of automorphisms of the surface and then construct an isomorphism of the Lie algebra and some well-known Lie algebra. Using the representation theory of Lie algebras we can then lift this isomorphism to an isomorphism of the given variety and some very well-known variety. Knowing the latter one leads to finding all rational point on the given one.

It turns out that the method is often successful also for other types of varieties provided the group of its automorphisms is "large enough". For example in [6] we generalized the method for both types of Del Pezzo surfaces of degree 8.

References

[1] Aigner, M., Szilágyi, I., Jüttler, B., and Schicho, J. Implicitization and distance bounds. In *Algebraic Geometry and Geometric Modelling* (2005), Mathematics and Visualization, Springer. to appear.

[2] Beck, T. Computing multivariate power series roots, February 2005. YMIS '05 (Sedano).

[3] Beck, T., and Schicho, J. Sparse parametrization of plane curves. *AAECC* (2005). to appear.

[4] Chen, F. Approximate implicitization of rational surfaces. In *Computational geometry (Beijing, 1998)* (2003), Amer. Math. Soc., pp. 57–65.

[5] Corless, R. M., Giesbrecht, M., Kotsireas, I., and Watt, S. Numerical implicitization of parametric hypersurfaces with linear algebra. In *Artificial intelligence and symbolic computation (Madrid, 2000)* (2001), Springer, pp. 174–183.

[6] de Graaf, W. A., Pílniková, J., and Schicho, J. Parametrizing del pezzo surfaces of degree 8 using lie algebras., 2005. preprint.

[7] de Graaf W. A., Harrison, M., Pílniková, J., and Schicho, J. A Lie algebra method for rational parametrization of Severi-Brauer surfaces. *Journal of Algebra*. to appear.

[8] Dokken, T. Approximate implicitization. In *Mathematical methods for curves and surfaces (Oslo, 2000)* (2001), Vanderbilt Univ. Press, pp. 81–102.

[9] Schicho, J. Computation of adjoints and the parametrization problem, 2005. invited talk at MAGMA workshop Algebraic Geometry and Group Theory, Warwick.

[10] Schicho, J. The parametric degree of rational surfaces. *Math. Zeitschr.* (2005).

[11] Schicho, J., and Szilágyi, I. Numerical stability of surface implicitization. *Journal of Symbolic Computation*, 40/6 (2005), 1291–1301.

[12] Szilágyi, I. A condition number for the implicitization problem, 2005. Computational Methods for Algebraic Spline Surfaces (COMPASS; Oslo 2005).

[13] Szilágyi, I., Jüttler, B., and Schicho, J. Local parametrization of cubic surfaces. *J. Symbolic Comput.* (2005). to appear.

F 1304: Symbolic Differential Computation

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

1 Results of the Project

This report covers the period from January 2005 until December 2005. During this period we have investigated factorization of linear partial differential operators, theoretical foundations for differential algebraic problems, numerical-symbolic methods for discrete geometric problems and analysis of differential equations

1.1 Factorization of Linear Partial Differential Operators

F. Winkler has worked jointly with E. Shemyakova on factorization of Linear Partial Differential Operators. This work is based on the work of Grigoriev, Tsarev and Schwarz. F. Winkler and E. Shemyakova introduce the new notion of obstacle to factorization, prove that is stable, and describe them for operators of low orders. For the second order operators they were noticed as famous Laplace invariants, and could be generalized to higher order operators. They also have developed an implementation and have started to consider "approximate" factorizations or obstacles to factorizations of LPDOs.

Winkler, Shemyakova and Kartashova have published their paper in [4, 5]. Shemyakova has presented the results in [23, 26, 24, 25] Winkler has presented the results in [27].

1.2 Theoretical foundations for differential algebraic problems

G. Landsmann has worked on theoretical foundations for differential algebraic problems. He has reported on this work in the joint publication [6]

1.3 Numerical-symbolic methods for discrete geometric problems

H. Gu and Dr. M. Burger (F1308) have worked together on numerical-symbolic approximation methods for a special class of partial differential equations derived from geometric problems. They use finite element method to approximate the solutions of parameter-dependent geometric problems, and investigate the possibility of using symbolic methods as a preprocessing step. Two different discretizations, namely a polynomial reformulation before discretization and a direct discretization of the divergence form are considered to perform the initial symbolic computation. The prolongation of the preprocessed symbolic solution can serve as a starting value for a numerical iterative method on a finer grid.

Gu and Burger have described their results in [21, 8]. Gu has presented the results in [7].

1.4 Analysis of differential equations

E. Kartashova has worked on the analysis of differential equations in year 2005. This work can be divided into three parts:

For linear PDEs (publications [22, 9, 16] and talks [19, 18, 10, 15]): Method of constructive factorization of arbitrary order LPDOs has been developed, invariants for this class of operators are found, these results will be further used for construction of approximate factorization to simplify numerical simulations with corresponding equations.

For nonlinear PDEs describing wave turbulence (publications [11, 17] and talks [13, 20, 12]): A new model of wave turbulence - laminated turbulence has been developed which is a generalization of the classical Kolmogorov-Arnold-Moser model; this model will be further applied for description of some known physical phenomena in laboratory plasma and in the Earth atmosphere.

For general theory of integrable differential equations (publications [1, 2, 3] and talk [14]): Work on the text book on computable aspects of integrability theory is in progress (collaboration with Prof. A. Shabat), conference ALISA-2005 has been organized, work on on-line encyclopedia of integrable systems ALISA will be carried out further in the frame of cooperation treaty with Steklov Math. Institute (Moscow, Russia) and Austrian-Russian project with Landau Institute for Theoretical physics (Chernogolovka, Russia).

References

[1] E. Kartashova, A. S. Computable integrability. chapter 1: General notions and ideas. RISC Report 2005-07, RISC Institute, JKU, 4232 Hagenberg, Austria, 2005.

[2] E. Kartashova, A. S. Computable integrability. chapter 2: Riccati equation. RISC Report 2005-08, RISC Institute, JKU, 4232 Hagenberg, Austria, 2005.

[3] E. Kartashova, A. S. Computable integrability. chapter 3: Integrability of linear pdes. RISC Report 2005-09, RISC Institute, JKU, 4232 Hagenber,g Austria, 2005.

[4] E. Kartashova, E. S., and Winkler, F. Implementation of a factorization algorithm for lpdos. In *Proc. of Workshop on Symbolic-Numeric Computation, Xi'an, China* (July 2005).

[5] E. Kartashova, F. W. Obstacle to factorization of lpdos. In *Proc. Transgressive Computing 2006, Granada, Spain* (2006).

[6] G. Landsmann, P. Mayr, J. S. A topological criterion for polynomiality. In *Algorithmic Algebra and Logic - Proc. A3L, Books on Demand GmbH, Norderstedt* (2005), S. Dolzmann, Seidl, Ed., pp. 155–158.

[7] Gu, H. Preprocessing for finite element discretizations of geometric problems, July 2005. Talk at the International Workshop "Symbolic and Numerical Computation".

[8] H. Gu, M. B. Preprocessing for finite element discretizations of geometric problems. In *Proc. of Workshop on Symbolic-Numeric Computation* (July 2005).

[9] Kartashova, E. Bk-factorization and darboux-laplace transformations. In *Proc. of CSC'05 (The 2005 International Conference on Scientific Computing, Las Vegas)* (June 2005), G. G. H. R. Arabnia, Ed., CSREA Press, USA, pp. 144–150.

[10] Kartashova, E. Bk-factorization and darboux-laplace transformations, June 2005. Contributed talk at CSC-05.

[11] Kartashova, E. Diophantine equations of nonlinear physics. part 1. RISC Report 2005-11, RISC Institute, JKU, 4232 Hagenberg, Austria, 2005.

[12] Kartashova, E. Discrete wave systems: model of laminated turbulence, Dec. 2005. Invited talk at Warwick Turbulence Symposium.

[13] Kartashova, E. Elements of integrability in nonlinear dispersive pdes, Mar. 2005. Invited colloquium talk at Mathematical Physics Seminar, Loughborough University, England.

[14] Kartashova, E. Encyclopedia alisa - main ideas and general structure, Oct. 2005. Invited colloquium talk at Steklov Institute for Mathematics, Russian Academy of Sciences, Moscow, Russia Loughborough University, England.

[15] Kartashova, E. General invariants of linear partial differential operators, Dec. 2005. Contributed talk at SFB Cooperation Meeting, Johannes Kepler University Linz.

[16] Kartashova, E. Hierarchy of general invariants for bivariate lpdos. *J. Theoretical and Mathematical Physics* (2005). to appear.

[17] Kartashova, E. A model of laminated turbulence. *Journal of Experimental and Theoretical Physics, Letters* (2005). to appear.

[18] Kartashova, E. On factorization of linear partial differential operators, Jan. 2005. Invited talk at "Workshop on symmetries, inverse problems and image processing".

[19] Kartashova, E. Order-reduction procedure for factorization of linear partial differential operators of arbitrary order, Feb. 2005. Invited talk at Conference "Solitons, boomerons and isochronious solutions to nonlinear systems".

[20] Kartashova, E. Wave turbulence theory for discrete systems, Sept. 2005. Invited colloquium talk at Landau Institute of Theoretical Physics, Russian Academy of Sciences, Chernogolovka, Russia.

[21] M. Burger, H. G. Numerical-symbolic methods for parameter-dependent geometric differential equations. SFB Report 2005-01, Johannes Kepler University, 4040 Linz, Austria, 2005.

[22] R. Beals, E. K. Constructive factorization of lpdo in two variables. *Journal of Theoretical and Mathematical Physics 145*, 2 (2005), 1510–1523.

[23] Shemyakova, E. Applications of bk method of linear partial differential operators factorization, May 2005. talk at Conference "Computer algebra", Dubna, Russia.

[24] Shemyakova, E. Families of factorizations of linear partial differential operators, Aug. 2005. talk at Conference "ACA'05", Nara, Japan.

[25] Shemyakova, E. Families of factorizations of linear partial differential operators, Dec. 2005. talk at Conference "ASCM'05", Seoul, South Korea.

[26] Shemyakova, E. A maple program for factorization of linear partial differential operators in two variables, June 2005. talk at Conference "SNMP'05", Kyiv, Ukraine.

[27] Winkler, F. On the factorization of linear differential operators, Nov. 2005. Talk at the workshop "Computer Algebra and Informatics" in Lomonosov Moscow State Univ., Faculty of Mechanics and Mathematics.

F 1305: Proving and Solving in Special Function Domains

Prof. Dr. P. Paule

Dr. S. Gerhold, Dr. M. Kauers, Dr. C. Schneider

DI C. Koutschan

1 Proving and Solving in Special Function Domains

The scientific output achieved in 2005 by the SFB project group F1305 is documented in the form of 21 publications: 8 articles were published in journals and 4 in conference proceedings; 9 technical reports have been produced, 4 of which are already accepted for journal publication. Additionally, two PhD-theses [9, 14] have been completed.

1.1 Identities

Various refined summation algorithms [20, 21, 22, 23, 24, 26] have been developed by Schneider that enable one to simplify and/or evaluate complicated multi-sum expressions. Examples of successful applications of these tools are: A computer proof of the "Totally symmetric plane partition" theorem [1], a quadruple sum expression that evaluates to zeta-functions [19, 25], proofs of identities that are needed for Padé approximation [5, 6], and the derivation of reciprocity laws of harmonic numbers that arise in the analysis of algorithms [18]. In addition, recurrences were computed that could speed up the computations in Finite Element Methods [2]; see project F1301.

Kauers and Schneider extended the summation algorithms of Schneider by allowing generic (unspecified) sequences within sums [17]. In [16] they illustrate how these algorithms can be used to discover new general identities.

In a joint effort, Paule, Gerhold, Kauers, Schneider, and Zimmermann could provide proofs of various identities in the Handbook of Mathematical Functions (Abramowitz/Stegun) whose original proofs have been lost [12]. One of of these identities is shown in the box below.

$$\frac{1}{z}\cos\sqrt{z^2-2zt}=\sum_{n=0}^{\infty}\frac{t^n}{n!}j_{n-1}(z) \qquad z\neq 0$$

where $j_n(z)$ are the spherical Bessel functions of the first kind.

In his Ph.D. thesis [14], Kauers presents a collection of algorithms for sequences which can be defined by nonlinear higher order difference equations. An implementation of these algorithms in form of a Mathematica package [15] 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. A large collection of example applications is included in the thesis.

1.2 Inequalities and Asymptotics

Gerhold and Kauers have proposed a procedure for automatically proving inequalities among expressions that are defined via recurrence equations [10]. With this procedure, it was possible to verify a large number of inequalities appearing in the literature by a computer procedure for the first time. A remarkable example is the computer proof of Turán's inequality for Legendre polynomials [11].

Inequalities are in general harder than identities, and the procedure of Gerhold and Kauers is not able to provide a proof for every true inequality to which it is applicable. A conjectured inequality which arose in the numerical work of J. Schöberl (F1319), for example, is in the right shape for the method of Gerhold/Kauers to apply, but the method fails to supply a proof. Attempts to prove this inequality by hand using asymptotic arguments have also failed so far. See [13] for some work that has been done by Gerhold, Kauers, and Schöberl on this inequality.

In joint work with J.P. Bell [3], Gerhold has obtained a fairly satisfactory result about the sign of oscillating linear recurrence sequences: If a C-finite sequence has no real positive dominating root, then its positivity set and its negativity set both have positive density. Moreover, the density can assume each value from $]0,1[$.

1.3 Non-Holonomicity

Non-holonomicity results give some evidence on the algorithmic complexity of a sequence, since values of holonomic sequences can be readily computed by the linear recurrence with polynomial coefficients that defines them. Flajolet, Gerhold, and Salvy [8] have shown by an asymptotic method [7] that the sequence $\mathrm{e}^{1/n}$ is not holonomic. Along the way, amusing asymptotic results like

$$\sum_{k=1}^{n}\binom{n}{k}(-1)^k\mathrm{e}^{1/k}\sim-\frac{\mathrm{e}^{2\sqrt{\log n}}}{2\sqrt{\pi}(\log n)^{1/4}}$$

have been obtained. A completely different approach has been pursued by Bell, Gerhold, Klazar, and Luca [4]. They show how the additional structure of sequences like $e^{1/n}$ and $n^{1/2}$, which are defined by the analytic functions $e^{1/z}$ and $z^{1/2}$, can be exploited more directly to establish their non-holonomicity.

References

[1] Andrews, G., Paule, P., and Schneider, C. Plane Partitions VI: Stembridgeś TSPP Theorem. *Adv. in Appl. Math. 34*, 4 (2005), 709–739.

