Special Research Program (SFB) F 013

Numerical and Symbolic Scientific Computing

Annual Report 2004

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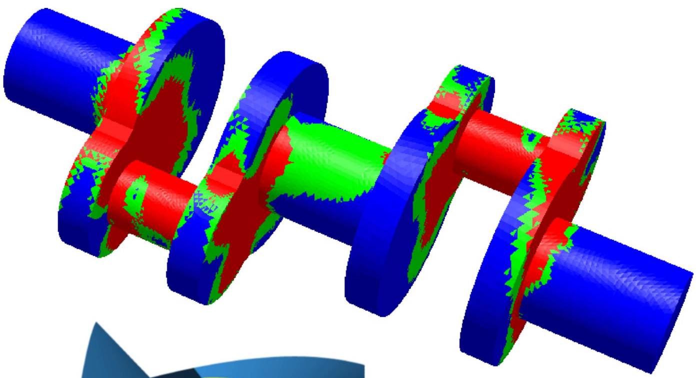

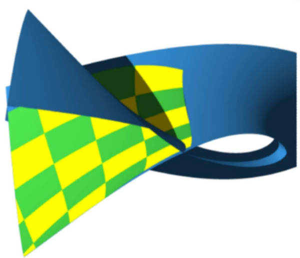

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Special Research Program SFB F013

“Numerical & Symbolic Scientific Computing”

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In March 2004 the SFB had successfully finished its second funding period: as a result of the peer-review organized by the FWF at the end of 2003, a third period (April 2004 to March 2008) had been granted. This Annual Report gives a summary of SFB results achieved in 2004.

Also for the third and last funding period, 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.

This overall goal in its essence is the same as defined in the original proposal written more than seven years ago. However, we note that during the evolution of the SFB the following minor changes have been made in its definition. In the proposal for the first funding period, instead of “geometrical” the term “graphical” was chosen. Since geometrical issues have started to play a stronger rôle, in the proposal for the second funding period, instead of “graphical” the term “geometrical and graphical” was chosen. Meanwhile scientific visualization tools are available (partly developed in F1301), and since different aspects of geometrical scientific computing are needed in almost all subprojects, for the last funding period the replacement of “geometrical and graphical” by “geometrical” was a natural decision.

As pointed out in the SFB Progress Report 2001–2003, 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*, also supplementary measures, like joint internal seminars between numerical and symbolic groups or a new target-oriented structure of the SFB status seminars, were introduced. As a result, the coherence between the numerical and symbolic groups has increased significantly. Instead of point-wise cooperations, a whole network of concrete links between numerics, symbolics, and geometry has emerged.

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 section “Transfer of Knowledge and Technologies”. 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.

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.

Acknowledgements: We express our thanks to the Austrian Research Fund (FWF), the University of Linz, the Government of Upper Austria, and the City of Linz for moral and financial support. Sincere thanks to all SFB members who helped with preparing this booklet.

Linz, May 2005 Peter Paule

F 1301: Scientific Part of the Service Project

Prof. Dr. P. Paule, Dr. J. Schöberl
DI V. Pillwein, Mag. B. Zimmermann

In the third funding period of the SFB the theme of the scientific part of subproject F1301 has been changed. The new major objectives 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.

1 High Order Finite Elements

The particular choice of high order finite element basis functions influences the necessary iteration number of iterative equation solvers. We construct basis functions in order to minimize the iteration number. The numerical analysis of such basis functions is given in [3]. We obtained the following two results [1] that allow an efficient implementation of these methods.

Edge-based basis functions Let $L_i(x), (i \geq 2)$, be the integrated Legendre polynomials, which are orthogonal w.r.t. the H^1 scalar product, satisfy a three-term recurrence and vanish at $\{-1, +1\}$. We define an edge-based basis $\varphi_i(x, y)$ using the extension procedure $\varphi_i^{(1)}(x, y) := \frac{1}{2y} \int_{x-y}^{x+y} L_i(s) ds$,

$$\varphi_i^{(2)}(x, y) = \varphi_i^{(1)}(x, y) - \frac{2y}{1 - x + y} \varphi_i^{(1)} \left(\frac{1 + x - y}{2}, \frac{1 - x + y}{2} \right),$$

$$\varphi_i(x, y) = \varphi_i^{(2)}(x, y) - \frac{2y}{1 + x + y} \varphi_i^{(2)} \left(-\frac{1 - x - y}{2}, \frac{1 + x + y}{2} \right).$$

The resulting extension operator preserves the polynomial order, is bounded in the sense that $\|\varphi\|_{H^1(T)} \leq c \|\varphi\|_{H^{1/2}_{00}(E)}$, and satisfies zero boundary conditions at the upper two edges. Using hypergeometric summation techniques, viz. the Multisum Package developed by K. Wegschaider, A. Riese and B. Zimmermann in F1305, it is possible to derive a recurrence relation for the functions $\varphi_i, (i \geq 2)$. The computed recurrence relation has the form

$$\varphi_i = a_i x \varphi_{i-1} + (b_i + c_i(x^2 - y^2))\varphi_{i-2} + d_i x \varphi_{i-3} + e_i \varphi_{i-4}, \qquad i \geq 6,$$

where the coefficients are rational functions in i. In applications the coefficients a_i to e_i are computed once and for all, and are stored in tables. The evaluation of p basis functions φ_i takes just $11p + \mathrm{O}(1)$ floating point operations.

Low energy vertex functions The idea is to use vertex shape functions that are constant along the level-sets of the standard hat-basis-functions, and to minimize the H^1 norm among this class of functions. This leads to the one-dimensional constrained minimization problem

$$\min_{\substack{v \in P^p \\ v(-1)=0, v(1)=1}} \int_{-1}^{1} (s - 1)^{d-1} (v'(s))^2 \, ds,$$

where d is the space dimension ($d = 2, 3$). Expanding v in terms of the Jacobi polynomials $P_i^{(d-2,-1)}$, $(1 \leq i \leq p)$, yields the algebraic minimization problem:

$$\min_{\substack{v \in \mathbb{R}^p \\ b^0 \cdot v = 0, b^1 \cdot v = 1}} v^T A v,$$

where

$$A_{i,j} = \int (s - 1)^{d-1} (P_i^{(d-2,-1)})'(s) (P_j^{(d-2,-1)})'(s) \, ds.$$

For the matrix entries $A_{i,j}$ we first use that the derivative of a Jacobi polynomial $P_i^{(\alpha,\beta)}$ is again a Jacobi polynomial (with shifted parameters α, β and i) and second that the $P_i^{(\alpha,\beta)}$ are orthogonal w.r.t. the weight function $w_{\alpha,\beta}(x) = (1-x)^\alpha (1+x)^\beta$. Solving the algebraic minimization problem results in the functions

$$u_p^2(x) = \left(\sum_{i=1}^{p} \frac{1}{i} \right)^{-1} \sum_{i=1}^{p} \frac{1}{i} P_i^{(0,-1)}(x),$$

$$u_p^3(x) = \frac{1}{p(p+2)} \sum_{i=1}^{p} \frac{2i+1}{i+1} P_i^{(1,-1)}(x)$$

in the two, resp. three dimensional case. Using the closure properties of holonomic functions, the software developed in F1305 [2] computes inhomogenous recurrence relations for the u_p^d, which can be used for a fast assemblance of the stiffness matrix.

2 Gröbner Bases

R. Hemmecke has developed a generic Gröbner bases framework in the programming language Aldor. This framework requires only a minimal set of properties from the domain of the actual Gröbner basis elements. In particular, commutativity is not assumed. Basically, we require only a function that checks for reducibility of an element by another element and a function that does the actual reduction. Furthermore a function is needed that computes the S-polynomial. Although our goal is to implement Gröbner bases for several kinds of (noncommutative) polynomial-like domains, it should be noted that the above notions are abstract so that they do not even need the existence of a multiplication. This abstractness makes it possible to use specially tailored efficient implementations of these functions in the domain in which the Gröbner basis elements live. In addition, it makes it possible to add new domains of computation for a Gröbner basis computation relatively easily.

An Aldor library has been produced that eases the communication with Mathematica and Maple.

3 Symbolic Integration and Summation of Special Functions

A *d-field in rational representation* is a field $C(X_1, \ldots, X_m)$ of rational functions, equipped with a finite set Θ of derivations and shifts. The derivations and shifts are given by their action on the X_i, the elements of C being constants. Many problems in symbolic summation and integration find their natural setting in d-fields in rational representation. For instance, the $\Pi\Sigma$-fields of Karr's indefinite summation algorithm are d-fields in rational representation of some special type.

Let (K_1, Θ_1) be a d-field in rational representation. Fixing a subset Θ_2 of Θ_1, and a subfield of K_2 of K_1, closed under Θ_2, defines a noncommutative ring $K_2[\Theta_2]$ of operators acting on K_1. Given f in K_1, Zimmermann's generalization of the Fasenmyer-Wilf-Zeilberger algorithm is about finding an annihilator A for f in the ring $K_2[\Theta_2]$. It can be used for computing recurrences and differential equations for sums and integrals that depend on free parameters. The fact that the algorithm is based on rational function representations does not mean that it is limited to the case of rational functions. Indeed, it goes beyond hypergeometric summation, which is well-studied, and includes the holonomic case.