[2] Bećirović, A., Paule, P., Pillwein, V., Riese, A., Schneider, C., and Schöberl, J. Hypergeometric summation algorithms for high order finite elements. SFB-Report 2006-8, J. Kepler Universität, Linz, 2006. Submitted.

[3] Bell, J. P., and Gerhold, S. The Positivity Set of a Recurrence Sequence. *Israel J. Math.* (2005). To appear.

[4] Bell, J. P., Gerhold, S., Klazar, M., and Luca, F. Non-holonomicity proofs for sequences defined via elementary functions. Submitted.

[5] Driver, K., Prodinger, H., Schneider, C., and Weideman, A. Padé approximations to the logarithm III: Alternative methods and additional results. *To appear in Ramanujan J.* (2006).

[6] Driver, K., Prodinger, H., Schneider, C., and Weideman, J. A. C. Padé approximations to the logarithm II: Identities, recurrences, and symbolic computation. *Ramanujan J. 11*, 2 (2006).

[7] Flajolet, P., Gerhold, S., and Salvy, B. On the non-holonomic character of logarithms, powers and the nth prime function. *Electronic Journal of Combinatorics 11*, 2 (2005), 1–16.

[8] Flajolet, P., Gerhold, S., and Salvy, B. Asymptotic analysis of the generating functions of certain closed form sequences. In preparation, 2006.

[9] Gerhold, S. *Combinatorial Sequences: Non-Holonomicity and Inequalities.* PhD thesis, RISC, J. Kepler Universität, Linz, 2005.

[10] Gerhold, S., and Kauers, M. A procedure for proving special function inequalities involving a discrete parameter. In *Proceedings of ISSAC'05* (2005), pp. 156–162.

[11] Gerhold, S., and Kauers, M. A computer proof of Turán's inequality. *Journal of Inequalities in Pure and Applied Mathematics 7*, 2 (2006).

[12] Gerhold, S., Kauers, M., Olver, F., Paule, P., Schneider, C., and Zimmermann, B. Computer proofs of some identities for bessel functions of fractional order. In preparation, 2006.

[13] Gerhold, S., Kauers, M., and Schöberl, J. On a conjectured inequality for a sum of Legendre polynomials. SFB-Report 2006-11, J. Kepler Universität, Linz, 2006.

[14] Kauers, M. *Algorithms for Nonlinear Higher Order Difference Equations.* PhD thesis, RISC, J. Kepler Universität, Linz, 2005.

[15] Kauers, M. SumCracker — a package for manipulating symbolic sums and related objects. SFB-Report 2005-21, J. Kepler Universität, Linz, 2005. Submitted.

[16] Kauers, M., and Schneider, C. Application of unspecified sequences in symbolic summation. *To appear in ISSAC'06* (2006).

[17] Kauers, M., and Schneider, C. Indefinite summation with unspecified sequences. *To appear in Discrete Math.* (2006).

[18] Kuba, M., Prodinger, H., and Schneider, C. Generalized reciprocity laws for sums of harmonic numbers. SFB-Report 2005-17, J. Kepler Universität, Linz, 2005. Submitted.

[19] Pemantle, R., and Schneider, C. When is 0.999... equal to 1? *To appear in Amer. Math. Monthly* (2006).

[20] Schneider, C. Degree bounds to find polynomial solutions of parameterized linear difference equations in ΠΣ-fields. *Appl. Algebra Engrg. Comm. Comput. 16*, 1 (2005), 1–32.

[21] Schneider, C. Finding telescopers with minimal depth for indefinite nested sum and product expressions. In *Proceedings of ISSAC'05* (2005), M. Kauers, Ed., ACM, pp. 285–292.

[22] Schneider, C. A new Sigma approach to multi-summation. *Adv. in Appl. Math. 34*, 4 (2005), 740–767.

[23] Schneider, C. Product representations in ΠΣ-fields. *Ann. Comb. 9*, 1 (2005), 75–99.

[24] Schneider, C. Solving parameterized linear difference equations in terms of indefinite nested sums and products. *J. Differ. Equations Appl. 11*, 9 (2005), 799–821.

[25] Schneider, C. Some Notes On "When is 0.999... equal to 1?". In *Mathematics, Algorithms, Proofs* (2005), no. 05021 in Dagstuhl Seminar Proceedings.

[26] Schneider, C. Simplifying sums in ΠΣ-extensions. SFB-Report 2006-13, J. Kepler Universität, Linz, 2006. Submitted.

F 1306: Nonlinear 3D Mechanical Problems

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

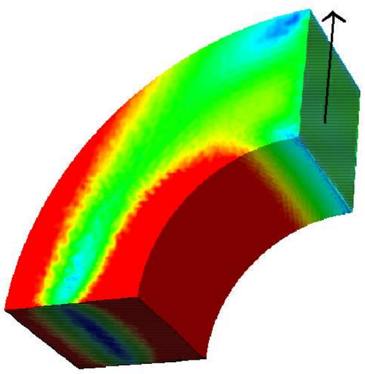

Figure 3: The yield function of an elastoplastic object under traction, fixed on the lower face.

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 non-zero. Figure 3 shows the yield function of an elastoplastic object, the plastic areas with permanent deformations are colored red. The evolution of the plastic strains in time 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, the displacements u and the plastic strains p, i.e.

$$f(u,p) = \min_{v,q} f(v,q), \qquad (2)$$

with incompressibility constraints to satisfy. The objective is smooth in the displacements, but non-smooth in the plastic strains, thus strategies for overcoming the non-smoothness are necessary.

The first class of algorithms is based on a regularization of the objective, where a modulus is smoothed for making the objective f_ϵ twice differentiable. Figure 4 shows the modulus $|p|$ and possible regularizations $|p|_\epsilon$ depending on the regularization parameter ϵ, ϵ is here chosen as 10^{-6}. The green

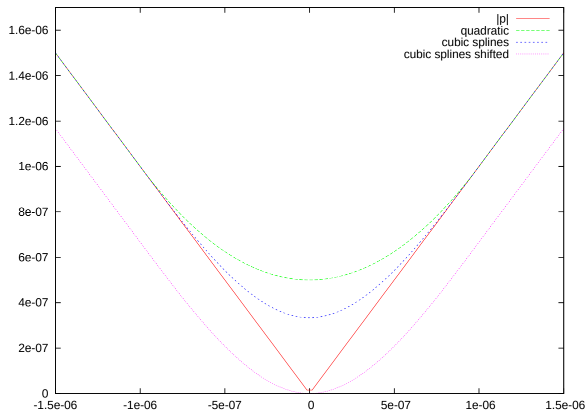

Figure 4: $|p|$ and its regularizations.

quadratic regularization within the interval $(-\epsilon, \epsilon)$ has a smooth first derivative, but the second derivative is piecewise constant and discontinuous, thus the local convergence of Newton type methods cannot be guaranteed. The blue piecewise cubic spline has a piecewise linear continuous second derivative, thus Newton type methods can be applied. The final choice is the pink regularization, where the blue cubic spline function is shifted into the origin, so that $|p|_\epsilon = 0$ holds for $p = 0$.

The algorithm is based on alternating minimization with respect to the two variables, and on the reduction of the objective to a quadratic functional with respect to the plastic strains. This can be interpreted as a linearization of the nonlinear elastoplastic problem.

The minimization problem with respect to the plastic part of the strain is separable and the analytical solution $p_\epsilon(u)$ can be calculated in explicit form. The minimization problem (2) formally reduces to

$$f_\epsilon(u) = \min_{v} f_\epsilon(v, p_\epsilon(v)). \qquad (3)$$

The displacement field is the solution of a linear Schur complement system after the elimination of plastic strains. The solution of this linear system can be efficiently computed by a multi-grid preconditioned conjugate gradient solver.

The second approach is provided by the Moreau-Yosida theory. It follows that the elastoplastic minimization problem can be considered a regularization itself. As the dependence of the strains on the displacements is given by a formula for $p(u)$, the Frechet derivative with respect to the displacements exists, and can be also computed explicitly. The second derivative exists everywhere apart from the elastoplastic interface, thus there it is replaced by a slant derivative and a quasi-Newton method is applied.

All regularization approaches are treated in the ongoing PhD thesis [3] of J. Kienesberger, the Moreau-Yosida approach was first discussed in the master's thesis [2] of our diploma student P. Gruber.

The algorithm was extended towards uniform p-adaptivity, where p denotes the polynomial degree of the ansatz functions for the finite element spaces of u and p. These high order polynomials were investigated and implemented by the Start project group "Y-192" of J. Schöberl. First results for elastoplastic problems were published in [4].

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 [1]. Such an 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. Numerical examples confirm an improved linear convergence rate, the performance of the algorithm in comparison with the more frequently applied maximum refinement rule is studied in Figure 5.

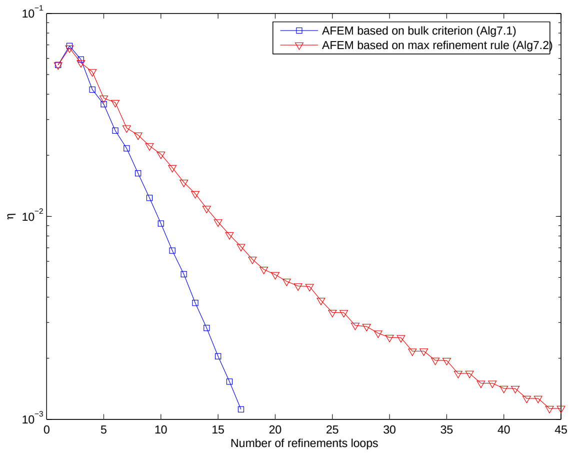

Figure 5: Comparison of the new adaptive algorithm (blue line) and the original algorithm based on the maximum refinement rule (red line). Note that using the new algorithm, the energy of the elastoplastic solution is linearly reduced with each refinement step.

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. So far, the only applied technique was an alternating minimization, whose convergence is known to be geometrical and global. They showed that symmetries can be utilized to obtain a more efficient implementation of the alternating minimization. For the first plastic time-step problem, which describes the initial elastoplastic transition, the exact solution for p_1 and p_2 could even be obtained analytically. In the later time-steps used for the computation of the further development of elastoplastic zones in a continuum, an extrapolation technique as well as a Newton-algorithm were proposed.

At last, J. Valdman cooperated with S. Repin (St. Petersburg) on reliable error estimates for the scalar nonlinear problem, where the nonlinearity is defined on a part of the boundary. Such system can be easily described as a variational inequality. They derived a-posteriori estimates of the difference between the exact solution of such type variational inequalities and any function lying in the admissible functional class of the problem considered. It is shown that the structure of the error majorant reflects properties of the exact solution. The majorants provide guaranteed upper bounds of the error for any conforming approximation and possess necessary continuity properties. In the series of numerical tests performed, it was shown that the estimates are explicitly computable, they provide sharp bounds of approximation errors, and they give high quality indication of the distribution of local (element-wise) errors. The joint work will be extended to problems of elasticity with so-called friction boundary conditions and to elastoplasticity as well.

References

[1] Carstensen, C., Orlando, A., and Valdman, J. A convergent adaptive finite element method for the primal problem of elastoplasticity. *Int. J. Numer. Methods Eng.* (2006). accepted.

[2] Gruber, P. Solution of elastoplastic problems based on Moreau-Yosida theorem. Master's thesis, Johannes Kepler University Linz, 2006.

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

[4] Kienesberger, J., and Valdman, J. An efficient solution algorithm for elastoplasticity and its first implementation towards uniform h- and p- mesh refinements. In *Proceedings of ENUMATH 2005.*

F 1308: Computational Inverse Problems and Applications

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

Dr. N. Bila, Dr. H. Egger, Dr. H.K. Pikkarainen, DI B. Hackl, DI A. Hofinger, DI R. Stütz, DI M.T. Wolfram

Dr P. Kügler (Basic Staff)

1 Stochastic Inverse Problems

A collaboration between H.W.Engl and A.Hofinger with S.Kindermann resulted in a publication on regularization methods for stochastic inverse problems that appeared in 2005 (cf. [11]). In this work it was demonstrated how the Prokhorov metric can be applied to linear inverse problems in order to derive results on convergence rates. Extensions to other stochastic error measures such as the Ky-Fan metric have been considered recently by A.Hofinger (cf. [13]).

H.Pikkarainen, who joined project F 1308 in fall 2005, wrote an article in which the results presented in her doctoral dissertation concerning electrical impedance process tomography were extended to a certain class of linear nonstationary inverse problems (cf. [18]). The novel contribution of the article is the analysis of the space discretization of the corresponding infinite-dimensional state estimation system.

Numerical implementation of the method introduced in this work was considered, in a possible one-dimensional model case in collaboration J.Huttunen (University of Kuopio, Finland). The effectiveness of the method introduced will be presented in a forthcoming article.

2 Iterative Regularization

Preconditioning: Especially for nonlinear and even large scale linear inverse problems, iterative regularization methods are an attractive, widely used alternative to classical regularization methods, like Tikhonov regularization. One of the drawbacks of iterative regularization algorithms, especially of simple methods like Landweber iteration, is that usually many iterations are needed in order to obtain optimal results. While for well-posed problems, preconditioning is very well understood and successfully used to accelerate iterative methods, the question of (optimal) preconditioning of iterative methods for ill-posed equations has not been analysed in detail so far. In joint publication with Prof. A. Neubauer (University Linz), H. Egger proposed a preconditioning strategy for Landweber iteration for inverse problems (cf. [10]). In his PhD. thesis (cf. [5]) on "Preconditioning Iterative regularization in Hilbert Scales", the construction of efficient preconditioners for large classes of linear and nonlinear ill-posed problems and for several iterative regularization methods under relatively mild assumptions was investigated. In a subsequent publication (cf. [6]), the acceleration of semiiterative regularization methods has been investigated. In recent research, so called Y-scale regularization methods are considered: while in standard regularization in Hilbert scales, scales of spaces over the the domain of the operator under consideration are used to either extend the range of optimal convergence of regularization methods or to accelerate iterative methods, scales of spaces over the range space of the operator are considered in Y-scale regularization. This allows to apply the idea of Hilbert scale regularization to new classes of problems (cf. [7]).

Convergence Analysis of Iterative Regularization: One of the drawbacks of iterative regularization methods is a saturation effect when the iteration is stopped by a discrepancy principle. Saturation can be partially overcome, i.e., better convergence rates can be achieved, if a more sophisticated a-posteriori stopping rule is considered. The possible improvement of convergence results by applying new a-posteriori stopping rules has been considered in [4]. Moreover, the use of semiiterative methods in each Newton step has been shown to yield a significant acceleration of the overall scheme.

For the convergence analysis of Newton-type regularization methods suitable decompositions of (differences of) certain polynomials (acting on noncommutative operators) are of importance. Such decompositions are investigated in an ongoing research of H. Egger and G. Regensburger (F1322).

3 Parameter Identification in Parabolic PDEs

Volatility Identification from Option Prices: Volatility is one of the key parameters in many stochastic models in mathematical finance. Earlier research on volatility identification in extended Black-Scholes models has been pursued [8]. In cooperation with Prof. B. Hofmann (TU Chemnitz), a new approach to volatility identification has been considered: if a special (non-parametric) structure of the local volatility surface is assumed, the parameter identification problem can be shown to decompose into two separate subproblems, whose solution is computationally much faster and more stable. A joint publication has been submitted (cf. [9]). Previous work on identification of volatilities by H.Egger and H.Engl has been completed and accepted for publication in 2005 (cf. [8]).

A collaboration of H.Egger with J.Sass (RICAM Mathematical Finance Group) has been started recently, which is is devoted to parameter identification in Levy-processes from observations of a state trajectory.

Semiconductor Inverse Dopant Profiling: The identification of doping profiles in semiconductor devices, previously investigated in this subproject in a stationary setting, has been reconsidered for an instationary model and transient measurements by M.T.Wolfram in her Diploma thesis (cf. [20]) and subsequent publications (cf. [21, 19]). The use of transient current and capacitance measurements yields additional information and thus allows better reconstruction of doping profiles, but also makes the inverse problem computationally more demanding. Tikhonov regularization and its computational implementation has been considered in this application starting from the case of diodes that can be reduced to one-dimensional flow models. The implementation of the approach for devices two- and three-dimensional flow behaviour is currently in progress. An analysis of the inverse problem showed that uniqueness in the case of a bipolar device cannot be expected without additional a-priori knowledge, which has to be incorporated in the regularization scheme (e.g. the prior in Tikhonov regularization). Moreover, an asymptotic analysis and problem reduction have been used to obtain a more efficient reconstruction scheme in the case of highly doped devices (which leads to a scaling limit in the underlying PDE-model). So far the latter has been applied only for unipolar devices, an extension to bipolar ones is in progress.

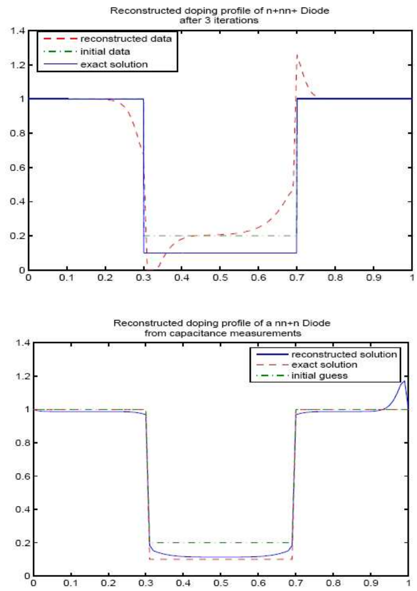

Figure 6: Reconstruction of a doping profile in a $n^{+}nn^{+}$ diode from current and capacitance measurements. .

4 Level Set Methods

Level set methods for geometric inverse problems and imaging tasks have been subject of research of several project members (M.Burger, B.Hackl, S.Kindermann). Besides the ill-posedness of geometric inverse problems, a crucial problem is their numerical solution. To deal with the ill-posed character, penalization perimeter is used frequently, while level set methods are widely used for the numerical solution. Although level set methods are supposed to allow topological changes, theory and practice show that this possibility is somehow limited. To force nonetheless topological changes, the concept of topological gradients was incorporated into level set methods. Topological gradients indicate where to force a topological change but do not provide information about the global influence of this change to the objective functional. Moreover, the widely used perimeter regularization is not topologically differentiable. For a suitable class of geometric inverse problems, first and a second order methods were developed by B.Hackl in order to estimate the change of the objective function with respect to the topology change (cf. [12]). These methods can deal also with perimeter regularization and provide global information about the influence of the topology change to the objective functional. The first order estimate is in principle very similar to the topological gradient, while the second order estimate is based on a quadratic minimization problem governed by another partial differential equation. While the first order method is very cheap and simple to implement, the second order method provides better estimates close to the solution. Both methods were incorporated into the level set methods and tested numerically, the resulting schemes turned out to provide a reliable change of topology during the reconstruction.

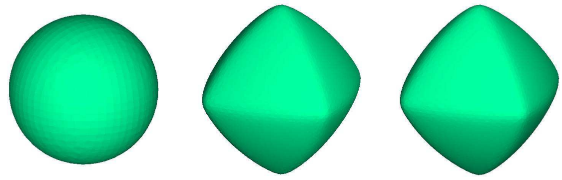

Figure 7: Evolution of a surface via curvature regularized anisotropic surface diffusion flow, computed via level set methods. .

Several applications of level set and related techniques in imaging problems have been considered in 2005. A first approach concerned a global relaxation technique for segmentation problems based on total variation minimization, which led to a simple level set technique (cf. [3]). Another investigation was related to the decomposition of images into cartoon, texture, and noise, where again a level set technique could be applied together with a suitable saddle-point formulation (cf. [15]). Finally, improved total variation techniques, which operate on the level sets of images, have been derived for the classical inverse problems of image denoising and deconvolution (cf. [1, 16, 17]).

Finally, the regularization and construction of level set methods for anisotropic flows as appearing in thermal faceting has been considered. Such problems pose various challenges due to the strong nonlinearities and the high order of the involved differential operators (cf. [2]).

5 Learning Theory

In the past years regularization methods for neural networks have been studied. In the chosen approaches it was always assumed that full measurements are given, nonetheless in practice only discrete, noisy observations at certain points are available. Using Koksma-Hlawka-type inequalities it could now be shown that the previously derived approaches also work in the discrete setup (cf. [14]). This work has been carried out in a collaboration between A.Hofinger and F.Pillichshammer (Financial Mathematics Institute, JKU Linz).

6 Further Activities

Within this subproject, the organization of two international workshops have been organized in 2005. The international workshop "Symmetries, Inverse Problems and Imaging" took place in Linz in January 2005, and the international workshop "Level Set Methods for Direct and Inverse Problems" took place in September 2005.

The results achieved in this subproject lead to invitations of project members to talks at various universities and at various conferences and workshops.

H.Egger finished his PhD-Thesis and graduated in August 2005.

References

[1] Burger, M., Gilboa, G., Osher, S., and Xu, J. Nonlinear inverse scale space methods. *Communications in Mathematical Sciences 4*, 1 (2006), 179–212.

[2] Burger, M., Hausser, F., Stöcker, C., and Voigt, A. A level set approach to anisotropic flows with curvature regularization. CAM-Report 06-02, UCLA, 2006. Submitted.

[3] Burger, M., and Hintermüller, M. Projected gradient flows for bv / level set relaxation. *PAMM 5* (2005), 11–14.

[4] Egger, H. Accelerated Newton-Landweber iterations for regularizing nonlinear inverse problems. SFB-Report 2005-03, SFB F013, 2005.

[5] Egger, H. *Preconditioning Iterative Regularization in Hilbert Scales*. PhD thesis, University Linz, August 2005.

[6] Egger, H. Semiiterative regularization in Hilbert scales. SFB-Report 2004-26, SFB F013, 2005.

[7] Egger, H. Y-scale regularization. SFB-Report 2006-07, SFB F013, 2006.

[8] Egger, H., and Engl, H. Tikhonov regularization applied to the inverse problem of option pricing: Convergence analysis and rates. *Inverse Problems* (2005). accepted.

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

[10] Egger, H., and Neubauer, A. Preconditioning Landweber iteration in Hilbert scales. *Numer. Math.* (2005). accepted.

[11] Engl, H. W., Hofinger, A., and Kindermann, S. Convergence rates in the Prokhorov metric for assessing uncertainty in ill-posed problems. *Inverse Problems 21* (2005), 399–412.

[12] Hackl, B. Methods for reliable topology changes for perimeter regularized geometric inverse problems. *submitted* (2006).

[13] Hofinger, A. *Ill-posed problems: Extending the deterministic theory to a stochastic setup*. PhD thesis, University Linz, April 2006.

[14] Hofinger, A., and Pillichshammer, F. Learning a function from noisy samples at a finite sparse set of points. Tech. rep., SFB F013, 2005. Submitted.

[15] Kindermann, S., and Osher, S. Saddle point formulation for a cartoon-texture decomposition. CAM-Report 05-42, UCLA, 2005. Submitted.

[16] Kindermann, S., Osher, S., and Xu, J. Denoising by bv-duality. CAM-Report 05-21, UCLA, 2005. Submitted.

[17] Osher, S., Burger, M., Goldfarb, D., Xu, J., and Yin, W. An iterative regularization method for total variation based image restoration. *Multiscale Modelling and Simulation* (2005). accepted.

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

[19] Wolfram, M. Semiconductor inverse dopant profiling from transient measurements. Tech. rep., Johannes Kepler University Linz, 2006. Submitted.

[20] Wolfram, M.-T. Semiconductor inverse dopant profiling from transient measurements. Master's thesis, Johannes Kepler University Linz, 2005.

[21] Wolfram, M.-T., and M.Burger. Inverse dopant profiling for highly doped semiconductor devices. In *Conference Proceedings of MATHMOD 2006* (2006).

F 1309: Multilevel Solvers for Large Scale Discretized Optimization Problems

Prof. Dr. Ulrich Langer, Prof. Dr. Heinz W. Engl,

Dr. Ewald Lindner, Prof. Dr. Walter Zulehner,

Roman Stainko, René Simon

1 Optimal Design Problems

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

During the last year, we not only continued our investigations on optimal design problems. Especially we focused our work on efficient solution techniques for large-scale indefinite linear systems of equations, that result from the optimality systems of optimal design and optimal control problems.

Topology optimization is by far the most general class of optimal design problems, as it does not a-priori assume the connection of the structural parts nor the position of the used material (and the position, shape and number of holes). Optimal control deals with the problem of finding a control function for a given system such that a certain optimality criterion is achieved. Here the control function does not describe a design, but other quantities in a system of partial differential equations. Although the way of posing the problems for optimal design and optimal control is very similar, the coefficient matrices of the resulting optimality systems have different patterns.

2 Topology Optimization

We continued our cooperation with Project F1308 with respect to the phase–field based approach to stress constrained topology optimization. Standard topology optimization methods fail when it comes to problems with local stress constraints due to lack of constraint qualifications. As a result the related set of feasible design has non-regular properties. A reformulation of the constraints, based on [5], overcomes this problem. We adapted this idea to our continuous problem formulation and added a parameter dependent Cahn–Hillard relaxation term to the objective for regularizing reasons. The problem is then solved for a decreasing sequence of this parameter. For solving the resulting optimization problems we used a primal-dual interior-point method, which is a very suitable method to attack very large scale problems. A picture showing the optimal material distribution of benchmark beam w.r.t. local von Mises stress constraints can be found in Figure 9 (red indicates material, blue indicates air), where Figure 8 shows the sketch of the problem. More information about this approach can be found in [1]. Moreover, a previ-

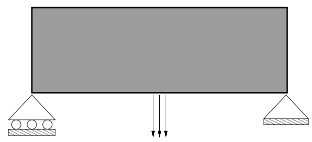

Figure 8: Sketch of a beam example

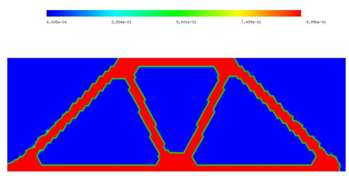

Figure 9: Optimal material distribution

ously developed adaptive multilevel approach for the minimal compliance problem is now published, see [3].

3 Preconditioning

Optimal design problems and optimal control problems are optimization problems that are governed 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 (e.g. describing the equilibrium of forces), 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 (KKT-system). This leads to large scale symmetric, but indefinite, saddle-point problems, like (4), which are solved by iterative methods.

$$\begin{pmatrix} A_{11} & A_{12} & B_1^T \\ A_{21} & A_{22} & B_2^T \\ B_1 & B_2 & 0 \end{pmatrix} \begin{pmatrix} q \\ u \\ \lambda \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ g \end{pmatrix} \quad (4)$$

But in order to exploit the potential speed-up, which is expected by these approaches, efficient solution techniques to solve the large scale linear systems are needed.

Multigrid methods certainly belong to the most efficient methods for solving large scale system. During the last year we used multigrid methods to solve systems of the form (4), resulting from one topology optimization problem and one optimal control problem. One of the most important ingredients of an efficient multigrid method is an appropriate smoother. In our work we considered a multiplicative Schwarz-type iteration method as a smoother in the multigrid method. Each iteration step of such a multiplicative Schwarz- type smoother consists of the solution of several small local saddle point problems over a patch of the finite element mesh, i.e. small local versions of the global saddle point problem (4). For detailed description of this smoothing method, we refer to [2].

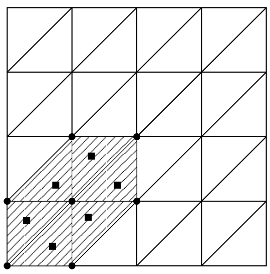

Figure 10: Patch of a local saddle point problem

3.1 An optimal control problem

In order to adapt this smoothing idea to an optimal control problem, we solved the KKT-system arising from the first order optimality conditions for a quadratic, elliptic optimal control problem by a multigrid method. Table 1 contains the (averaged) convergence rates for different numbers of smoothing steps. The numerical results show the typical multigrid behavior, namely the independence of the convergence rate of the grid level and the improvement of the rates with an increasing number of smoothing steps.

Level	Unknowns	Smoothing steps 1+1	3+3	5+5
4	2114	0.1837	0.0231	0.0071
5	8322	0.1897	0.0251	0.0068
6	33026	0.1913	0.0255	0.0080
7	131586	0.1930	0.0265	0.0079

Table 1: Convergence rates, V-cycle

3.2 An optimal design problem

We applied a multigrid method with the above mentioned smoothing technique to the KKT-system of the stress constrained topology optimization problem, treated in [1]. Table 2 lists the convergence rates of a numerical example and it shows the typical multigrid convergence behaviour, i.e., convergence rates that are asymptotic independent of the grid level and an asymptotic constant number of iterations. For more details we refer to [4].

Level	Unknowns	Smoothing steps 1+1 Iterations	Conv. Factor
4	725	39	0.621
5	2853	25	0.478
6	11333	24	0.460
7	45189	22	0.427
8	180485	22	0.425

Table 2: Convergence rates for a W-cycle and an error reduction by a factor of 10^{-8}.