Example: For the integral

$$f(n, \omega) = \int_{-\infty}^{\infty} J_n(t) e^{-i\omega t} dt,$$

where J denotes Bessel's J-function, the algorithm computes annihilators in the following rings:

1. in $C(n, \omega)[S_n]$, i.e., recurrences:
$$(S_n^2 + 2i\omega S_n - 1) \cdot f(n, \omega) = 0.$$
2. in $C(n, \omega)[D_\omega]$, i.e., differential equations:
$$\big(i(\omega^2 - 1)D_\omega^2 + 3i\omega D_\omega + (1 - i)n - i - 1)\big) \cdot f(n, \omega) = 0.$$
3. in $C(n, \omega)[D_\omega, S_n]$:
$$(D_\omega S_n + i\omega D_\omega + i\,(n + 1)) \cdot f(n, \omega) = 0.$$

The new algorithm is implemented in the Mathematica program `mdf`. All three examples took less than 1 second to compute.

The *termination* of the algorithm, i.e., the existence of annihilators, was studied. Zimmermann was able to prove a new existence theorem. It generalizes an existence theorem from the previous year that dealt only with a smaller class of d-fields, the class of d-fields with nested depth two.

A method for improving the *efficiency* of this algorithm was developed. It is based on the well-known idea of using a finite field as a (computationally) cheap homomorphic image of a ring of polynomials. Based on the notion of black box polynomials, the notion of a *black box difference ring* is introduced. The main point here is that rings of polynomials can be equipped with any shift, while its elements can still be represented as black boxes. These black boxes can not only be added and multiplied, but also shifted efficiently.

For a function depending on several parameters, it is usually much cheaper to compute partial relations than it is to compute ordinary relations. Therefore it is natural to use partial relations for proving identities. However, the problem of proving initial conditions becomes harder with partial relations. First progress in this direction was made.

All this will be part of a PhD thesis of B. Zimmermann on Symbolic Definite Integration and Summation of Special Functions (in preparation).

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

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

Dr. W. Windsteiger, Dr. T. Kutsia, Dr. M. Rosenkranz, Dr. F. Piroi, Dr. M. Marin

DI A. Craciun, DI N. Popov, DI L. Kovacs, DI Camelia Rosenkranz

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 started 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) [2]. Our group is in the center of international research in this area [1].

The case studies in the area of functional analysis are developed in close cooperation with the subproject F 1322, and resulted in a novel approach to solving differential equations using symbolic techniques [23]. This research addresses also an important aspect of MKM: lifting knowledge to the inference level. This was done by the creation of a simplifier on congruence classes of noncommutative polynomials (where each congruence class represents an operator like differentiation or integration). Such a simplifier then has the practical purpose of solving two-point boundary value problems on the operator level. The activity in presented in more detail in the respective section of this report.

The case study on Groebner Bases theory is developed in the context of using the respective mathematical knowledge base for the automated synthesis of the Buchberger algorithm [3], using a powerful and novel approach introduced by Buchberger [5].

The same approach is also studied in the context of basic algorithmic domains (e. g. tuples/lists) [4]. Moreover, the usage of mathematical knowledge about integers is studied in the frame of program verification [8, 21], which led to interesting interactions to combinatorial techniques (subproject F 1305) [9, 10].

The interplay between proving, solving, and computing in the context of real numbers was also studied in conjunction with problems from algebraic geometry [7, 6, 22].

A special issue was the continued developement of the tools for the management and exploration of mathematical knowledge: interactivity, focus windows, label management, and other [20, 18, 19].

Equational Reasoning. The progress includes the generalization of earlier results of the project on reasoning with sequence variables and flexible arity symbols. The paper [11] and its full version [12] describe a sound and complete unification procedure that enumerates a minimal complete set of solutions of term equations with sequence variables and sequence functions. The procedure has been implemented in ρLog. Implementation details can be found in [14], and more experiments with evaluation strategies in ρLog are described in [15, 16, 17]. Furthermore, [13] presents a study of the meta-mathematical implications of extending predicate logic with sequence variables and sequence functions.

The methods developed by us for reasoning with sequence variables and flexible arity symbols have found applications in the fields like automated deduction, constraint logic programming, XML processing, and formal methods in software engineering. In automated deduction, the unification procedure was implemented in the equational prover of the Theorema system. In constraint logic programming, on the basis of the unification procedure the constraint solving module of the CLP(Flex) language was built. In XML processing, the procedure was incorporated into the XCentric language through CLP(Flex). Both languages CLP(Flex) and XCentric have been developed at the University of Porto, Portugal. In formal methods, techniques for processing expressions with flexible arity symbols were used to formalize nested statecharts in the Uniform Modeling Language (UML) state machines (University of Malaga, Spain).

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F 1303: Proving and Solving over the Reals

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

1 Singularity Analysis

In previous phases of the project, we used resolution as the main method for analysis of the singularities of an algebraic variety (see [6, 7]). There is a resolution algorithm for varieties in arbitrary dimension, but it is very complex. Therefore we looked for alternative methods. In particular, we wanted to implement the algorithm [2] for computing solutions of a quasi-ordinary polyomial in the ring of multivariate Puiseaux series. To do this, we needed to finitely represent algebraic power series. Such a representation was suggested in [3]. But then we observed that exact representation of the intermediate results is not really necessary, because for expansion up to a given order it suffices to work with approximate roots throughout. We could devise and implement an algorithm for computing approximate roots in a multivariate polynomial ring [5]. In particular, we can use this method to approximate algebraic power series up to any desired order. This observation makes it possible to devise a data type for representation and manipulation of algebraic power series in finite terms. Such a representation was implemented in Aldor and presented in [4].

2 Topology of Level Curves

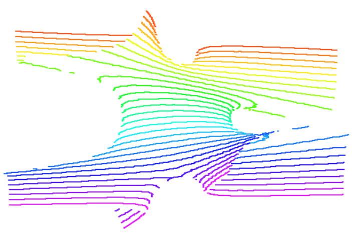

Figure 1: Level curves of a cubic surface.

There exist already algorithms for computing the *topological type* of a plane real algebraic curve (see e.g. [11]). Here, two plane curves are said to have the same topological type if there exists an embedded homeomorphism of one to the other. In some situations, one wants to compute the topological type of a curve depending on a parameter. In a collaboration with J. G. Alcazar and J. R. Sendra from the University of Alcala, Spain, we developed an algorithm for doing this [1]. The idea is to study the set of parameters where the topological type may change. We showed that these parameters are roots of the repeated discriminant, using methods from cylindrical algebraic decomposition.

3 Stability of Implicitization

There are various methods for converting a parametric surface with rational parametrization into implicit form (for instance one can use Gröbner bases, see [12]). In many applications the input is given in terms of floating point numbers, and it is not necessary to compute an exact implicitization, an approximate is also sufficient, such as computed in [8, 9, 10]. Of course, there arises an important question: how precise can we say something about the output?

In [14], we introduced a condition number for the implicitization problem. It depends not only on the input parameters, but also on the estimation of the degree of the output implicitization; if the degree is changing, then the number of coefficients in the output is different, and we have a completely different numerical problem. The output error can then be estimated in terms of the input error and the condition number.

It is planed to extend this result in order to estimate also the geometric error, in terms of the Hausdorff distance, in a cooperation with B. Jüttler and M. Aigner from subproject 1315.

4 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. For particular classes of varieties, for instance for Del Pezzo surfaces of degree at least 5, the Hasse principle holds: a solution exists if and only if we have local solvability, meaning that we have a solution modulo powers of prime numbers. Moreover, if we have one rational solution of a Del Pezzo surfaces of degree at least 5, then we can compute a rational parametrization, which in turn gives *all* rational solutions of the equation system.

In order to find rational solutions in this special situation, we developed the *Lie algebra method* for diophantine equations, in colaboration with M. Harrison, University of Sydney, and Willem de Graaf, University of Sydney / RICAM, Academy of Sciences. The idea, first presented at [13], is to compute the Lie algebra of the group of complex automorphism of the algebraic variety, and to use classification results for Lie algebras in order to construct an isomorphism to a "standard Lie algebra", which is the Lie algebra of a simpler variety Y. Then we lift the isomorphism of Lie algebras to an isomorphism of varieties, and this reduces the original problem to the problem of finding rational points on Y; which is a much simpler problem.

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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 September 2003 until December 2004. During this period we have investigated theoretical and practical methods for the numerical computation of Gröbner bases, the use of symmetry analysis in symbolic differential elimination, symbolic methods in the solution analysis of PDEs related to the Mumford-Shah functional, numerical-symbolic methods for parameter dependent geometric differential equations, and the problem of factorization of linear partial differential operators.