References

[1] Burger, M., and Stainko, R. Phase–field relaxation of topology optimization with local stress constraints. To appear in *SIAM Journal on Control and Optimization*, 2006.

[2] Schöberl, J., and Zulehner, W. On Schwarz-type smoothers for saddle point problems. *Numerische Mathematik 95*, 2 (2003), 377–399.

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

[4] Stainko, R. An optimal solver to a kkt-system. Tech. Rep. 15, Special Research Program SFB F013, JK University of Linz, April 2006.

[5] Stolpe, M., and Svanberg, K. Modeling topology optimization problems as linear mixed 0–1 programs. *International Journal for Numerical Methods in Engineering 57*, 5 (2003), 723–739.

F 1315: Numerical and Symbolic Techniques for Algebraic Spline Surfaces

Prof. Dr. J. Schicho, Prof. Dr. B. Jüttler
Dr. P. Chalmovianský, Dr. E. Wurm

The on–going work in this subproject was devoted to several tasks.

Algebraic subdivision [2] We continued to analyze a novel geometrically motivated subdivision scheme for curve design. Starting from an initial sequence of points with associated normals, we refine by generating new elements until we reach a sufficiently smooth limit curve. Our method is among the first which has been defined solely by using geometric information. It has been shown to generate tangent continuous limit curves. In addition, it preserves circles, i.e., if the data are taken from a circular segment, then the method truly reproduces that curve. An example is shown in Figure 11.

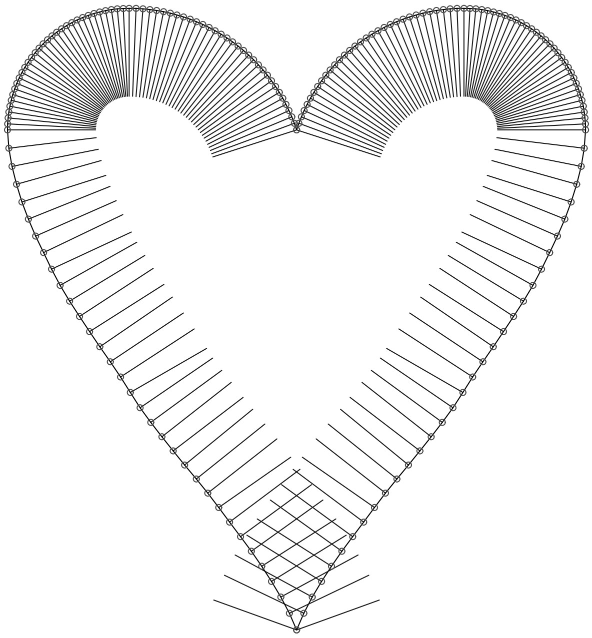

Figure 11: Circle-preserving subdivision

Approximate parameterization of space curves [1] A space curve can be obtained by intersecting two implicitly defined surfaces. We propose a new technique for generating a piecewise rational approximation. Our approach uses a combination of predictor and corrector steps in the space of rational parametric representations. It is able to fully exploit the power of the rational representations, using both the control points and their "weights" for optimization. See Figure 12 for an example.

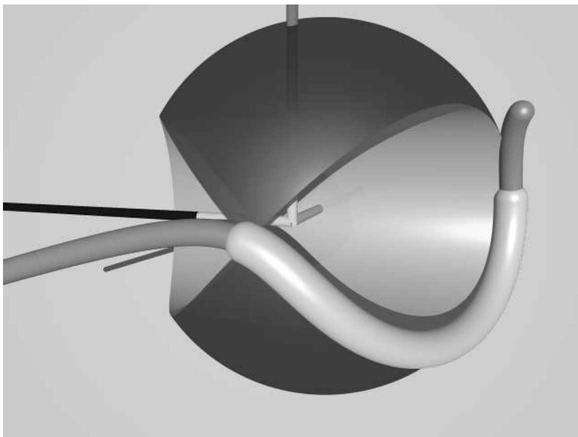

Figure 12: Approximate parameterization of an implicitly defined space curve

Approximate algebraic techniques for curves and surfaces [4] A survey paper covering several aspects of approximate algebraic techniques for designing, analyzing and visualizing curves and surfaces has been presented as a keynote talk at the 21st Spring Conference on Computer Graphics. Among other topics, it covers visualization via ray-tracing and a procedure for orthogonalizing the implicit definition of a space curve.

Approximate parameterization of surfaces [6] A region-growing type technique for the generating rational surface patches on implicitly defined surfaces has been proposed. It combines minimizing a function measuring the deviation from the implicit surface with terms controlling the inner geometry of the surface. In the case of truly rational algebraic surfaces, it gives results which are virtually exact. See Figure 13 for an example.

Comarison of techniques for approximate implicitization [5] Based on industrial benchmark data, several techniques for approximate implicitization of freeform surfaces by spline functions have been compared. The comparison was based on criteria such as computational efficiency, reproduction of low-degree implicit representations, and the possibility of avoiding unwanted "phantom branches".

Other activities The co–investigator of this subproject (B. Jüttler) served as the program chair of the 21st Spring Conferenc on Computer Graphics [3].

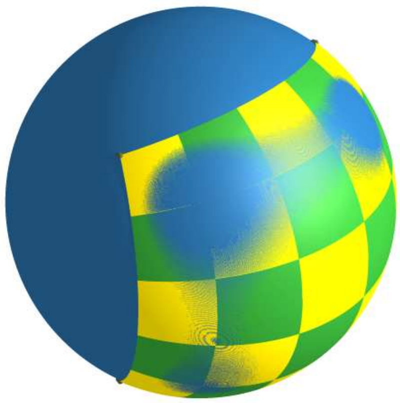

Figure 13: Approximate rational parameterization of an implicitly defined surface

He has greatly been supported by Dr. P. Chalmovianský during the reviewing and selection process.

References

[1] Chalmovianský, P., and Jüttler, B. A predictor–corrector–type technique for the approximate parameterization of intersection curves. *SFB Report* (2005). No. 2005-10.

[2] Chalmovianský, P., and Jüttler, B. A non–linear circle-preserving subdivision scheme. *Advances in Computational Mathematics* (in press).

[3] Jüttler, B., Ed. *Proc. 21st Spring Conference on Computer Graphics*. Comenius University Press / ACM Siggraph, 2005.

[4] Jüttler, B., Chalmovianský, P., Shalaby, M., and Wurm, E. Approximate algebraic methods for curves and surfaces and their applications. In *Proc. SCCG 2005* (2005), Comenius University Press / ACM Siggraph, 200.

[5] Shalaby, M. F., Thomassen, J. B., Wurm, E. M., Dokken, T., and Jüttler, B. Piecewise approximate implicitization: Experiments using industrial data. In *Algebraic Geometry and Geometric Modelling*, B. Mourrain, M. Elkadi, and R. Piene, Eds. in press.

[6] Wurm, E., Jüttler, B., and Kim, M.-S. Approximate rational parameterization of implicitly defined surfaces. In *The Mathematics of Surfaces XI* (2005), R. Martin, H. Bez, and M. Sabin, Eds., Springer LNCS 3604, pp. 434–447.

F1322: Computer Algebra for Pure and Applied Functional Analysis

Prof. Dr. B. Buchberger, Prof. Dr. H.W. Engl
Dr. M. Rosenkranz, Dr. G. Regensburger

In the year 2005, we have extended various *ideas and techniques* crucial to the project (described below in some more detail): The structure of integro-differential rings provides a natural framework for expressing the operators pertinent to boundary value problems, which lie at the heart of this project. In the course of giving a lecture, we have investigated the possibilities of the so-called Mikusiński calculus, a classical method for treating initial value problems, dating back to the sixties; we believe there is quite some potential in this forerunner (so to say) of symbolic functional analysis.

As one example of a *nonlinear* "boundary value problem", we constructed an analytic solution of the Riccati equation (somehow the simplest such problem possible). Another attack onto the area of nonlinear problems was established through so-called max-plus semirings, which provide a natural structure for studying the (generalized) solutions of certain nonlinear ODEs with multi-point boundary conditions. We have also made some advances in constructing optimized wavelets (e.g. for compression of image data), started already in 2004.

Integro-Differential Rings. This class is a natural generalization of the well-known differential rings [8, 9]. The essential difference is that they contain the indefinite integral as an additional operation, together with some axioms to the effect of making the integral "almost inverse" to the given derivation. This is necessary because we want to solve boundary value problems with parametrized right-hand side, so the operation of integration must be available explicitly (not only implicitly as in the case of Ritt-Kolchin's differential algebra). It turns out that the corresponding integro-differential polynomials (analogous to the differential polynomials of differential algebra) are exactly the Green's polynomials of [11, 10].

The Mikusiński calculus. Giving a precise algebraic basis to Heaviside's ideas of an "operator calculus" for solving initial value problems for certain linear ODEs, the crucial point is to create the quotient field for the convolution ring of continuous functions. The result is a practical calculus where solving a differential equation means dividing by the corresponding differential operator. We have embarked on transferring these ideas to the situation of boundary value problems (the classical Mikusiński calculus is intrisically restricted to initial value problems due to the commutativity of convolution). A first draft on some new ideas in this vein are to be found in the lecture notes [13].

The Riccati problem. It is given by the differential equation $u' + u^2 = f$ with the initial condition $u(0) = 0$. In contrast to the standard situation where f is some fixed right-hand side, we regard f as a symbolic parameter, keeping in the spirit of boundary value problems. (It is for this reason that we still refer to the Riccati problem as a "boundary value problem" even though it has only one "boundary point" since it is of first order!) It is well known that the above problem has no Liouvillian solution for generic f, therefore we have constructed an analytic solution [12]. The formula for the Taylor coefficients of u turned out to be quite complicated, involving sums over certain integer partitions and compositions as well as trees that "specialize" them.

Max-plus Semiring. Another focus of our work was on nonlinear differential equations and semirings starting from a suggestion of Martin Burger at the SFB-Statusseminar 2005. We surveyed the relevant literature on idempotent and pseudo analysis in connection with differential equations [6]. The max-plus semiring, where the addition is replaced by the maximum and the multiplication by the sum, showed to be particularly useful for symbolic computation. We developed a symbolic method to compute generalized solutions for nonlinear first-order ordinary boundary value problems of the form $f(x, y'(x)) = 0$ where we assume that we have a (symbolic) representation of the solutions of the initial value problem. We can add arbitrary constants to a solution of such a differential equation, and the maximum (or minimum) of two solution is again a generalized solution, possibly nondifferentiable at some points. Thus max-plus (or min-plus) linear combinations of solutions are again (generalized) solutions. Using this observation, we showed that the existence and uniqueness of a max-plus linear combination solving a given boundary value problem can be translated to the analogous questions for a corresponding max-plus linear system. An implementation for max-plus linear systems and the method for the computer algebra system Maple is already available.

Wavelets. We also continued our work on symbolic computation and wavelets and extended results on parametrized wavelets based on joint work with Otmar Scherzer [7] in several directions [2, 3, 4].

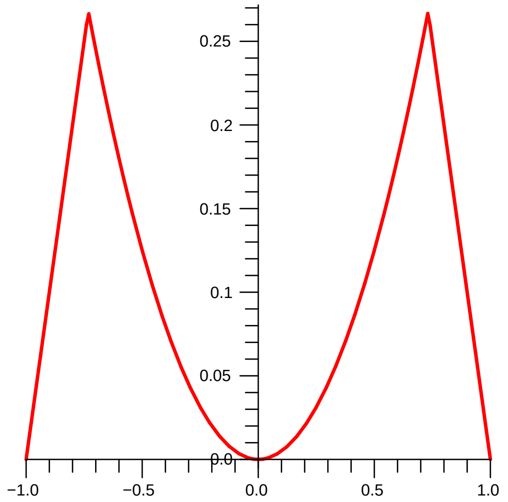

Figure 14: The generalized min-plus solution of the differential equation $x - y' - y'^2 x + y'^3 = 0$ with boundary conditions $y(-1) = y(0) = y(1) = 0$

See in particular the SFB-report [5] where new parametrizations of filter coefficients of scaling functions and wavelets are obtained using Gröbner bases which were introduced by Bruno Buchberger.

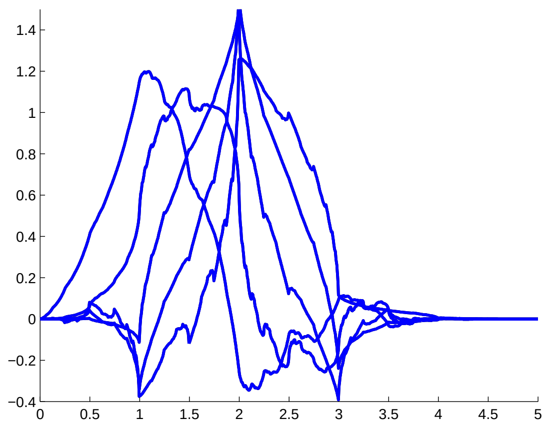

Figure 15: Parametrized wavelets (6 filter coefficients)

References

[1] Buchberger, B., Rosenkranz, M., et al. Theorema: Towards computer-aided mathematical theory exploration. *Journal of Applied Logic to appear* (2006).

[2] Regensburger, G. Construction and applications of parametrized wavelets. Workshop on Inverse Problems, Obergurgl, April 2005.

[3] Regensburger, G. Construction of parameterized wavelets using gröbner bases. ACA 2005, Conference on Applications of Computer Algebra, Nara, Japan, August 2005.

[4] Regensburger, G. Parametrized wavelets and algebraic curves. Workshop on Resolution of Algebraic Varieties, September 2005.

[5] Regensburger, G. Parametrizing compactly supported orthonormal wavelets by discrete moments. Tech. Rep. 2005-23, SFB F013, 2005. `http://www.sfb013.uni-linz.ac.at/`.

[6] Regensburger, G. Semirings, idempotent analysis and differential equations. Workshop on "Level Set Methods for Direct and Inverse Problems", Special Session on Symbolic Computation and PDEs, RICAM Linz, September 2005.

[7] Regensburger, G., and Scherzer, O. Symbolic computation for moments and filter coefficients of scaling functions. *Ann. Comb. 9*, 2 (2005), 223–243.

[8] Rosenkranz, M. Integro-differential rings and operators. SFB Statusseminar, Strobl, April 2005.

[9] Rosenkranz, M. Linear two-point boundary value problems in symbolic computation: A new approach. Foundations of Computational Mathematics (FoCM'05), Santander, Spain, July 2005.

[10] Rosenkranz, M. New symbolic computation methods for the exact solution of two-point boundary value problems. Algorithmic Information Theory (AIT'05), Vaasa, Finland, May 2005.

[11] Rosenkranz, M. New symbolic method for solving linear two-point boundary value problems on the level of operators. *Journal of Symbolic Computation 39*, 2 (February 2005), 171–199.

[12] Rosenkranz, M. Symbolic solution of nonlinear bvps? - first steps and considerations. Workshop on Inverse Problems, Obergurgl, April 2005.

[13] Rosenkranz, M. Symbolic computation methods for functional analysis. Lecture notes, 2006.

SFB F013: Numerical and Symbolic Scientific Computing

Coherence within the SFB

- **Cooperation between F1301, F1305 and F1306**

  Summation and Finite Elements. In F1301, Prof. P. Paule and Prof. J. Schöberl have continued to apply summation techniques from F1305 to the construction of high order finite elements [2], which are also relevant to F1306. Besides hypergeometric summation, C. Schneider's Sigma approach can be used to compute recurrence relations for sums involving orthogonal polynomials. This allows fast assemblance of the stiffness matrix ([1]).

  V. Pillwein and B. Zimmermann applied methods from symbolic computation to find recurrences for high order finite element basis functions, which are initially given by hypergeometric sums. These results allow an efficient implementation of the iterative equation solvers. They applied Fasenmyer's method for definite hypergeometric summation (implemented in Wegschaider's package `MultiSum`) and effective closure properties for P-finite functions (implemented in `GeneratingFunctions`).

  New shape functions for tetrahedra. S. Beuchler from F1306 and V. Pillwein constructed high order basis functions for the second order boundary value problem $-\nabla(A(x,y)\nabla u) = f$ on a tetrahedral mesh and proved the sparse structure of the resulting system matrix. Currently they are conducting numerical experiments to investigate further properties of these basis functions and applying symbolic summation methods to derive recurrences for these shape functions.

  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.

- **Cooperation between F1302, F1322, and F1308**
  As pointed out in the previous reports, project F1322 was born by a nontrivial cooperation between projects F1302 and F1308. Naturally, this interaction has been maintained and has gained new impetus. 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). This line of research is now strengthened by considering wider classes of practically relevant operators (for more details see the section about F1322): ill-posed problems (first results have been obtained), operators with symbolic parameters (full solution of the the generic Sturm problem!), nonlinear problems (following some recent ideas by Martin Burger from F1308).

- **Cooperation between F1302, F1305, and F1303**
  In the context of analysis and verification of programs (expressed both in functional and imperative style), we are using 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).

- **Cooperation between F1302 and F1301**
  In the context of our case study on Groebner 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 Groebner Bases.

- **Cooperation between F1303 and F1304**
  We continued in cooperation – with G. Landsmann, subproject 1304, and P. Mayr from the department of algebra – which started promisingly last year. In a study of polynomial functions over linear groups we applied topological methods for real and complex manifolds. We could answer the question whether a transposition is a polynomial function in the matrix group, for cases of infinite fields of real and complex numbers.

- **Cooperation between F1303 and F1315**
  Another cooperation was to combine the stability analysis for the implicitization problem

obtained in our group by the stability analysis of implicit equations obtained in subproject 1315. Together with B. Jüttler and M. Aigner we extended the result to finding a geometric error in terms of the Hausdorff distance.

- **Cooperation between F1304 and F1308**
  H. Gu has cooperated with M. Burger (F1308) for symbolic and numeric computation of geometric problems.

- **Cooperation between F1304 and others**
  On the topic of factorization of differential operators we have discussed symbolic-numeric methods with other groups in the SFB.

- **Cooperation between F1305, F1301 and F1306**
  In F1301, Prof. P. Paule and Prof. J. Schöberl have continued to apply summation techniques from F1305 to the construction of high order finite elements [2], which are also relevant to F1306. Besides hypergeometric summation, C. Schneider's Sigma approach can be used to compute recurrence relations for sums involving orthogonal polynomials. This allows fast assemblance of the stiffness matrix ([1]).

- **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 nonsmooth minimization problem for the unknown plastic-strain increment matrices p_1 and p_2. So far, the only applied technique was an alternating minimization, whose convergence is known to be geometrical and global. They showed that symmetries can be utilized to obtain a more efficient implementation of the alternating minimization. For the first plastic timestep problem, which describes the initial elastoplastic transition, the exact solution for p_1 and p_2 could even be obtained analytically. In the later time-steps used for the computation of the further development of elastoplastic zones in a continuum, an extrapolation technique as well as a Newton-algorithm were proposed. A joint paper is in preparation.

- **Cooperation between F1308 and F1306**
  A collaboration between A. Hofinger with J. Valdman was concerned with the acceleration of algorithms in multiyield-plasticity. In multi-surface elastoplasticity a system of nonlinear equations must be solved in each timestep, for every grid-point of the finite element grid, the solution of this problem is therefore a time-critical step. An extrapolation technique was successfully applied to this problem and could reduce the computation time by approximately a factor of ten. A joint paper will be finished in 2006.

- **Cooperation between F1308 and F1309**
  A collaboration of M. Burger and R. Stainko (F1309) on the use of level set techniques for topology optimization (cf. [3]) has been continued. An important recent development was the construction of a one-shot multigrid method for linear problems arising in each step of the previously derived iterative scheme for topology optimization with stress constraints. This novel approach, based on local patch smoothers, yields an efficient method that turns out to be robust with respect to the discretization size and other parameters appearing in the problem (cf. [4]).

- **Cooperation between F1308 and F1322**
  A cooperation of H. Egger with G. Regensburger (F1322) on the use of noncommutative polynomial decomposition for the analysis of iterative regularization methods has been continued.
  Recently, a collaboration between these projects on the use of novel algebraic techniques for Hamilton-Jacobi equations has been started, based on a tutorial on level set methods given at the annual SFB Seminar in Strobl. The idea of the approach is to consider so-called pseudo-linearity of certain nonlinear partial differential equations (linearity after suitable change of the addition and multiplication operators) for the symbolic construction of solutions. In the case of Hamilton-Jacobi equations, the so-called max-plus algebra (a semiring instead of a field), is of particular importance, which led to the development of symbolic computation techniques for the min-plus linear algebra. Joint work on the application of symbolic computation techniques for min-plus linear equations.

- **Cooperation between F1309 and F1308**
  In a close cooperation between R. Stainko (F1309) and Dr. M. Burger (F1308) we developed a new approach to topology optimization problems with local stress constraints. The approach leads to large-scale optimization problems that are solved with a primal-dual interior-point method. Most of the computational time of such methods is spent by solving large-scale optimality systems. A resulting spin-off project deals with the construction of an optimal solver to these large-scale optimality systems using multigrid methods.

- **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 started to establish

a new cooperation with 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. The subject matter of Symbolic Functional Analysis is situated at the interface between computer algebra and functional analysis. 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 system of F1302. The leading theme of inverse problems in F1308 provides an ample field of studying operator problems relevant in practical applications (e.g. parameter-to-solution maps and their inverses); the discussion and research along these lines is ongoing.

- **Cooperation between F1322 and F1301**
As anticipated in the project proposal, the role of noncommutative polynomials is seen to be more and more relevant in formulating and solving various operator problems (e.g. boundary value problems) based on integro-differential rings. Hence project F1322 can profit crucially from the noncommutative polynomial tools prepared in project F1301. The expertise in solving parametric polynomial systems has also already shown to be useful for the construction of parametrized wavelets and this line of research will be continued in 2005.

- **Cooperation between F1322 and F1303**
Motivated by a talk of Josef Schicho (F1303), a new line of research was established in a cooperation on quadratic forms over fields where the main issue is to find and prove identities by the aid of Gröbner bases. For constructing the Witt ring, one defines a new addition and multiplication on equivalence classes of quadratic forms. Every element of the Witt ring can then be represented by a polynomial over the integers modulo suitable relations. Using this structure, a statement of the form "some identity holds provided certain assumed identities hold" can be decided by computing a Gröbner basis for the polynomials corresponding to the assumptions and checking if polynomial corresponding to the claimed identity reduces to zero modulo the Gröbner basis. Often one also wants to find a concrete coordinate representation of the isomorphism connecting the equivalent quadratic forms; this can be achieved by tracing the Gröbner basis computation.

- **Cooperation between F1322 and F1304**
As explained in the main text, we think of the class of integro-differential rings as a natural extension of the classical notion of differential rings, prominently used in the area of differential algebra, which is one of the main research topics in project F1304. These connections and the interplay between these two viewpoints have been discussed extensively in the series of seminars on differential equations (see below).

- **Cooperation between F1322 and F1305**
The theory of D-modules, one of the focal points in project F1305, provides an alternative approach to differential equations, in some sense dual to the one we employ in symbolic functional analysis: Instead of describing the solution of a given differential equation as a function built from certain primitives, the differential equations themselves (actually only some canonical ones) are used as a specification of functions.

- **Seminar on Differential Equations**
The seminar series "Symbolic Computation for Differential Equations: Quantitative and Qualitative Methods", initiated by Buchberger in 2004, has extended over the year 2005 in altogether 10 seminar sessions (first seminar on 20 January, last seminar on 7 October). Approximately 20 people were attending these seminars on a regular basis, and this has brought together people from virtually all subprojects of the SFB (of course preferentially those with a symbolic background). Furthermore, the seminar has also involved researchers from RICAM.

References

[1] A. Becirovic, P. Paule, V. Pillwein, A. Riese, C. Schneider, and J. Schöberl. Hypergeometric Summation Methods for High Order Finite Elements. Technical Report 2006-8, SFB F013, J. Kepler University Linz, 2006.

[2] A. Bećirović, P. Paule, V. Pillwein, A. Riese, C. Schneider, and J. Schöberl. Hypergeometric summation algorithms for high order finite elements. SFB-Report 2006-8, J. Kepler Universität, Linz, 2006. Submitted.

[3] M. Burger and R. Stainko. Phase-field relaxation of topology optimization with local stress constraints. SFB Report 04-35, University Linz, 2004.

[4] R. Stainko and M. Burger. A one-shot approach to topology optimization with stress constraints. Preprint, Johannes Kepler University Linz, 2005. Submitted.

SFB F013: Numerical and Symbolic Scientific Computing

National and International Cooperations

1 Cooperations

- **Number of multinomial coefficients**
In an external cooperation with G. E. Andrews and A. Knopfmacher, B. Zimmermann studied the asymptotics of the number $M(n)$ of distinct values taken by multinomial coefficients with upper entry n [1]. They show that both $p_P(n)/M(n)$ and $M(n)/p(n)$ tend to zero as n goes to infinity, where $p_P(n)$ is the number of partitions of n into primes and $p(n)$ is the total number of partitions of n. To use methods from commutative algebra – in particular Gröbner bases – they encode partitions and multinomial coefficients as monomials.

- **RWTH Aachen (Germany)**
The cooperation of Dr. V. Levandovskyy with Prof. E. Zerz on constructive methods of algebraic analysis has been continued. In recent articles [3], [4] we have studied algorithms for commutative and non–commutative structures, arising in connection with Control Theory.

- **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 of finite difference schemes for linear PDEs with constant coefficients. Among other, we work on the symbolic von Neumann stability analysis as well as the dispersion analysis.

- **University of Sevilla (Spain)**
The Singular library for computations with algebraic D–modules dmod.lib [2] has been released as the result of a joint work of Dr. V. Levandovskyy and J. Morales. The tools, implemented in the library are of interest for F1304 and F1305. Together with Prof. F. Castro we continue investigating algorithms for local algebraic and analytic settings in D–module theory.

- **The project CreaComp**
This project, started in summer 2004, has a volume of 72 man-months and aims at the construction of and contents developement for a novel e-learning platform for mathematics, covering theory exploration, construction of mathematical models, and automatic reasoning (proving). The project is funded by the JKU Linz and is 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 will buil-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 will implement some of the newest concepts in e-learning, like constructive and exploratory learning. For implementing such concepts it is crucial to use the natural style and natural language proving capabilities of Theorema, because the lessons have to be 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, on the period Oct.2002 - Dec.2005. The results of this research are to be applied in concrete industrial environments inside software companies in Romania and Austria. During 2005 we have participated in applied projects with Alcatel Timisoara, and we are currently starting another project with Siemens VDO Timisoara.

- **University of Innsbruck**
Within the FWF project Explicit Resolution and Related Methods in Algebraic Geometry and Number Theory we continued in a successful series of joint seminars, this year held in Tirol. We applied Groebner basis techniques for recursive expansion of algebraic power series, a result which is latex used for analyzing singularities of algebraic varieties.

- **University of Sydney,**
University of Trento
We developed and implemented algorithms for parametrizing various types of surfaces by exploring the use of the Lie algebra of the variety. Some of the related algorithms are planned

to be included into packages distributed with MAGMA.

- **RICAM**
J. Schicho together with J. Kraus, RICAM, developed a coarse grid correction and interpolation method based on the splitting of element matrices into so-called *edge matrices*. The problem was finding such a splitting in the most efficient way.

- **Cooperation with Prof. Scott McCallum**
Prof. Scott McCallum of Macquarie University in Sydney, Australia, has visited RISC for a month in May 2005. E.Kartaschova has started a cooperation with Prof. McCallum on using cylindrical algebraic decomposition for deciding approximate factorizability of differential operators.

- **Workshop on Integrability of PDEs**
In June 2005 the workshop ALISA was held at the university of Linz. ALISA was organized by E. Kartaschova, with the goal of forming a project group on research in the theory of integrability. Colleagues from several European countries participated in the workshop. Unfortunately, this activity did not yet lead to an application for a EU project, but it might in the future.

- **Joint work with Dr. H. Herrmann, TU Berlin**
Dr. H. Herrmann, a theoretic physicist from TU Berlin will visit our research group. He is currently doing some research on the heat conduction problems. H. Gu will cooperate with him by using symbolic-numerical computing method and investing the convergence properties of some specific heat conduction equations.

  They also plan to write a joint paper which should be submitted to [5].

- **INRIA Paris**
The long term cooperation with Prof. Paule's group was continued in a joint paper [9] on holonomic sequences by P. Flajolet, B. Salvy (both INRIA Paris) and S. Gerhold. Prof. Flajolet has been member of the PhD thesis committee of S. Gerhold (Nov. 2005). Further joint papers are in preparation.

- **International universities**
Several joint articles have been published/accepted in cooperation with Helmut Prodinger (University of Stellenbosch, South Africa) [10, 8, 7], with George E. Andrews (The Pennsylvania State University) [6], and with R. Pemantle (University of Pennsylvania) [11].