1.1 Numerical computation of Gröbner bases

In his PhD thesis A. Kondratyev has dealt with the problem of numerical computation of Gröbner bases of zero-dimensional polynomial systems. It is well known that the computation of a Gröbner basis cannot be generally executed in floating-point arithmetic by a standard approach. This, however, would be highly desirable for practical applications. In his dissertation [8], advised by H.J. Stetter and F. Winkler, A. Kondratyev has presented an approach for computing Gröbner bases numerically. It is an elaboration of the idea of a stabilized Gröbner basis computation initially proposed by Stetter. Kondratyev has implemented his algorithm, the program is available online. Some of the main ideas of this approach to numerical computation of Gröbner bases have been presented at the CASC conference in St.Petersburg [1].

1.2 Characteristic Sets

In his diploma thesis C. Aistleitner has been implementing characteristic sets for differential polynomials [2]. He has created a highly generic implementation which can be linked to many different computer algebra systems.

His work has been supported by a research fellowship (Kleine Forschungsbeihilfe).

1.3 Symmetry analysis in differential elimination

Transformations which leave a given differential equation invariant are commonly known as Lie symmetries. They form a group, a so-called Lie group. The basic idea here is to find a group of symmetries of a differential equation and then use this group to reduce the order or the number of variables appearing in the equation. The knowledge of a one-parameter group of symmetries of an ordinary differential equation of order n allows to reduce the problem of solving this equation to that of solving a new differential equation of order $n-1$ and integrating.

In symbolic treatment of DEs the ultimate goal is a symbolic solution. However, this is rarely achieved. But it is also of great importance to decide whether a system of DEs is solvable. If there are solutions, then we can derive differential systems in triangular form such that the solutioins of the original system are the (non-singular) solutions of the output system. Deriving symmetries helps in verifying numerical schemes for solution approximation. In case the given system consists of differential algebraic equations, we may get a complete overview of the algebraic relations which the solutions must satisfy.

These theoretic ideas and computer algebra methods have been presented at a conference in Vienna in 2003 [11] and a polished form has been published in [3].

1.4 Symbolic methods in the solution analysis of PDEs

H. Gu has worked together with S. Kindermann (F1317) on the denoising and signal recovery problems within the framework of signal processing. For signal and image processing, one important task is the segmentation problem, i.e. to split a given signal or image into several disjoint regions where the signal or image is homogeneous. Gu and Kindermann use the Energy methods on the denoising equation by minimizing a Mumford-Shah functional leading to a variational problem. They could discretize the obtained weak formulation in a finite element space, in order to analyze the reconstructed solutions. They use a new variational transformation which can turn the finite element scheme into an algebraic system, so that the discrete form can be simplified by eliminating most of the variables with the aid of symbolic computation. The obtained solutions are implicit functions which only depend on parameters, so that one can investigate their changing value on each partition grid nodes by plotting their function curve on Maple software. That also provides the possibility for determining appropriate parameters in the denoising equations so that the finite element formulatioin can be uniquely solved by Newton type methods. For the large-scale denoising problems the obtained finite element solution on the coarse grid partition can be a good initial guess for further Newton recorrective iterations.

Gu and Kindermann have described their results in [5, 6]. Gu has presented the results in [4].

1.5 Numerical-symbolic methods for parameter dependent geometric differential equations

H. Gu and M. Burger (F1308) have worked together on numerical-symbolic approximation methods for some parameter-dependent elliptic geometric equations. In order to perform a detailed analysis of the discretizaion methods they have investigated a model problem related to mean curvature type equations. This work has been described in [9]. Publications are planned for the year 2005.

1.6 Factorization of linear partial differential operators

Together with R. Beals (of Yale University) E. Kartashova has studied conditions under which a partial differential operator of arbitrary order n in two variables or ordinary linear differential operator admits a factorization with a first-order factor on the left. The factorization process consists of solving, recursively, systems of linear equations, subject to certain differential compatibility conditions. In the generic case of partial differential operators one does not have to solve a differential equation. In special degenerate cases, such as ordinary differential operators, the problem is finally reduced to the solution of some Riccati equation(s). Kartashova gave an invited talk at a workshop on “Integrable Systems” in Guernavaca, Mexico in November 2004 [7]. A first paper is accepted for publication [10].

E. Shemyakova is currently working on a Maple implementation.

1.7 Geometric computation

In previous phases of the project F1304 we have worked on algorithms in geometric computation, in particular on parametrization algorithms for algebraic curves. A talk on this topic was given by F. Winkler during a visit of Charles University Prague [12].

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F 1305: Proving and Solving in Special Function Domains

Prof. Dr. P. Paule
DI Dr. A. Riese, DI Dr. C. Schneider
DI S. Gerhold, DI M. Kauers

1 Proving and Solving in Special Function Domains

The scientific output achieved in 2004 by the SFB project group F1305 is documented in the form of 15 publications: 3 articles came out in journals and 3 in conference proceedings; 9 technical reports have been produced, 6 of which are already accepted for journal publication. Additionally, one diploma thesis [23] has been completed; it is closely related to the project work.

1.1 Identity Proving

The summation theory of difference fields has been developed further by C. Schneider in a series of articles [22, 18, 15, 21, 17, 19], and the algorithmic results have been implemented in his summation package Sigma [16]. Given these new features we managed to show that a double sum involving harmonic numbers that arose in the analysis of an optimization algorithm evaluates to a sum of products of values of the zeta function [14].

$$\sum_{j,k=1}^{\infty} \frac{\mathrm{H}_j(\mathrm{H}_{k+1}-1)}{jk(k+1)(j+k)} = -4\zeta(2) - 2\zeta(3) + 4\zeta(2)\zeta(3) + 2\zeta(5)$$

Particular emphasis has been put on special function applications. More precisely, we developed a general framework that enables one to deal with summation problems involving quite general objects that can be described by a linear recurrence, like orthogonal polynomials [20]. This ansatz opens up a completely new class of applications. For instance, in joint work with G. E. Andrews (Pennsylvania State University) the celebrated "Totally Symmetric Plane Partition Theorem" (Stembridge, 1995) now can be proven almost automatically with the package Sigma [4, 1].

M. Kauers has developed a decision procedure for the zero equivalence problem in difference rings [9, 10]. In this way one can prove identities, e.g., involving continued fractions, that were out of the scope of all previous algorithms. The algorithm was implemented as a Mathematica package [11]. The method may be applied to free difference fields [10, 8]. This allows the treatment of expressions involving unspecified sequences x_n as subexpressions, which arise, e.g., in the theory of symmetric functions. We investigated whether other algorithms can be generalized in an analogous way. Necessary conditions on a difference field K were worked out that make it possible to apply Karr's algorithm to K [12]. It was shown that the free difference field satisfies these conditions.

In joint work with P. J. Larcombe (Derby, UK), A. Riese and B. Zimmermann have introduced a method for computing indefinite products of matrices of rational functions [13]. They have applied the method in the proof of an identity involving definite sums and a definite integral. The proof uses the Mathematica package OreSys, developed by S. Gerhold in F1305 work, for uncoupling a system of linear difference equations.

1.2 Inequality Proving

A modification of M. Kauers's algorithm has led to a procedure for proving positivity, and hence inequalities, of sequences defined by difference fields [8]. By this method, it was possible to prove certain nontrivial inequalities for the first time by symbolic computation methods. Prominent examples of inequalities that can now be proven automatically include the inequalities of Cauchy-Schwarz, Levin and Weierstrass.

S. Gerhold has investigated the positivity of C-finite sequences, i.e., sequences that satisfy linear recurrences with constant coefficients. A partial result that clarifies the behaviour in some non-trivial cases has been achieved [7] and is currently being extended in joint work with Jason P. Bell (Ann Arbor, Michigan).

1.3 Non-Holonomic Sequences

Holonomic sequences, i.e., those that satisfy linear recurrences with polynomial coefficients, play an important role in symbolic summation. Only a handful of methods for proving non-holonomicity, which can be viewed as a lower bound for the complexity of a sequence, is available. S. Gerhold has extended this toolbox and showed that some sequences, e.g., $(n^n)_{n\geq 0}$ and $(\sqrt{n})_{n\geq 0}$, are not holonomic [6]. This article has triggered many reactions and the results have been significantly extended by asymptotic methods in joint work with P. Flajolet and B. Salvy (INRIA Paris) [5]. The cooperation is being continued and promises also new insight into the asymptotics of certain sequences.

1.4 Partitions

In cooperation with G. E. Andrews (PennState, USA), A. Riese and P. Paule have continued to apply Riese's package Omega, which implements MacMahon's Partition Analysis. They have derived closed forms for the generating functions of plane partitions with certain constraints [2, 3].

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

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DI J. Kienesberger, Dr. J. Valdman
Dr. S. Beuchler, Prof. Dr. W. Zulehner

This project is concerned with the development of adaptive multilevel solvers for 2D/3D Solid Elasto-plastic Problems. This period we focused on the improvement of the existing solver and its analysis.

Considering only purely elastic material laws in mathematical models does not suffice many real life applications. A modification to make the model more realistic is an additional term in the stress-strain relation describing plastic behavior. The governing equations describing this phenomenon are then the equilibrium of forces, the non-linear relationship between strain and stress, the linear dependence of the strain on the displacements and the Prandtl-Reuß normality law describing the time evaluation of plastic materials.

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

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

under incompressibility constraints. The functional f depends on the displacement u smoothly and on the plastic part of the strain p non-smoothly. Therefore the term with the plastic part of the strain is regularized, thus a modified minimization problem $\tilde{f}(u,p) = \min$ is differentiable and standard (Newton type) methods apply.

The algorithm is a successive sub-space optimization method: In the first step, the Schur-Complement system for the displacement variable u is solved by a multigrid preconditioned conjugate gradient (MPCG) method. It has been shown applying symbolic calculation techniques in Maple that the resulting elasto-plastic linear system of equations is spectrally equivalent to the linear system of equation from pure elasticity, with constants depending on material parameters and the regularization parameter only [4]. Thus the use of the elastic preconditioner for this elasto-plastic system is sufficient and the convergence of MPCG guaranteed.

The second step, namely the minimization in the plastic part of the strain p, splits into a large number of local optimization problems. The linear incompressibility constraint is resolved by projecting the problem onto a hyperplane, where the constraint is satisfied exactly.

In addition to the regularization technique described above, there is another approach developed with the new diploma student Peter Gruber. The objective is split in the following way:

$$f(u,p) = \frac{1}{2}||\varepsilon(u) - p||_C^2 + \varphi(p) + \text{linear terms}$$

with $||x||_C^2 := (Cx){:}x$ and $:$ being the scalar product of matrices. Due to the special structure of the problem and the internal dependence of p on the total strain $\varepsilon(u)$, the well known Moreau-Yosida theorem from convex analysis states that the functional $\hat{f}(u) = f(u, p(\varepsilon(u)))$, no matter whether the relation $p = p(u)$ is non-smooth, is already differentiable and special semi-smooth Newton methods can be taken into account for the numerical treatment.

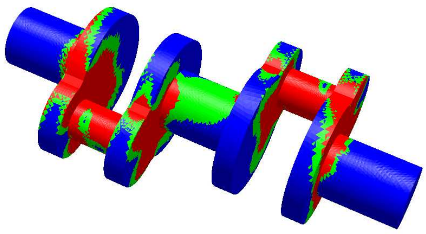

Figure 2: Example of two-yield plasticity distribution.

J. Valdman together with M. Brokate and C. Carstensen published his results on analysis [1] and numerical treatment [2] of multi-yield plasticity models. The main feature of the multi-yield models is higher number of plastic strains $p_1, \ldots, p_N$ used for more realistic modeling of the elasto-plastic transition. It was possible to prove the existence and uniqueness of the corresponding variational inequalities and design a FEM based solution algorithm. Since the structure of the minimization functional in the multi-yield plasticity model remains the same as for the single-yield model discussed above, a direct modification of an existing elastoplasticity package [3] as a part of the Netgen/NGSolve software was feasible [5]. In addition to older Matlab examples, a new 3D calculation performed in Netgen/NGSolve was added [2]. Figure 2 displays (blue) elastic, (red) first and (green) second plastic deformational zones of the shaft model. As the preparation for the next paper concerning h-adaptivity, numerous experiments in Matlab were performed.

It is well known that the local minimization problem in the multi-yield case, i.e., the dependence between $p_1, \ldots, p_n$ and $\epsilon(u)$ can not be expressed directly anymore and its analytic treatment requires simultaneous solving of system of polynomials. Even in the two-yield case with two plastic strains p_1 and p_2, the original system for $\xi_1 = ||p_1||$ and $\xi_2 = ||p_1||$ reduces for instance to a polynomial of the 8th degree in ξ_2. Together with B. Buchberger and W. Windsteiger from Project F1302 we managed to calculate the Gröbner base which gives insight to the structure of solutions of the simultaneous system. It has also been confirmed that no explicit formula can be found and the local minimization problem needs to be solved approximatively for general material parameters and deformation states. Alternatively, in cooperation with Project F1303 a combined numerical-symbolic method based on the Synaps package was tested.

J. Kienesberger and J. Valdman extended the already existing 3D quasi-static solver [3] towards uniform p adaptivity. The previous version worked for linear displacements and constant (plastic) strains respectively. Now the elasto-plastic solver can handle higher polynomial 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 Joachim Schöberl. Figure 3 shows the von-Mises stress approximated by a 4th degree polynomial an each element.

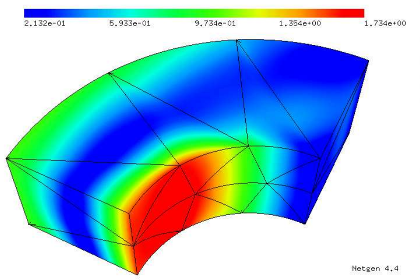

Figure 3: Von Mises stress using polynomials of 4th degree.

According to the theory and other numerical experiments, the p-method yields good approximation results for smooth functions. If the solution is singular (e.g. in corners, changing boundary conditions, or along the elasto-plastic interface), the approximation property fails and can only be restored using h- or combined hp-methods. Therefore, a special effort was made on detecting the interface between the elastic and plastic zones. First attempts in order "catch" an elasto-plastic interface were using the h-adaptive version only. Figure 4 is the result of an adaptive refinement process identifying the interface. An element is marked for refinement if one of its neighboring elements sharing a common edge/face in 2D/3D is in a different (elastic or plastic) phase.

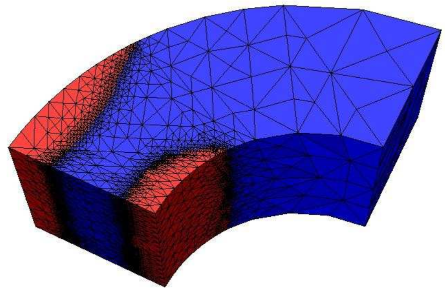

Figure 4: Illustration of h-interface adaptivity.

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F 1308: Computational Inverse Problems and Applications

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Dr. N. Bila, DI H. Egger, DI B. Hackl, DI A. Hofinger

DI P. Kügler (Basic Staff)

R. Stütz (Diploma Student)

1 Iterative Regularization

Preconditioning: Besides the convergence behavior, i.e., the capability generating good approximations for a solution of an inverse problem in the presence of data noise, the overall computational effort of an implementation may serve as a measure for the "quality" of a regularization method. Since a discretiztaion of an ill-posed problem typically leads to ill-conditioned systems, many iterations have to be performed to get a reasonable approximation. In a joint paper [10] with A. Neubauer (University Linz), H. Egger showed that Landweber iteration for linear and nonlinear inverse problems can be efficiently preconditioned in Hilbert scales and the number of iterations can essentially be reduced to the square root, e.g., 10000 $\to$ 100. In [6] the corresponding results for linear problems were generalized to semiiterative regularization methods, yielding another reduction of the number of iterations by a square root factor, e.g., 100 $\to$ 10. In both cases, optimal converence rates of the preconditioned iterative regularization methods could be proven, and the theoretical results were verified in several numerical examples (see Figure 5 for an illustration of the speed-up). Reports concerning preconditioning of the conjugate-gradients method for linear problems and of Newton-type iterations for nonlinear problems are in preparation.

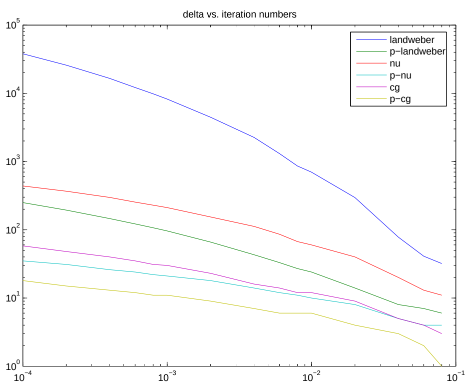

Figure 5: Comparison of iteration numbers needed for standard and preconditioned methods until stopping criterion is satisfied .

Convergence Analysis of Newton-type Iterations: Due to the ill-posedness, the Newton iteration cannot be applied directly to the solution of inverse problems in general. Instead, the (ill-posed) linearized equations have to be solved by some regularization method, e.g., by iterative regularization methods. In [15], a Newton-Landweber method was formulated, in which the linearized equations are solved by Landweber iteration. In [7], H. Egger showed that alternatively faster semiiterative regularization methods can be used, and thereby the overall number of (inner) iterations can be reduced to the square root. Moreover, he showed that in case of *a-posteriori* stopping the convergence rates for smooth solutions can be improved, if a bound on the lower number of iterations is included in the stopping criterion.

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).

2 Parameter Identification in Parabolic PDEs

Identification of nonlinearities: In several applications, e.g., in heat transfer at high temperatures, physical parameters depend on the solution of certain (partial differential) equations governing the evolution of the system, e.g., the thermal conductivity itself depends on the temperature. In order to be able to predict the evolution of a physical system, a precise knowledge of these parameters, i.e., their dependence on the state (temperature) is necessary, and thus the identification of these nonlinearities from easily accessible measurements of the state is of high interest. In a joint work of H. W. Engl and H. Egger with M. V. Klibanov (UNCC Charlotte) [8], identifyability (uniqueness) and stable reconstruction of a temperature dependent source term in nonlinear parabolic equation from a simple set of boundary measurements of the Neuman data was investigated by means of Carleman estimates.