- **Humboldt-University of Berlin:**
Dr. J. Valdman together with Prof. C. Carstensen and Dr. A. Orlando (both Berlin) established an adaptive finite elements algorithm for the solution of elasto-plastic problems. This cooperation led to a technical report and was also accepted as a journal publications in Math. Methods Appl. Sci.

- **Petersburg Department of Steklov Institute of Mathematics:** Prof. S. Repin and Dr. Jan Valdman and started to work on reliable error estimates for the scalar nonlinear problem, where the nonlinearity is defined on a part of the boundary. A joint paper is in preparation.

- **Inverse Problem of Endocardiology**
In this context a model problem is studied, which is related to a new method for diagnosing heart diseases. The resulting equations describe an inverse, time-dependent Cauchy-problem, which is well-known to be severely ill-posed. The construction and implementation of a real-time algorithm for this problem has been considered in a collaboration between A. Hofinger and R. Celorrio (University of Zaragoza, Spain), resulting in a joint paper [16].

- **Parameter Identification in Mathematical Finance**
In a cooperation with T.Hein and B. Hofmann (TU Chemnitz), a decomposition of the volatility surface into term-structure and smile has been investigated (cf. [17]). For a suitable multiplicative decomposition of the volatility surface, the identification problem in the Black-Scholes equation splits up into two subproblems, which can be tackled separately and more efficiently.

- **Total Variation Regularization**
In collaboration of M.Burger with S. Osher, G. Gilboa and J. Xu (University of California, Los Angeles), the construction, analysis, and implementation of nonlinear inverse scale space methods based on total variation regularization has been considered (cf. [13]). Nonlinear inverse scale space methods arise as a limit (for decreasing step size) of an iterative regularization method constructed previously by the authors and generalize the important concept of inverse scale space methods to the degenerate case of total variation techniques.

  In another collaboration of S.Kindermann with S.Osher and J.Xu, the so-called G-norm was used for the denoising (cf. [19]). The G-norm can be roughly seen as dual of the bounded variation norm and was introduced by Y.Meyer as a suitable norm for highly oscillatory signals. It turned out, that it is natural to use it for bounded variation regularization problems. It has been shown in [] that it can be computed by the level-set method and that it is leads to new noise filters for highly degraded images.

A further collaboration with S.Osher was concerned with the decomposition of images into cartoon, texture, and noise. For this sake a saddle-point formulation was introduced and analyzed (cf. [18]).

- **Level Set Methods**
  A collaboration with H. Ben Ameur (ENIT Tunis) concerned with the mathematical analysis of inclusion detection problems in thermoelasticity has been continued, and a joint paper has been finished in 2005 (cf. [12]).

  In cooperation with M. Hintermüller (University Graz) a relaxation technique linking total variation and level set methods has been considered, and their numerical solution by projected gradient flows has been investigated (cf. [15]).

  A collaboration with F. Hausser, C.Stöcker, and A.Voigt (all CAESAR Crystal Growth Group, Bonn) has been concerned with the use of curvature regularization for anisotropic surface evolution laws exhibiting backward diffusion phenomena. Level set methods for the resulting high-order regularized problem have been developed and implemented, and applications to the thermal faceting of material surfaces have been investigated (cf. [14]).

  In collaboration of S.Kindermann with M.Alves and A.Leitao (University of Florianopolis), the application of level set methods for elliptic Cauchy-Problems has been investigated.

- **Stochastic Inverse Problems**
  In collaboration with J.Huttunen (University of Kuopio), the development of a numerical method for electrical impedance process tomography including stochastic modeling has been investigated.

- **Technical University of Copenhagen (DTU):**
  R. Stainko continued his cooperation with the *TOPOPT*–group around Prof. Dr. M. Bendsoe and Prof. Dr. O. Sigmund, especially with Dr. M. Stolpe, about various aspects of modelling, formulating and solving various topology optimization problems.

- **SINTEF Applied Mathematics (Norway)**
  Dr. T. Dokken (SINTEF, coordinator) and Prof. B. Jüttler and four other European partners **(University of Cantabria, Spain; University of Nice and INRIA, France; think3, Italy, University of Oslo, Norway)** are involved in a IST–FET research project within the Fifth Framework Programme of the European Commission. The project has been successfully completed in September 2005.

- **University of Science and Technology of China, Hefei**
  An ongoing cooperation with Prof. Falai Chen on approximate μ–bases led to a joint publication, which has been accepted for publication in Geometric Modeling and Processing 2006.

- **RICAM**
  Like other parts of the SFB, project F1322 is conducted over the Radon Institute for Applied and Computational Mathematics (RICAM). In particular, the two postdocs M. Rosenkranz (part of the SFB throughout 2004) and G. Regensburger (joined the SFB in November 2004) are employed b RICAM. The interdisciplinary environment of this instutition provides an additional incentive to cross-group (in particular symbolic-numerical) cooperations.

- **Seminar on Differential Equations**
  The series of seminars "Symbolic Computation for Differential Equations: Quantitative and Qualitative Methods" was also addressed to the research groups of RICAM, and there was some crucial input from their side as well, in particular one talk by Stefan Müller on modelling biochemical systems.

2 Guests

- **Prof. Lajos Ronyai:** MTA SZTAKI,Budapest, Hungary, February 20–23, 2005, Cooperation with Dr. W. de Graaf, DI J. Pilnikova und Prof. J. Schicho
- **DI Vera Nübel:** TU München, Germany, March 1–2, 2005, Talk: "Eine rp-Adaptive finite-elemente-Diskretizierung fr physikalisch nichtlineare Probleme"
- **Prof. Manuel Bronstein:** INRIA Sophia Antipolis, April 10–14, 2005, Talk: "Discussion of ongoing research in symbolic integration"
- **a.Univ-Prof. Dr. Alfio Borzi:** Karls-Franzens-University Graz, Austria, April 21–22, 2005, Talk: "Space-time multigrid methods for solving unsteady optimal control prolbems"
- **DI Niels Lubbes:** Netherlands,April 24–25, 2005, Talk
- **DI Brian Moore:** TU München, Germany, April 25, 2005,
- **DI Zsolt Minier:** Cluz-Napoca, Rumania, May 1–2, 2005,
- **Dr. Tor Dokken:** SINTEF ICT, Appl. Mathem., Norway, May 9–12, 2005, Talk, research cooperation
- **Prof. Dr. Myung-Soo Kim:** Seoul National University, May 9–12, 2005, Talk, research cooperation
- **Prof. Dr. A. Karger:** Karlsuniversität Prag, MFF, Czech Republic, May 17–19, 2005, Talk, research cooperation
- **Dr. Ray Sarrasa:** General Motors Research, USA, June 26–28, 2005, Talk
- **Prof. Dr. Rolf Rannacher:** Ruprecht-Karls-University Heidelberg, Germany, June 9–12, 2005, Invited Speaker at COSCOMP 2005, Vienna
- **Prof. Dr. Peter Hilton:** State University of New York, USA, June 29, 2005, Talk at the J. Kepler Syposium: "Paradoxes in Traditional Thinking"
- **Dr. Shojiro Sakata:** University of Electro-Communications, Tokyo, Japan, June 2005, Talk: "Some remarks on 1D/mD linear recurrences and their applications"
- **a.Univ-Prof. Dr. Alfio Borzi:** Karls-Franzens-University Graz, Austria,July 13 -, 2005, Research Cooperation with R. Stainko u. R. Simon.
- **DI Erik Lindgren:** KTH Stockholm, Sweden,July 24–25, 2005, Talk, research cooperation on Level Set Methods
- **Prof. Dr. Dominique Foata:** University of Strassburg, France,Oct. 2–3, 2005,
- **Dr. Hend Benameur:** Ecole National d'Ingenieurs de Tunis, February 8–20, 2005, Cooperation with Dr. Martin Burger and DI Benjamin Hackl on geometric Inverse Problems and Level Set Methods
- **Prof. Dr. Alexey B. Shabat:** L.D. Landau, Inst. f. Theoretical Physics, Russia, April 22–May 3, 2005, Talk: "Classification of systems of ODEs describing integrable interactions of particles on the line."
- **Prof. Robert Corless:** University of Western Ontario, Canada, June 8–12, 2005, Invited Speaker at COSCOMP 2005, Vienna
- **Prof. Dr. Alexander Mikhailov:** University of Leeds, United Kingdom, June 12–18, 2005, Participated at ALISA, Talk at the RISC
- **Prof. Sergvey Tsarev:** Krasnoyask State Reda gog. University, Russia, June 8–17, 2005, Participated at ALISA
- **Prof. Keith O. Geddes:** University of Waterloo, Canada, June 8–16, 2005, Invited Speaker at COSCOMP 2005, Vienna
- **Prof. Dr. John Christopher Eilbeck:** Heriot-Watt University MACS, United Kingdom,July 13–17, 2005,
- **Prof. Dr. Alexey B. Shabat:** L.D. Landau, Inst. f. Theoretical Physics, Russia, July 3–31, 2005, Collaboration on the subject "Computable Integrability", preparing of a paper on general invariants of LPDES of arbitrary order
- **Prof. Dr. Alexey B. Shabat:** L.D. Landau, Inst. f. Theoretical Physics, Russia, August 1–29, 2005, Collaboration on the subject "Integrable Systems", plainlevel-like equations and special funktions; preparation of Austrian-Russian project (beginning in 2006)
- **Dr. Dalibor Lukas:** VSB-Technical University Ostrava, Czech Republic, Aug. 29–Sep. 25, 2005, Cooperation concerning the construction of optimal solution techniques for optimality systems using multigrd methods
- **DI Hossein Teimoori Faal:** Institute f. Advanced Studies in Basic Sciences, Iran, Sep. 11–18, 2005, Cooperation: "Symbolic Summation"
- **Prof. Masahiko Sato:** Kyoto University, Japan, Sep. 10–22, 2005,

3 Lectures at other Universities

- **V. Levandovskyy:** "Non-commutative Groebner basics: from the theory to the implementation in the Computer Algebra System SINGULAR:PLURAL", Invited colloquium talk at University of Granada, Spain, November 2005.
- **V. Levandovskyy:** "Computer Algebra System SINGULAR:PLURAL and non-commutative Groebner bases in theory and applications", Invited colloquium talk at University of Sevilla, Spain, November 2005.
- **B. Buchberger:** Theorema: A System for Formal Mathematics. Invited colloquium talk at North Carolina State University, Dept of Computer Science, March 2005.
- **B. Buchberger:** A Historic Introduction to Gröbner Bases. Invited talk at Summer School on Gröbner Bases and Applications, Zanjan, Iran. July 2005.
- **W. Windsteiger:** Wie erfinde ich mathematische Algorithmen? Wie beweise ich mathematische Algorithmen? Presentation given at Schwerpunktfach Mathematik, Europagymnasium Auhof, December 15, 2005.
- **W. Windsteiger:** An Automated Theorem Prover for Set Theory within the Theorema System. Invited colloquium talk at Institute for Algebra, Charles University Prague. April 2005.
- **T. Kutsia and M. Marin:** Matching with Regular Constraints. Invited talk at Austria-Japan Summer Workshop on Term Rewriting, Obergurgl, Austria. August, 2005.
- **B. Buchberger:** Algorithmische Beweisverfahren: Das Ende der Mathematik? Invited colloquium talk at Kepler Symposium, Universität Linz. April 2005
- **B. Buchberger:** Mathematik: Die Kunst des effektiven Handelns. Invited colloquium talk at MathSpace, Wien. May 2005.
- **B. Buchberger:** Algorithm Synthesis in Theorema: Case Study Gröbner Bases. Invited colloquium talk at University of Edinburgh, School of Informatics. June 2005.
- **Tudor Jebelean:** Combining Logic and Computer Algebra in Theorema. Invited colloquium talk at the University of Tsukuba, Japan. December 2005.
- **B. Buchberger:** Algorithm Synthesis by Lazy Thinking: Case Study Gröbner Bases. Invited colloquium talk at DFKI, Saarbrücken.
- **Tudor Jebelean:** University of Timisoara, Romania. November 2005. Blocked lecture (8 hours) on automated reasoning techniques and their implementation in Theorema.
- **Tudor Jebelean:** University of Cluj, Romania. July 2005. Blocked lecture (8 hours) on automated reasoning techniques and their implementation in Theorema.
- **J. Pílniková** gave a talk on parametrizing Severi-Brauer surfaces at the Comenius University in Bratislava.
- **J. Pílniková** gave a talk on splitting central simple algebras over the rational numbers at the University of Trento.
- **J. Schicho** gave an invited talk on computation of adjoints and the parametrization problem at the Magma workshop "Algebraic Geometry and Group Theory" in Warwick.
- **J. Schicho** gave an invited talk on sparse parametrization of algebraic curves and surfaces at COMPASS 2005, Oslo.
- **J. Schicho and G. Bodnár** gave talks at Algorithmic Algebra and logic 2005, Passau. J. Schicho talked on a topological criterion for polynomiality, and G. Bodnár talked on computing centers of blowups for birational projective morphisms of varieties.
- **J. Schicho and J. Pílniková** gave talks at MEGA 2005, Sardinia. J. Schicho talked on the parametric degree of rational surfaces, and J. Pílniková talked on a Lie Method for rational parametrization of Severi-Brauer surfaces.
- **J. Pílniková** gave a talk on rational parametrization via Lie algebras II at the Magma workshop "Algebraic Geometry and Group Theory" in Warwick.
- **J. Pílniková** gave a talk on using Lie algebras to parametrize certain types of algebraic varieties II at the Workshop on Lie Algebras, their Classification and Applications in Trento.
- **J. Pílniková** gave a talk on Splitting Central Simple Algebras of degree 4 at Darstellungstheorietage and Nikolaus Conference in Aachen.
- **I. Szilágyi** gave a talk on a condition number for the implicitization problem at COMPASS 2005, Oslo.
- **E.Kartaschova** has visited the Max-Planck-Institut für Mathematik in Leipzig and given a lecture on factorization of LPDOs.
- **E.Shemyakova** has participated in a workshop on computer algebra and its applications to physics in Dubna, Russia, a given a talk on her implementation of a factorization algorithm for low order differential operators.