Volatility Identification from Option Prices: Another parameter identification problem governed by a parabolic equation arises in mathematical finance. There, the identification of the volatility surface from quoted market prices of liquidly traded options is of high interest. Once the volatility has been identified, and thus the stochastic model of the underlying asset has been specified, many financial derivatives depending on the same underlying can be priced correctly, e.g., by Monte-Carlo simulations. In [9] H. W. Engl and H. Egger analyzed the stable solution of the *inverse problem of option pricing*, i.e., the identification of the volatility surface from quoted market prices of European Vanilla options, by means of Tikhonov regularization. The theoretical results derived in [9] were also used for a fast numerical implementation. The results were presented at UNCC Charlotte. In a cooperation started with B. Hofmann (TU Chemnitz), a decomposition of the volatility surface into term-structure and smile shall be investigated in more detail. For a suitable multiplicative decomposition of the volatility surface, the overall identification problem splits up into two subproblems, which can be tackled separately and more efficiently. A corresponding report is in preparation.

Online Parameter Estimation: Online (or real-time) parameter estimation finds practical applications both by itself and as part of an adaptive control system. In the infinite dimensional case, the literature discusses online algorithms for parameter estimation in parabolic or hyperbolic partial differential equations that require spatially distributed data and their differentiation with respect to the space variables. In recent work by P.Kügler (cf. [16]), an online parameter estimation algorithm applicable to PDEs as well as ODEs has been developed, which allows for partial state observations and makes data differentiation unnecessary. Numerical examples are presented.

3 Level Set and Phase-Field Methods

In collaboration with subproject F 1309 (cf. [4]), a phase-field method for structural optimization with local stress constraints has been constructed. Using reformulations of constraints and the phase-field approach, this resulted in a linearly constrained quadratic optimization problem, whose feasible set satisfies all common constraint qualifications (in contrast to all standard formulations of this problem). The resulting discrete problems have been solved using interior-point methods and continuation with respect to the phase-field parameter (see Figure 6 for illustrations of results).

In 2004, B. Hackl also started to investigate modified notions of topological derivatives, which allow also the treatment of topologically non-differentiable problems (like perimeter regularized problems). These investigations already lead to a first publication [2] on this subject joint with

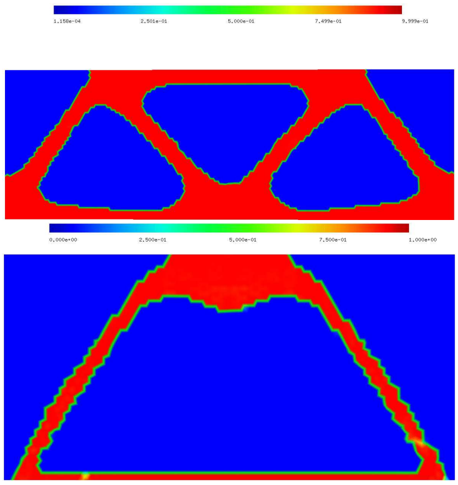

Figure 6: Optimal topologies obtained for a load on bottom (above) and a load on top (below).

M. Burger and W. Ring (TU Graz)

4 Neural Networks

After the successful investigations of Tikhonov-type methods in preceding years, we have now investigated iterative methods for the training of neural networks. It turned out already in previous work that convergence criteria for standard iterative regularization methods are not satisfied for network training, and even examples of non-convergence have been found (cf. [13]). For this reason we focused on *greedy algorithms* based on training one network node after the other. The first paper in this context, including a detailed analysis of convergence and regularization properties, has been published recently (cf. [3]). In recent work, an adaptive version of the greedy algorithm has been constructed (cf. [14]), which extends the work in [3] to a more general setting.

5 Stochastic Inverse Problems

A collaboration between H.W.Engl and A.Hofinger with S.Kindermann (now UCLA, before University Linz / SFB F 013) resulted in a publication on regularization methods for stochastic inverse problems (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. This work extends a former paper by H.W.Engl and A.Wakolbinger [12], and is a promising step towards a unified framework for treating deterministic and stochastic inverse problems.

6 Inverse Problems in Electrocardiology

In cooperation with the applied mathematics department of the university of Zaragoza, an inverse problem in electrocardiography has been investigated (cf. [5]). The problemn under consideration is concerned with the reconstruction of electric potentials on the cardiac surface via remote measurements. In particular we considered a new approach, where the electrodes are not placed on the patient, e.g., his or her chest, but where a balloon with electrodes on its surface is inserted into the heart using a catheter, and the measurements are taken in the interior. A fast method has been developed allowing to solve the severely ill-posed problem in real-time, i.e., a physician can utilize the information resulting from the regularized solution during the examination.

7 Further Activities

A. Hofinger participated in two study groups with industry in Canada, the "Seventh PIMS MITACS Graduate Industrial Math Modelling Camp" and the "Eighth PIMS MITACS Industrial Problem Solving Workshop", which resulted in two publications (cf. [1, 17]).

Within this subproject, the organization of two international workshops started in 2004. 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" will take place in Linz in September 2005.

The results achieved in this subproject lead to invitations of project members to talks at various universities (e.g. Princeton, Columbia, Chemnitz, Duisburg-Essen, Erlangen-Nürnberg, Zaragoza) and at various conferences and workshops.

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F 1309: Multilevel Solvers for Large Scale Discretized Optimization Problems

Prof. Dr. U. Langer, Prof. Dr. H.W. Engl, Dr. E. Lindner, Prof. Dr. W. Zulehner, Dr. D. Lukáš, DI R. Stainko, Dipl.Math. R. Simon

1 Optimal Design Problems

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

During the last year, we continued our investigations on optimal design problems. Especially we focussed our work on efficient solution techniques for topology and shape optimization problems. The first one is by far the most geneneral 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). Shape optimization, on the other hand, deals with the optimal shape of the boundary of a given structure, whereas the basic topology is maintained. In design process shape optimization can be seen as a post processing tool of topology optimization.

2 Topology Optimization

We finished our investigations with respect to the minimal compliance problem. Here we aim for an optimal material distribution such that the resulting structure is as stiff as possible under loading. The algorithm we introduced is based on a multilevel solution idea and gave good results and performance for several benchmark problems. Figure 7 shows a coarse solution to the 3D cantilever beam problem on the first level, whereas Figure 8 shows a much smoother optimal design on a higher level. For more details see [5].

Furthermore, we successfully applied material interpolation techniques from mechanical problems to optimization problems for magnetostatics. Here we managed to successfully constructed a multilevel algorithm in 2D and incorporated a nonlinear state equation in 3D. Corresponding pictures can be seen in Figure 9, whereas blue donotes the optimal design in the 2D picture.

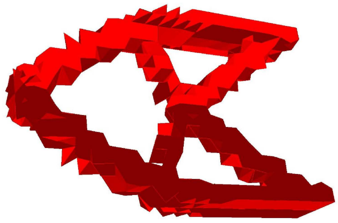

Figure 7: Coarse design with 8100 elements

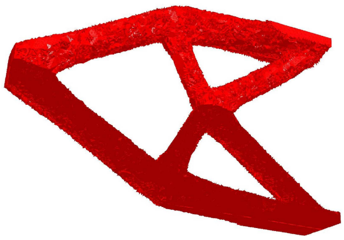

Figure 8: File design with 1410880 elements

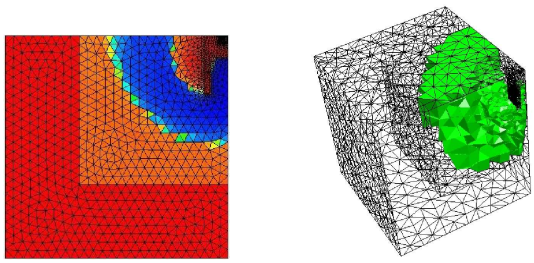

Figure 9: Optimal designs of a electromagnet in 2D and 3D

In a close cooperation with Project F1308 we developed and worked out a method for solving topology optimization problems with local stress constraints. Standard method fail when it comes to problems with local stress constraints. Moreover, the minimization of mass without material failure under loading it is one of the hottest topics in this field. As a starting point for our approach we picked up an previously published idea, see [4], which consists of a reformulation of the stress constraints such that their original unregular properities are overcome. We adapted this idea to our continous 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 10 (red indicates material, blue indicates air). Figure 11 shows the von Mises stress distribution of the corresponding design. More information about this approach can be found in [3].