- **F.Winkler** has visited the Universidad de Alcalá in Madrid, and given a lecture on computer algebra and factorization of differential operators.
- **C. Schneider:** "Analysis of Algorithms and Symbolic Summation" in the frame of the European Erasum/Socrates programme. Invited colloquium talk at West University of Timisoara, Faculty of Mathematics and Computer Science, Romania, May 2005.
- **P. Paule:** "Partition Analysis: MacMahon's Dream Came True", Invited talk at Festkolloquium for Prof. J. Cigler, University of Vienna, Austria, 30. September 2005.
- **P. Paule:** "Partitionsanalysis: MacMahon's Traum wurde Wirklichkeit", Invited talk at TU Graz, Austria, 2. December 2005.
- **B. Jüttler** visited the IT University of Denmark, the Institute of Geometry of the TU Graz, the Dept. of Mathematics of the University of Science and Technology of China (Hefei), the Dept. of Mathematics of Zhejiang University (Hangzhou, China), General Motors Research (USA), and the Dept. of Mathematics of the University of Siena (Italy) and gave presentations related to on–going research in the SFB.

References

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

[2] Levandovskyy V. and Morales, J. A Singular 3.0 library for computations with algebraic D-modules dmod.lib, 2006.

[3] Levandovskyy, V. and Zerz, E. Computer algebraic methods for the structural analysis of linear control systems. *PAMM*, 5:717–718, 2005.

[4] 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.

[5] H. Herrmann, H. Gu, G. Rueckner, J. Siebert, and W. Muschik. Close-to-fourier heat conduction equation for solids: Motivation and symbolic-numerical analysis. In *ATTI della ACCADEMIA PELORITANA DEI PERICOLANTI Classe di Scienze Fisiche, Matematiche e Naturali*, 2006. to be submitted.

[6] G. Andrews, P. Paule, and C. Schneider. Plane Partitions VI: Stembridgeś TSPP Theorem. *Adv. in Appl. Math.*, 34(4):709–739, 2005.

[7] K. Driver, H. Prodinger, C. Schneider, and A. Weideman. Padé approximations to the logarithm III: Alternative methods and additional results. *To appear in Ramanujan J.*, 2006.

[8] K. Driver, H. Prodinger, C. Schneider, and J. A. C. Weideman. Padé approximations to the logarithm II: Identities, recurrences, and symbolic computation. *Ramanujan J.*, 11(2), 2006.

[9] P. Flajolet, S. Gerhold, and B. Salvy. On the non-holonomic character of logarithms, powers and the nth prime function. *Electronic Journal of Combinatorics*, 11(2):1–16, 2005.

[10] M. Kuba, H. Prodinger, and C. Schneider. Generalized reciprocity laws for sums of harmonic numbers. SFB-Report 2005-17, J. Kepler Universität, Linz, 2005. Submitted.

[11] R. Pemantle and C. Schneider. When is 0.999... equal to 1? *To appear in Amer. Math. Monthly*, 2006.

[12] H. B. Ameur, M. Burger, and B. Hackl. Cavity identification in linear elasticity and thermoelasticity. *Mathematical Methods in the Applied Sciences*, 2005. submitted.

[13] M. Burger, G. Gilboa, S. Osher, and J. Xu. Nonlinear inverse scale space methods. *Communications in Mathematical Sciences*, 4(1):179–212, 2006.

[14] M. Burger, F. Hausser, C. Stöcker, and A. Voigt. A level set approach to anisotropic flows with curvature regularization. CAM-Report 06-02, UCLA, 2006. Submitted.

[15] M. Burger and M. Hintermüller. Projected gradient flows for bv / level set relaxation. *PAMM*, 5:11–14, 2005.

[16] R. Celorrio and A. Hofinger. A real-time solution for an inverse Cauchy problem in cardiology. Technical report, SFB F013, 2005.

[17] H. Egger, B. Hofmann, and T. Hein. On decoupling of volatility smile and term structure in inverse option pricing. *Inverse Problems*, 2006. accepted.

[18] S. Kindermann and S. Osher. Saddle point formulation for a cartoon-texture decomposition. CAM-Report 05-42, UCLA, 2005. Submitted.

[19] S. Kindermann, S. Osher, and J. Xu. Denoising by bv-duality. CAM-Report 05-21, UCLA, 2005. Submitted.

SFB F013: Numerical and Symbolic Scientific Computing

Statistical Appendix

1 Monographs, PhD Theses, Diploma Theses

[1] Gerhold, S. *Combinatorial Sequences: Non-Holonomicity and Inequalities*. PhD thesis, RISC, J. Kepler University Linz, 2005.

[2] Kauers, M. *Algorithms for Nonlinear Higher Order Difference Equations*. PhD thesis, RISC-Linz, Johannes Kepler Universität Linz, 2005.

[3] Semrad, M. Special functions, computer proofs and the dlmf. Master's thesis, RISC, J. Kepler University Linz, 2005.

[4] Wolfram, M.-T. Semiconductor inverse dopant profiling from transient measurements. Master's thesis, Johannes Kepler University Linz, 2005.

2 Publications

[1] Aigner, M., and Jüttler, B. Robust computation of foot points on implicitly defined curves. In *Mathematical methods for curves and surfaces: Tromsø 2004* (2005), Mod. Methods Math., Nashboro Press, Brentwood, TN, pp. 1–10.

[2] Beals, R., and Kartashova, E. Constructively factoring linear partial differential operators in two variables. *TMPh (Journal of Theoretical and Mathematical Physics) , Springer 145*, 2 (2005), 1510–1523.

[3] Beals, R., and Kartashova, E. Constructively factoring linear partial differential operators in two variables. *TMPh (Journal of Theoretical and Mathematical Physics) , Springer 145*, 2 (2005), 1510–1523.

[4] Beuchler, S., and Schöberl, J. New shape functions for triangular p-fem using integrated jacobi polynomials. *Num. Math.* (2005). (submitted).

[5] Brokate, M., Carstensen, C., and Valdman, J. A quasi-static boundary value problem in multi-surface elastoplasticity: Part 2 – Numerical solution. *Mathematical Models and Methods in Applied Sciences 28*, 8 (2005), 881 – 901.

[6] Buchberger, B., Craciun, A., Jebelean, T., Kovacs, L., Kutsia, T., Nakagawa, K., Piroi, F., Popov, N., Robu, J., Rosenkranz, M., and Windsteiger, W. Theorema: Towards computer-aided mathematical theory exploration. *Journal of Applied Logic* (2005), –. To appear.

[7] Burger, M., and Hofinger, A. Regularized greedy algorithms for network training with data noise. *Computing 74*, 1 (2005), 1–22.

[8] Burger, M., and Osher, S. A survey on level set methods for inverse problems and optimal design. *European J. Appl. Math.* (2005). To appear.

[9] Dokken, T., and Jüttler, B., Eds. *Computational methods for algebraic spline surfaces*. Springer-Verlag, 2005. Papers from the ESF Exploratory International Workshop (COMPASS) held in Kefermarkt, September 29–October 3, 2003.

[10] Egger, H., and Engl, H. Tikhonov regularization applied to the inverse problem of option pricing: Convergence analysis and rates. *Inverse Problems 21* (2005), 1027–1045.

[11] Egger, H., Engl, H., and Klibanov, M. Global uniqueness and Hölder stability for recovering a nonlinear source term in a parabolic equation. *Inverse Problems 21* (2005), 271–290.

[12] Egger, H., and Neubauer, A. Preconditioning Landweber iteration in hilbert scales. *Numerische Mathematik 101* (2005), 643–662.

[13] Engl, H., and Kügler, P. Nonlinear inverse problems: theoretical aspects and some industrial applications. In *Multidisciplinary methods for analysis, optimization and control of complex systems* (2005), J. P. V. Capasso, Ed., Mathematics in Industry, Springer, pp. 3 – 48.

[14] Engl, H. W., Hofinger, A., and Kindermann, S. Convergence rates in the Prokhorov metric for assessing uncertainty in ill-posed problems. *Inverse Problems 21* (2005), 399–412.

[15] Flajolet, P., Gerhold, S., and Salvy, B. On the non-holonomic character of logarithms,

powers and the nth prime function. *Electronic Journal of Combinatorics 11*, 2 (2005), 1–16.

[16] Gerhold, S. Point Lattices and Oscillating Recurrence Sequences. *Journal of Difference Equations and Applications 11*, 6 (2005), 515–533.

[17] Gu, H., and Burger, M. Preprocessing for finite element discretizations of geometric problems. In *Proceedings of The International Workshop of Symbolic and Numerical Computation, Xi'an, China.* (2005).

[18] Jüettler, B., Chalmoviansly, P., Shalaby, M., and Wurm, E. Approximate Algebraic Methods for Curves and Surfaces and their Applications. In *21st Spring Converence on Computer Graphics* (2005), Comenius University Press / ACM Siggraph 2005.

[19] Kartashova, E. BK-factorization and Darboux-Laplace transformations. In *Proceedings of The 2005 International Conference on Scientific Computing, June 20-23 Las Vegas* (2005), H. R. Arabnia and G. Gravvanis, Eds., CSREA PRESs, USA, ISSN: ISSN: 1-932415-62-9, pp. 144–150.

[20] Kartashova, E. Hierarchy of general invariants for bivariate lpdos. *TMPh (J. Theoretical and Mathematical Physics), Springer to appear* (2005).

[21] Kartashova, E. A model of laminated turbulence. *Letters JETP (Journal of Experimental and Theoretical Physics, Letters; Springer to appear* (2005).

[22] Kartashova, E., Shemyakova, E., and Winkler, F. Implementation of a factorization algorithm for lpdos. In *Proc. of Workshop on Symbolic-Numeric Computation, Xi'an, China* (2005).

[23] Kauers, M., Ed. *Proceedings of the 2005 International Symposium on Symbolic and Algebraic Computation (ISSAC'05)* (2005), ACM Press.

[24] Kovacs, L., Popov, N., and Jebelean, T. Verification environment in theorema. *Annals of Mathematics, Computing and Teleinformatics (AMCT) 1*, 2 (2005), 27–34.

[25] Landsmann, G., Mayr, P., and Schicho, J. A topological criterion for polynomiality. In *Algorithmic Algebra and Logic - Proc. A3L, Books on Demand GmbH, Norderstedt* (2005).

[26] Levandovskyy, V. and Zerz, E. Computer algebraic methods for the structural analysis of linear control systems. *PAMM 5* (2005), 717–718.

[27] L.He, S.Osher, and M.Burger. Iterative total variation regularization with non-quadratic fidelity. *J. Math. Imag. Vision* (2005). To appear.

[28] M.Burger, and M.Hintermueller. Projected gradient flows for bv / level set relaxation. *PAMM 5* (2005), 11–14.

[29] Osher, S., Burger, M., Goldfarb, D., Xu, J., and Yin, W. An iterative regularization method for total variation based image restoration. *Multiscale Modelling and Simulation 4* (2005), 460–489.

[30] Rosenkranz, M. New symbolic method for solving linear two-point boundary value problems on the level of operators. *Journal of Symbolic Computation 39* (2005), 171–199.

[31] S. Hein, W. K., and Schöberl, J., Eds. *Acoustic Resonances in a 2D Slat Cove and 3D Open Cavity* (2005), no. 2005-2867, AIAA / CEAS Aeroacoustics Conference.

[32] Sir, Z., and Juettler, B. Spatial Pythagorean Hodograph Quintics and the Approximation of Pipe Surfaces. In *The Mathematics of Surfaces XI* (2005), vol. 3604 of *Springer Lecture Notes on Computer Science*.

[33] Šír, Z., and Jüttler, B. Constructing acceleration continuous tool paths using pythagorean hodograph curves. *Mechanism and Machine Theory 40*, 11 (2005), 1258–1272.

[34] Šír, Z., and Jüttler, B. Euclidean and Minkowski Pythagorean hodograph curves over planar cubics. *Computer Aided Geometric Design 22*, 8 (2005), 753–770.

[35] Šír, Z., and Jüttler, B. Lifting cubics into (Minkowski) space. In *Mathematical methods for curves and surfaces: Tromsø 2004* (2005), Mod. Methods Math., Nashboro Press, Brentwood, TN, pp. 315–326.

[36] Wurm, E., Jüettler, B., and Kim, M.-S. Approximate Rational Parameterization of Implicitly Defined Surfaces. In *he Mathematics of Surfaces XI* (2005), vol. 3604 of *Springer Lecture Notes on Computer Science*.

3 Conference Talks

[1] Buchberger, B. Algorithm synthesis by lazy thinking: Case study gröbner bases. Invited colloquium talk at DFKI, Saarbrücken, November 14-15 2005.

[2] Buchberger, B. Algorithm synthesis in theorema: Case study gröbner bases. Invited colloquium talk at University of Edinburgh, School of Informatics, June 23 2005.

[3] Buchberger, B. Algorithmic algorithm invention in the theorema project. Invited talk at Conference on Algorithms and Information Theory, May 16-18 2005.

[4] Buchberger, B. Algorithmic algorithm synthesis: Case study gröbner bases. Invited talk at East Coast Computer Algebra Day, March 12 2005.

[5] Buchberger, B. Algorithmische beweisverfahren: Das ende der mathematik? Invited colloquium talk at Kepler Symposium, Universitt Linz, April 20 2005.

[6] Buchberger, B. Formal mathematical theory exploration in theorema (4 lectures). Invited talk at Summer School on Theoretical Computer Science, Marktoberdorf, August 3-13 2005.

[7] Buchberger, B. From gröbner bases to automated theorem proving and back. 3 lectures. Invited talk at Summer School on Gröbner Bases and Applications, July 9-22 2005.

[8] Buchberger, B. A historic introduction to gröbner bases. Invited talk at Summer School on Gröbner Bases and Applications, July 9-22 2005.

[9] Buchberger, B. Introduction to gröbner bases. Invited talk at Introduction to Gröbner Bases, May 16-18 2005.

[10] Buchberger, B. Lazy thinking: A new method for algorithm synthesis. Invited colloquium talk at Workshop 201cAlgebraic and Numeric Algorithms and Computer-Assisted Proofs201d. Research Center Schloss Dagstuhl, Germany, September 26-30 2005.

[11] Buchberger, B. Mathematik: Die kunst des effektiven handelns. Invited colloquium talk at MathSpace, Wien, May 12 2005.

[12] Buchberger, B. Symbolic computation: Current trends. Invited talk at International Workshop on Advanced Computing and Analysis Techniques in Physics Research, May 22-27 2005.

[13] Buchberger, B. Theorema: A system for formal mathematics. Invited colloquium talk at North Carolina State University, Dept of Computer Science, March 15 2005.

[14] Buchberger, B. A view on the future of symbolic computation. Invited talk at ISSAC 2005 (International Symposium on Symbolic and Algebraic Computation), Bejing, July 25-27 2005.

[15] Burger, M. BV / Levelset relaxation of topology optimization problems. Invited minisymposium talk at GAMM 2005, Luxemburg, 2005.

[16] Burger, M. The choice of regularization functionals in inverse problems and imaging. Workshop on Symmetries, Inverse Problems, and Imaging, Linz, 2005.

[17] Burger, M. Level set methods for shape optimization and reconstruction. Plenary talk at ALGORITMY 2005, Podbanske, SK., 2005.

[18] Burger, M. Parameter identification in partial differential equations. 6 lectures at the Winter school on inverse problems, Geilo, Norway, 2005.

[19] Burger, M. Some aspects of surface diffusion. University Oslo, 2005.

[20] Burger, M., and Hackl, B. Level set methods for geometric inverse problems. Inverse Problems Workshop, Obergurgl, Austria, April 2005.

[21] Burger, M., and Stainko, R. Phase-field relaxation of topology optimization with local stress constraints. First Austrian Numerical Analysis Day, April 2005.

[22] Carstensen, C., Orlando, A., and Valdman, J. "adaptive finite element analysis in computational elastoplasticity with guaranteed convergence". Miniworkshop "Error-Estimates", Special Radon Semester 2005, Linz, November 2005.

[23] Chalmovianský, P. Approximation algorithms using algebraic curves and surfaces. TU Ostrava, April 2005.

[24] Egger, H. Preconditioning iterative regularization in Hilbert scales. GAMM-Conference, Luxembourg, March 2005.

[25] Egger, H. Preconditioning iterative regularization methods. Workshop on Inverse Problems, Obergurgl, April 2005.

[26] Egger, H. Some aspects of iterative regularization. Workshop on symmetries, inverse problems and image processing, RICAM, January 2005.

[27] Egger, H., and Regensburger, G. Decomposition of noncommutative polynomials in the convergence analysis of iterative regularization methods. SFB Statusseminar, Strobl, April 2005.

[28] Gerhold, S. Recurrence Relations and Inequalities. Invited colloquium talk at INRIA Rocquencourt, November 2005.

[29] Gu, H. Preprocessing for finite element discretizations of geometric problems. International Workshop of Symbolic and Numerical Computation, Xi'an, China, 2005.

[30] Hackl, B. Level sets, phase field and topological gradients in inverse problems. Workshop on "Level Set Methods for Direct and Inverse Problems", Linz 2005, September 2005.

[31] Hackl, B. Topological derivative and the level set method for geometric inverse problems. SIAM Annual Meeting, New Orleans, USA, July 2005.

[32] Hofinger, A. A real-time solution for an inverse cauchy problem in cardiology. Lake Arrowhead, June 2005.

[33] Hofinger, A. A real-time solution for an inverse Cauchy problem in cardiology. SFB Status seminar, Strobl, Austria, March 2005.

[34] Hofinger, A. A real-time solution for an inverse cauchy problem in cardiology. Obergurgl, April 2005.

[35] Hofinger, A. A real-time solution for an inverse cauchy problem in cardiology. SFB Status seminar, Strobl, Austria, 2005.

[36] Kartashova, E. BK-factorization and Darboux-Laplace transformations. Contributed talk at CSC-05 (International Conference on Scientific Computing), June 20-23, Las Vegas, USA, 06 2005.

[37] Kartashova, E. Discrete wave systems: model of laminated turbulence. Warwick Turbulence Symposium, University of Warwick, Warwick, UK, 12 2005.

[38] Kartashova, E. Elements of integrability in nonlinear dispersive pdes. Mathematical Physics Seminar, Loughborough University, England., 03 2005.

[39] Kartashova, E. Encyclopedia alisa - main ideas and general structure. Steklov Institute for Mathematics, Russian Academy of Sciences, Moscow, Russia, 10 2005.

[40] Kartashova, E. General invariants of linear partial differential operators. SFB Cooperation Meeting, 12 2005.

[41] Kartashova, E. On factorization of linear partial differential operators. Invited talk at "Workshop on symmetries, inverse problems and image processing", January 2005.

[42] Kartashova, E. On factorization of linear partial differential operators. generic case. "Workshop on symmetries, inverse problems and image processing", RICAM, 01 2005.

[43] Kartashova, E. Order-reduction procedure for factorization of lpdo of arbitrary order. Conference "Solitons, boomerons and isochronious solutions to nonlinear systems", 02 2005.

[44] Kartashova, E. Wave turbulence theory for discrete systems. Landau Institute of Theoretical Physics, Russian Academy of Sciences, Chernogolovka, Russia., 09 2005.

[45] Kovacs, L. Imperative program verification in theorema. Contributed talk at Theorema-Ultra-Omega'05 Workshop, Department of Computer Science, University of Saarbruecken, Germany, November 14-15 2005.

[46] Kovacs, L., and Jebelean, T. An algorithm for automated generation of invariants for loops with conditionals. Contributed talk at Computer-Aided Verification on Information Systems Workshop (CAVIS05), 7th International Symposium on Symbolic and Numeric Algorithms for Scientific Computing (SYNASC05), September 25-29 2005.

[47] Kovacs, L., and Jebelean, T. Generating invariance properties by recurrence solving and groebner basis computation in the theorema system. Contributed talk at Dagstuhl Seminar 05311: Verifying Optimizing Compilers, 31 July- 5 August 2005.

[48] Kovacs, L., and Jebelean, T. Polynomial invariant generation by algebraic and combinatorial methods. Contributed talk at SFB Cooperation Meeting, Johannes Kepler University Linz, December 19 2005.

[49] Kovacs, L., and Jebelean, T. Using combinatorial and algebraic techniques for automatic generation of loop invariants. Contributed talk at SFB Statusseminar, Strobl, Austria, April 1 2005.

[50] Kovacs, L., Popov, N., and Jebelean, T. A verification environment for imperative and functional programs in the theorema system. Satellite of 2nd Balkan Conference in Informatics, 17-19 November, Ohrid. Contributed talk at 2nd South-East European Workshop on Formal Methods (SEEFM05), "Practical dimensions: Challenges in the business world", Ohrid, FYR of Macedonia, 18-19 November 2005.

[51] Kutsia, T. Context sequence matching for xml. Contributed talk at the 1th International Workshop on Automated Specification and Verification of Web Sites (WWV'05), Valencia, Spain, March 15 2005.

[52] Kutsia, T., and Marin, M. Can context sequence matching be used for xml querying? Contributed talk at the 19th International Workshop on Unification (UNIF'05), Nara, Japan, April 22 2005.

[53] Kutsia, T., and Marin, M. Matching with regular constraints. Invited talk at Austria-Japan Summer Workshop on Term Rewriting, Obergurgl, Austria, August 10 2005.

[54] Kutsia, T., and Marin, M. Matching with regular constraints. Contributed talk at 12th International Conference on Logic for Programming, Artificial Intelligence, and Reasoning, LPAR'05, December 2 2005.

[55] Kutsia, T., and Marin, M. Matching with regular constraints. Contributed talk at Theorema-Omega'05 Workshop, November 14 2005.

[56] Levandovskyy, V. Computer Algebra System SINGULAR:PLURAL and non-commutative Groebner bases in theory and applications. Invited colloquium talk at University of Sevilla, 25.11 2005.

[57] Levandovskyy, V. Non-commutative Groebner basics: from the theory to the implementation in the Computer Algebra System SINGULAR:PLURAL. Invited colloquium talk at University of Granada, 18.11. 2005.

[58] Paule, P. Computer Algebra Proofs of Frank Olver's Problems. Invited talk at the Editorial Meeting of the Digital Library of Mathematical Functions (DLMF), National Institute of Standards and Technology (NIST), Gaithersburg, USA, 6. May 2005.

[59] Paule, P. Computer Algebra Tools for Special Functions in Physics. Invited talk at the Theoretical Physics Lab, NIST, Gaithersburg, USA, 9. May 2005.

[60] Paule, P. Contiguous Relations and Creative Telescoping. Invited talk at the International Conference on Difference Equations, Special Functions and Applications, Munich, Germany, 29. June 2005.

[61] Paule, P. Partition Analysis: MacMahon's Dream Came True. Invited talk at Festkolloquium for Prof. J. Cigler, University of Vienna, Austria, 30. September 2005.

[62] Paule, P. Partitionsanalysis: MacMahon's Traum wurde Wirklichkeit. Invited talk at TU Graz, 2. December 2005.

[63] Paule, P. Plane Partitions Revisited. Invited talk at Special Session Algebraic Combinatorics, Joint Meeting of AMS, DMV, and ÖMG, Mainz, Germany, 15. June 2005.

[64] Paule, P. Special Functions and Computer Algebra. Invited talk at Dagstuhl Seminar: Mathematics, Algorithms, Proofs, 10. January 2005.

[65] Pikkarainen, H. State estimation approach to nonstationary inverse problems: discretization error and filtering problem. The Eleventh Inverse Days, Helsinki, Finland, December 2005.

[66] Piroi, F., and Kutsia, T. The theorema environment for interactive proof development. Contributed talk at 12th International Conference on Logic for Programming, Artificial Intelligence, and Reasoning, LPAR'05, December 3 2005.

[67] Popov, N. Functional program verification in theorema. Contributed talk at Theorema-Ultra-Omega'05 Workshop, November 14 2005.

[68] Popov, N., and Jebelean, T. The role of algebraic simplification in the verification of functional programs. Contributed talk at SFB Statusseminar, Strobl, Austria, April 01 2005.

[69] Regensburger, G. Construction and applications of parametrized wavelets. Workshop on Inverse Problems, Obergurgl, April 2005.

[70] Regensburger, G. Construction of parameterized wavelets using gröbner bases. ACA 2005, Conference on Applications of Computer Algebra, Nara, Japan, August 2005.

[71] Regensburger, G. Parametrized wavelets and algebraic curves. Workshop on Resolution of Algebraic Varieties, Kaiserhaus, September 2005.

[72] Regensburger, G. Semirings, idempotent analysis and differential equations. Workshop on "Level Set Methods for Direct and Inverse Problems", Special Session on Symbolic Computation and PDEs, RICAM Linz, Workshop on "Level Set Methods for Direct and Inverse Problems", Special Session on Symbolic Computation and PDEs, RICAM Linz 2005.

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

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

[75] Rosenkranz, C., Hemmecke, R., Jebelean, T., and Buchberger, B. Mathematical knowledge management in the frame of verification and synthesis of generic algorithms for groebner bases. Contributed talk at SFB Statusseminar, Strobl, Austria, April 1 2005.

[76] Rosenkranz, C., and Piroi, F. Organizational tools in theorema. Contributed talk at Theorema-Ultra-Omega Workshop, November 14-15 2005.

[77] Rosenkranz, M. Integro-differential rings and operators. SFB Statusseminar, Strobl, April 2005.

[78] Rosenkranz, M. Linear two-point boundary value problems in symbolic computation: A new approach. Foundations of Computational Mathematics (FoCM'05), Santander, Spain, July 2005.

[79] Rosenkranz, M. New symbolic computation methods for the exact solution of two-point boundary value problems. Algorithmic Information Theory (AIT'05), Vaasa, Finland, May 2005.

[80] Rosenkranz, M. Symbolic solution of nonlinear bvps? - first steps and considerations. Workshop on Inverse Problems, Obergurgl, April 2005.

[81] Schneider, C. Finding telescopers with minimal depth for indefinite nested sum and product expressions. Contributed talk at ISSAC'05, Beijing, China, 27. July 2005.

[82] Schneider, C. When is 0.999... equal to 1? Invited talk at Special Session Algebraic Combinatorics, Joint Meeting of AMS, DMV, and ÖMG, Mainz, Germany, 16. June 2005.

[83] Shemyakova, E. Applications of bk method of linear partial differential operators factorization. talk at Conference "Computer algebra", Dubna, Russia, May 2005.

[84] Shemyakova, E. Families of factorizations of linear partial differential operators. talk at Conference "ACA'05", Nara, Japan, August 2005.

[85] Shemyakova, E. Families of factorizations of linear partial differential operators. talk at Conference "ASCM'05", Seoul, South Korea, December 2005.

[86] Shemyakova, E. A maple program for factorization of linear partial differential operators in two variables. talk at Conference "SNMP'05", Kyiv, Ukraine, June 2005.

[87] Stainko, R. Phase–field relaxation of topology optimization with local stress constraints. Workshop on Level Set Methods for Direct and Inverse Problems, Linz, September 2005.

[88] Stainko, R. Phase–field relaxation of topology optimization with local stress constraints. IUTAM Symposium on Topology Design Optimization of Structures, Machines and Materials, Rungsted, Denmark, November 2005.

[89] Stainko, R. Phase-field relaxation of topology optimization with local stress constraints. Technical University of Denmark, February 2005.

[90] Stainko, R., and Burger, M. Phase–field relaxation of topology optimization with local stress constraints. IPAM Inverse Problems Reunion Conference, Lake Arrowhead, June 2005.

[91] Stainko, R., and Burger, M. Phase–field relaxation of topology optimization with local stress constraints and an optimal KKT-solver. Workshop on Dircet and Inverse Field Computations in Mechanics, Linz, November 2005.

[92] Stütz, R. Estimation of discontinuous solutions of ill-posed problems using adaptive grid techniques. SFB Status Seminar Strobl, Austria, March 2005.

[93] Stütz, R. Estimation of discontinuous solutions of ill-posed problems via the moving grid approach. Workshop Inverse Problems, Obergurgl, Austria, April 2005.

[94] Valdman, J. Fast solve for elastoplasticity. Talk at the conference Enumath 2005, Santiago de Compostela, Spain, 2005., July 2005 2005.

[95] W., W. Symbolic solution techniques for the elastoplasticity problem. Contributed talk at SFB Statusseminar 2005, 31.3.2005 2005.

[96] Windsteiger, W. An automated theorem prover for set theory within the theorema system. Invited colloquium talk at Institute for Algebra, Charles University Prague, April 25 2005.

[97] Windsteiger, W. Creacomp: Neue mglichkeiten im e-learning fr mathematik. Invited colloquium talk at Research Net Upper Austria: Brennpunkt Forschung, 22. April 2005.

[98] Windsteiger, W. The creacomp project: Theorema for computer-supported teaching and learning of mathematics. Contributed talk at Theorema-Ultra-Omega'05 Workshop, November 14 2005.

[99] Windsteiger, W. Theorema: A system for mathematical theory exploration. Invited colloquium talk at Institute for Algebra, Charles University Prague, April 26 2005.

[100] Winkler, F. On the factorization of linear differential operators. Talk at the workshop "Computer Algebra and Informatics" in Lomonosov Moscow State Univ., Faculty of Mechanics and Mathematics, November 2005.

[101] Wolfram, M.-T. Semiconductor inverse dopant profiling from transient measurements. Inverse Problems Reunion Conference, Lake Arrowhead, June 2005.

4 SFB Technical Reports

2005

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