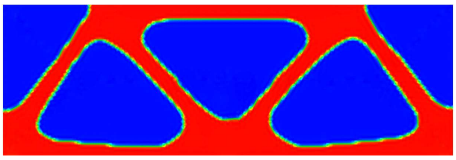

Figure 10: Material distribution

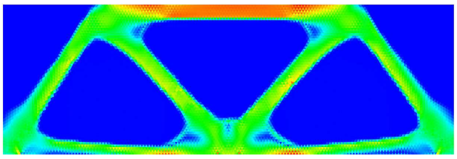

Figure 11: Von Mises stress distribution

3 Shape Optimization and Geometrical Aspects

During the last year we considered suitable geometrical descriptions for the boundaries of the structures we want to optimize. This was done in the framework of a cooperation with Project F1315. Since we used nested multilevel techniques for shape optimization problems, it turned out that Béziér curves or surfaces are proper representations of shapes, because they allow to intruduce a nested hierarchy of them. We tested this improved approach with linear magnetostatics in 3D successfully. For details see [2].

Moreover, also in cooperation with Project F1315, we started to tackle the integration of topology and shape optimization in the following way. Firstly we solve a coarsly discretized topology optimization problem. Then, we identify the boundary of the resulting structure and approximate the shapes using Béziér parametrization. Finally, we proceed with the multilevel shape optimization algorithm. In particular we optimize the Béziér parameters in such a way, that the difference between the Béziér curve and the boundary of the structure is minimized by means of least squares. In Figure 12 we see on the left the optimal shape approximation (illustrated by the red line) of the 2D design in Figure 9 and on the right we see it for the whole magnet.

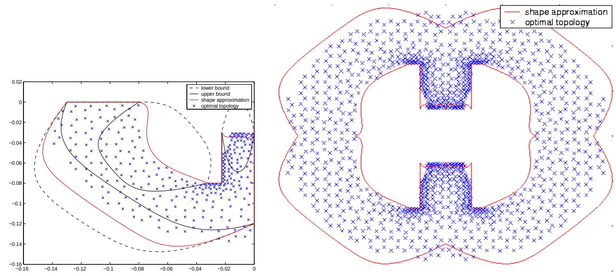

Figure 12: Approximation of shapes arising from 2D topology optimization

4 Preconditioning

Unlike in the classical nested approaches, the state equation (e.g. describing the equilibrium of forces) is treated as a constraint in all-at-once approaches (see, e.g. [1]. These methods lead to large scale saddle-point problems which are solved by iterative methods. But in order to exploit the potential speed-up which is expected by these approaches, efficient preconditioning of these large scale linear system is needed. We began to investigate the construction of such preconditioners to our optimal design problems. Which is also our current focus of work and will be in the future.

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F 1315: Numerical and Symbolic Techniques for Algebraic Spline Surfaces

Prof. Dr. J. Schicho, Prof. Dr. B. Jüttler
Dr. P. Chalmovianský, DI J. Gahleitner

During the first year of the third funding period, the work in this subproject concentrated on methods for approximate parameterization and on the analysis of space–filling line congruences and their relation to universal parameterizations. In addition, several other activities and cooperations with other subprojects took place.

Approximate parameterization

Monoids, as algebraic curves with a rational parameterization, were used for approximate parameterization of planar curves by J. Gahleitner in [6]. He finished his Ph.D. thesis and left the university, taking up a post of an high school teacher.

An algorithm of approximate parameterization via planar rational Bézier curves was published in [3]. The objective function combines the Sampson distance, a penalty function for the weight of the approximate curve and a regularization term based on the length of the projective control polygon of the curve. According numerical experiments, this technique is able to almost reproduce exact parameterizations. More recently, this technique has been extended to surfaces by E. Wurm (cooperating university staff) [12], see Figure 13 for an example.

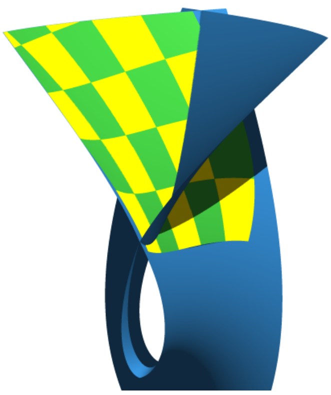

Figure 13: Approximate parameterization of a surface

Currently, P. Chalmovianský focuses on the formulation of the approximate parameterization of intersection curve as an ODE problem. The reformulation is used for the higher order approximation in predictor step when extrapolating approximate curve.

Universal parameterizations and line congruences

K. Rittenschober (cooperating university staff), who is due to finish her Ph.D. thesis in 2005, continued to study the connection between universal parameterizations and line congruences. She obtained new results on the system of chord of a twisted cubic, which can be used to define a parameterization mapping for parameterizing Veronese surfaces. In addition, she analyzed the connection of this mapping, and of the line congruences corresponding to cubic ruled surfaces, to universal parameterizations. While the final results will be presented in her thesis, some of them have meanwhile been accepted for publication [9].

Other activities

A circle-preserving subdivision scheme based on local algebraic fits has been developed. The convergence of the curves generated by such a process to a fair limit curve was proved and a paper has been submitted [4]. Earlier results on fairness criteria for algebraic curves have meanwhile been published [5].

The robustness of implicit representations with respect to small numerical errors has been studied by M. Aigner (cooperating university staff) [2]. In this work, it was also shown that this robustness can be enhanced via multiplication with auxiliary factors, see Figure 14 for an example. The two figures show the scalar fields $||\nabla f||$ associated with an algebraic curve $f = 0$ before (left) and after (right) multiplying it with an auxiliary factor. After this procedure, the critical region (red) has shrunk a lot. This process may help to improve the geometric robustness of implicitization results.

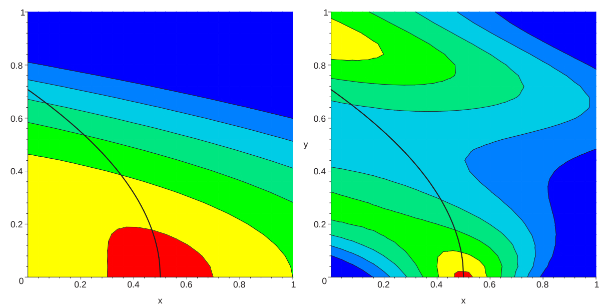

Figure 14: Robustness enhancement

More recently, M. Aigner developed robust methods for footpoint computation, demonstrating that implicitly defined curves and surfaces are particularly well suited for this task [1].

Earlier results of M. Shalaby (who left the project in September 2003) on spline implicitization have meanwhile been published [7].

Cooperations

The parameterization of the boundary of a certain region is an important issue in shape modeling, and P. Chalmovianský continued to collaborate with D. Lukáš of subproject F1309 on this issue.

A new cooperation was established between subprojects F1303 and F1315, addressing local methods for parameterizing cubic surfaces. This lead to a manuscript, which is currently under review [10].

Another cooperation between subprojects F1303 and F1308 was devoted to monotonicity-preserving interproximation of B-H curves. Here, the task is to generate a sensible curve from experimental data, taking side–conditions into account. This led to an improvement of existing earlier tools within the SFB and led to a joint paper [8]

An external cooperation with E. Wings (Procom GmbH, Aachen, Germany) on tool path generation for NC machining led to the publication [11]. In this research we used algebraic spline surfaces for bounding the distance to the target surface, in order to guarantee the accuracy of the tool path.

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F1322: Computer Algebra for Pure and Applied Functional Analysis

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

As defined in the project proposal [4], *symbolic functional analysis* has been introduced as an innovative research initiative that aims at developing constructive techniques for relevant fragments of functional analysis. In the view of the TH∃OREM∀ project F1302, these techniques may be classified roughly into three categories: understanding and analyzing crucial properties encountered in functional analysis ("proving"), simplifying complicated terms with respect to some complexity measure ("computing"), and finding instances for general or concrete operator statements ("solving").

The focus was laid on solving / computing with operator identities, a classical case being linear two-point *boundary value problems*, studied extensively in the PhD thesis [9]. Such problems can be formulated as searching for a Green's operator G such that $TG = 1$ and $B_1G = \cdots = B_mG = 0$, where T is a linear ODE operator of arbitrary order n and $B_1, \ldots, B_n$ are linear boundary operators involving derivatives of order up to $n-1$. Since these operators can be seen as noncommutative polynomials, Gröbner bases can be applied explicitly [11] or implicitly [10].

Naturally, the next steps to explore are concerned with various *generalizations* of these problems (see the project proposal for a more detailed list). In 2005, we have started to analyze the following generalizations, treated in the paragraphs below.

- Up to now, we have restricted our attention to well-posed problems in the sense that there is exactly one G for the given boundary value problem. However, in the applications one often meets *ill-posed problems* where exact solutions may not exist or may not be unique (besides being instable with respect to the data).
- It is near at hand to explore PDEs instead of ODEs, meaning that the differential operator T may contain *partial derivatives* with respect to several variables.
- Orthogonally to the ODE/PDE issue, it is of utmost interest to remove the linearity restriction, thus allowing *nonlinear differential operators* like $Tu = u' - u^2$.
- Another interesting way to generalize the usual formulation of boundary value problems is to allow for *symbolic parameters* to appear in T and/or $B_1, \ldots, B_n$.

Besides these more practical questions, we have also analyzed the underlying theory from a new perspective: As pointed out in [10], the fundamental data structure in our new approach to boundary value problems is a certain quotient ring of noncommutative polynomials that we have named the Green's polynomials. It turned out that one can subsume these Green's polynomials together with the well-known differential polynomials from Ritt-Kolchin differential algebra [8, 7] and with the equally well-known Weyl polynomials of D-module theory [3, 5] under a new polynomial concept that we have called *integro-differential polynomials*. We will give a short summary of these ideas in the last paragraph below.

Ill-posed Problems. Following a suggestion of the referee, we have investigated in [10] the two-point boundary value problem $-u'' = f, u'(0) = u'(1) = 0$. This problem is ill-posed for two reasons: First of all, the solution u exists only for those f that fulfill the solvability condition $\int_0^1 f(x)\,dx = 0$. And second, if this condition is fulfilled, the solution is unique only up to a constant. The solution algorithm discussed in [9] would break down on this example because the nullspace matrix becomes singular. However, we can still apply our method by a suitable transformation: Uniqueness is restored by imposing the condition that the L^2 norm of u be minimal; existence is enforced by projecting the given f onto an admissible subspace. This leads to the operator problem $-D^3G = D$ with side conditions $LDG = RDG = FG = 0$, where F is the definite integration operator. This problem can now be solved by our standard approach; one obtains the classical *modified Green's function* as in [15], page 216.

Partial Derivatives. We have started to investigate boundary value problems for linear PDEs. As a first simple example, we have considered the *Dirichlet problem for the Poisson equation* $\Delta u = f$ on the unit square as treated on page 333f of [6]. Instead of the right-inversion formula in [9], one needs here a fundamental solution to start with; it can be computed by the help of the Fourier transform. Following our standard method, one has to compute the nullspace projector, which amounts to solving the Laplace equation with certain Dirichlet boundary conditions. Putting things together, one gets a series representation of the Green's function $g(x, y, \xi, \eta)$. Work on this issue is still in a preliminary state, see the forthcoming technical report [12].

Nonlinear Problems. As a first example of a nonlinear boundary value problem, we have studied the simple equation $u' - u^2 = f$ with homogenous "boundary condition" $u(0) = 0$. In this case, one cannot expect any Green's function in terms of elementary functions as one can show easily [14]. As a first way out, we have derived a power-series expansion of $u(x) = \sum u_n x^n$ in terms of $f(x) = \sum f_n x^n$, thus solving the boundary value problem in an analytic setting [14]. It turned out that the recurrence problem generated for u_n is of an interesting combinatorial nature: It is of course again nonlinear and inhomogeneous, but it has also an order that grows with n, and the solution u_n turns out to be another series over partitions of n, where the "indeterminates" are f_n and the coefficients are built from compositions and trees refining the partitions of n.

Symbolic Parameters. Following another crucial suggestion of the referee, we have also investigated in [10] a first example with symbolic coefficients, namely the *generic Sturm problem* $u'' + au' + bu = f$ with unmixed boundary conditions $\alpha u(0) + \beta u'(0) = \gamma u(1) + \delta u'(1) = 0$. Here $a, b, \alpha, \beta, \gamma, \delta \in \mathbb{C}$ are symbolic parameters that have to fulfill certain regularity conditions such that the solution u is uniquely determined. It turns out that the standard method of [9] can be applied just as before. The only difference is that the multiplication operators are no longer taken from an algebra over $\mathbb{C}$ but rather over the rational-function field $\mathbb{C}(a, b, \alpha, \beta, \gamma, \delta)$. The Green's operator of this problem can finally be written in a compact form if it is factored and expressed in terms of the Wronskian of the chosen fundamental system; the corresponding result can then be easily compared with the literature like on page 195 of [15].

Integro-Differential Rings. The algebraic structure behind our method can be formulated nicely by the new concept of *integro-differential rings*, bringing together two crucial concepts: differential rings [8, 7] for modeling derivatives, Baxter rings [1, 2] for modeling integrals. In addition to the four axioms coming from these theories, we stipulate that the "derivation" be a left inverse of the "integration". The corresponding notion of polynomials is a direct generalization of differential polynomials (= those integro-differential polynomials that do not have an integral indeterminate). It subsumes also the Weyl algebra [3, 5] by introducing a compositional structure as for any other polynomial domain; the Green's polynomials are the linear subsegment of this structure. One particularly interesting feature of integro-differential rings is that they provide a natural way of introducing evaluation in terms of their derivation and integral. Hence the corresponding polynomial structure inherits boundary operators, and we need not stipulate them as indepenent operations. See the forthcoming report [13] for details.

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SFB F013: Numerical and Symbolic Scientific Computing

Coherence within the SFB

- **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, F1306, and F1303**
  The *Theorema* system and its underlying *Mathematica* computing engine are used in order to study the behaviour of the Buchberger algorithm for computing the Groebner Bases in the context of specific problems arising in the modeling of the Plastic Strain phenomena. By using the specific structure of this type of problems, one can obtain significant speed improvements.

- **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 others**
  Whereas geometric multigrid methods use hierarchical information in order to do coarse grid correction and interpolation, algebraic multigrid methods, such as studied in subproject F1306, use only the stiffness matrix itself, or the element matrices from which it is assembled. J. Kraus, RICAM, Austrian Academy of Sciences, developed a coarse grid correction and interpolation method based on the splitting of element matrices into so-called *edge matrices*. A priori, it was not clear under which such a splitting exists and how to find it in the most efficient way. Symbolic/algebraic methods were here helpful in two ways. First, we gave an algebraic criterion for the existence of a splitting. Second, we gave formula for computing a splitting assuming the criterion is fulfilled. Another cooperation – with G. Landsmann, subproject 1304, and P. Mayr from the department of algebra – was the application of topological methods for real and complex manifolds in order to solve a problem that appeared in a study of polynomial functions over linear groups. For the case of finite fields, it has been shown that transposition is a polynomial function in the matrix group, i.e. it can be expressed with the terms of group theory. For infinite fields, nothing was known previously; we could answer this question for the field of rationals, reals, and complex numbers. 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. As a result, we obtain information on the geometric stability of implicitization. Another cooperation with J. Valdman, subproject 1306, was to use symbolic methods in an algebraic subproblem that arose in the context of elasto-plasticity. Instances of a system of algebraic equations had to be solved as fast as possible. In this situation, it turned out that the symbolic approach was *inferior*; it could

not compete with the numeric approach. Our explanation was that the problem was numerically well-behaved: it seemed to be well conditioned and it was no problem to find good starting points for iterative methods.

- **Cooperation between F1304 and others**
The cooperation with project F1317, specifically between H. Gu and S. Kindermann has been continued in 2004. H. Gu has also cooperated substantially with M. Burger of F1308. On the topic of factorization of LPDOs we have presented our approach several times at internal SFB meetings, and a cooperation with project F1306 is currently being developed.

- **Summation and Finite Elements**
In F1301, Prof. P. Paule and Dr. J. Schöberl have continued to apply summation techniques from F1305 to the construction of high order finite elements, 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.

- **Cooperation between F1306 and others**
Prof. B. Buchberger, Dr. W. Windsteiger and Dr. J. Valdman calculated Gröbner basis for the two-yield minimization problem. Its structure confirms the former expectation, that there can be no analytic formula found for two-yield plastic strains p_1, p_2 - displacement u relation. In order to test the speed of an existing iterative algorithm, the numerical calculation in terms of a third part SYNAPS software was tested together with F1303. In project F1301-19, Prof. P. Paule and Dr. J. Schöberl work on special function techniques to construct algorithms for high order finite elements. These high order finite elements are applied in project F1306 for the mechanical problems. On the other side, these non-linear problems are challenges for the high order algorithms.

- **Cooperation between F1308 and F1322**
If Newton-type iterations are applied to the solution of (ill-posed) inverse problems, at each (outer) Newton-step a linearized ill-posed problems has to be solved. This can be done in a stable way by iterative regularization methods. A Newton-Landweber method of this type has been propopsed and analyzed earlier in [2]. For a convergence analysis the decomposition of the difference of certain polynomials of noncommutative operators has been utilized. In principle also faster semiiterative methods can be used for the regularized solution of the linear systems in each Newton-step. However, in contrast to Landweber iteration, a decomposition of the polynomials for general semiiterative methods is not at hand. In a cooperation of H. Egger with G. Regensburger (F1322), suitable decomposition of noncommutative polynomials for iterative regularization methods are investigated and shall finally lead to a convergence analysis of faster Newton-type iterations.

- **Cooperation between F1308 and F1309**
In collaboration of M. Burger and R. Stainko (F1309), the use of level set techniques for topology optimization has been investigated. Since preliminary numerical experiments indicated that level set methods cannot improve the efficiency and accuracy compared to standard material interpolation schemes for simple problems such as minimizing compliance, we started to investigate structural optimization with local stress constraints. Due to the high number of local constraints and possible degeneracies of admissible sets, this problem is one of the most challenging in topology optimization, and it is of high practical importance. Moreover, standard material interpolation schemes do not yield satisfactory solutions in this case, which is a good motivation for considering new approaches. In [3] a new phase-field approach for this problem has been constructed, whose main ingredients are a reformulation of bilinear equations into linear equalities and subsequent relaxation using phase-field methods.

- **Cooperation between F1308 and F1306**
A collaboration with subproject F 1306 has been started recently with the aim of tracking the evolution of elasto-plastic interfaces in computational plasticity via level set methods. The motivation for this approach is that the interface needs to be known accurately in order to construct suitable adaptive grids and subsequently achieve high accuracy in finite element solutions. The derivation of a motion law for the elasto-plastic interfaces involves several techniques usually used for level set methods in shape optimization (e.g. shape sensitivity calculus).

- **Cooperation between F1309 and F1315**
Dr. D. Lukáš (09) started a cooperation with Dr. P. Chalmoviansky (15) about the approximation of boundaries and shapes of coarse optimal designs resulting from topology optimization problems. Using Béziér curves and surfaces, their parameters are optimized in such a way, that the difference between the Béziér curve and the boundary of the structure is minimized by means of least squares. This smooth boundary representation allows then a continuative shape optimization of the optimal design. A joint paper about this approach is planned.

- **Cooperation between F1309 and F1308**
In a close cooperation between R. Stainko

(09) and Dr. M. Burger (08) a new approach to topology optimization problems with local stress constraints was developed. First, a reformulation of the constraints allows a problem formulation with a fixed number of constraints and a convex design space. Second, a parameter dependent Phase–Field relaxation is applied to the problem, which yields convergence of minimizers to 0-1 designs. The resulting optimization problems are finally solved with a primal-dual interior-point method. This new approach is summerized and described in a joint paper, submitted to *SICON*.

- **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 cooperation with between G. Haase and B. Jüttler, about automatic simplification of domains for FEM. This will be further pursued in the final year of the second funding period.

- **Cooperation between F1322, F1302, and F1308**
As obvious from the project proposal, F1322 was created from a symbiosis between projects F1302 and F1308. It benefits from bringing together the symbolic expertise from F1302 with the functional analysis know-how from F1308. The crucial link is that certain operators that are relevant in the abstract treatment of functional analysis can be modeled by noncommutative polynomials, which can be manipulated efficiently by Gröbner bases methods. In particular, the solving engine for linear two-point boundary value problems—which is continually extended to cover more problem types—is implemented in the 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**
The speaker's project F1301 is concerned with generic Gröbner bases in various polynomial domains, including commutative as well as noncommutative rings. As observed in the project proposal of F1301, the original setting of Green's polynomials as introduced in [4] is a prototypical example of such a generalized "Gröbner domain". As we have explained above, the formulation in terms of integro-differential polynomials provides an even smoother and also a more general notion of polynomial whose applicability for Gröbner bases methods has to be investigated.

- **Cooperation between F1322 and F1304**
Symbolic differential computation is of course intimately connected with symbolic functional analysis, the subject matter of F1322. As explained above, our current focus is on boundary value problems, whose main component is the differential equation defining the problem. In the case of symbolic functional analysis, we leave the function on the right-hand side of this differential equation symbolic, and we ask for the operator that maps it to the solution of the equation. In the case of symbolic differential computation, the focus is more on finding and representing the solutions of concrete equations. Of course there are a lot of connections among these two viewpoints. For example, in our standard approach to solving BVPs, we presume a given "symbolic solver" for homogeneous differential equations, that may of course be provided by the approach of F1304.

- **Cooperation between F1322 and F1305**
We have already remarked that attacking more general classes of BVPs is often associated with having to deal with infinite sums in the solution operators; see for example [5] for a PDE example and [6] for a nonlinear example. Up to now, our solution methods have been rather adhoc, but we expect a more systematic approach to benefit greatly in the future from using formal summation methods (e.g. in the framework of special functions).

- **Seminar on Differential Equations**
Buchberger organized a monthly seminar with the title "Symbolic Methods for Differential Equations" in which all SFB groups and also groups from the RICAM institute are taking part for finding out possible interactions between the topics treated in SFB 1322 and the other groups within SFB F013 and RICAM. Approximately 15–20 people are attending these seminars regularly, and a couple of new interactions are evolving from this seminar, e.g. an EU project proposal on symbolic methods for differential equations. The seminar is continued in 2005, and there are concrete plans for extending the discussion to numerical issues and their interaction with the symbolic methods (scheduled by Buchberger and Engl for the summer semester 2005).

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SFB F013: Numerical and Symbolic Scientific Computing

National and International Cooperations

1 Cooperations with other Research Institutions

- **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 Meet-MATH 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 2004 we have participated in applied projects with Alcatel Timisoara, and we are currently starting another project with Siemens VDO Timisoara.

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

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

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

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

- **University of Cantabria**
  In 2004, J. Schicho was general chair of the annual International Symposium for Symbolic and Algebraic Computation, which was held in Santander. T. Beck, I. Szilágyi, and J. Pílniková did the publicity work for this conference.

- **University of Innsbruck**
  In a series of joint seminars, which has been held 2 times in Tyrol and once in Upper Austria, we developed a method for resolution of singularities based on plane blowing ups. The idea is to perform the blowing up operations in such a way that no additional variables need to be introduced, because the blownup variety

is covered by open subsets of the affine space. A priori, it is not clear that such a covering is possible.

- **University of Sydney**
  We implemented an algorithm for solving quadratic forms in arbitrary many variables in the computer algebra system MAGMA. We also collaborated in the development of the Lie algebra method for solving diophantine equations.

- **University of Alcala**
  We developed a method for the computation of the topological type of level curves of an algebraic surface.

- **Joint Ph.D. thesis of Kondratyev with Prof. Stetter, TU Wien**
  The Ph.D. thesis of A. Kondratyev was jointly advised by F. Winkler of J. Kepler University Linz (F1304) and Prof. H.J. Stetter of the Technical University Wien. It was a very successful cooperation, combining numerical and symbolic algorithmic mathematics.

- **Factorization of LPDOs and integrability of PDEs**
  E. Kartashova has participated in the international workshop on "Integrable Systems" in Guernavaca, Mexico in November 2004. During this visit she has cooperated with R. Beals of Yale University on a new approach to factorization of LPDOs.

  Currently we are organizing a group of researchers in integrability with the goal of applying for a European project.

- **INRIA Paris**
  The long term cooperation with Prof. Paule's group was continued in a joint paper [5] on holonomic sequences by P. Flajolet, B. Salvy (both INRIA Paris) and S. Gerhold.

- **Humboldt-University of Berlin and TU Munich (Germany)**
  Dr. J. Valdman has cooperated with Prof. C. Carstensen (Berlin) and Prof. M. Brokate (Munich) on analysis and numerical solution of multi-yield models in elastoplasticity. This cooperation led to 2 journal publications until now.

- **St. Petersburg State Polytechnical University (Russia)**
  Prof. U. Langer and Prof. V.G. Korneev published a survey article in the "Encyclopedia of Computational Mechanics" (Chapter 19 in Part I) that was edited by E. Stein, R. de Borst and Th.J.R. Hughes, and that was published by John Wiley & Sons in 2004.

- **Dept Mathematics, Reading (UK)**
  Dr. J. Schöberl and PD Dr. J. Markus Melenk worked together on preconditioning for scalar problems and aspects of fast implementation. M. Melenk visited Linz several times, a joint paper is in preparation.

- **Identification of Nonlinearities in Parabolic Equations**
  In cooperation of F1308 with M V. Klibanov (UNCC Charlotte) the stable identification of nonlinear source terms in parabolic equations has been investigated. Inverse problems of this type are of interest e.g. in heat transfer at high temperatures. It was shown in [3] that such nonlinearities can be stably reconstructed from a single set of boundary measurements in a simple experimental setup. The theoretical stability results were illustrated by several numerical test examples. The results of the numerical simulations further suggest that some of the conditions needed for the analysis can even be further relaxed.

- **Newton-Kaczmarcz Methods**
  In collaboration with B. Kaltenbacher (University Erlangen-Nürnberg) regularizing Newton-Kaczmarcz methods have been developed (cf. [2]), which offer a possibility for the efficient solution of inverse problems with a high number of measurements (such as e.g. impedance tomography) with restricted memory requirement.

- **Total Variation Regularization**
  In collaboration with Stan Osher and Jinjun Xu (University of California, Los Angeles), Don Goldfarb and Wotao Yin (Columbia), a novel iterative regularization method for image denoising has been constructed (cf. [4]). This new scheme is able to remedy a systematic error in standard total variation denoising, namely a decrease of the variation in the image and consequently yields improved reconstructions compared to the standard approach.

- **Level Set Methods**
  A collaboration with Marc Droske and Martin Rumpf (University Duisburg-Essen) on constructing level set methods for higher-order geometric flows (such as Willmore flow) has been started. The main idea of the new approach is to construct semi-implicit methods on a narrow band, and to use continuation by solving eikonal equations on an outer band in order to avoid artificial boundary values on the narrow band.

  The continuation of a collaboration with H. Ben Ameur (ENIT Tunis) is concerned with the mathematical analysis of inclusion detection problems in thermoelasticity. In particular the effect of having more boundary measurements compared to a previously discussed problem in plain elasticity as well as the incorporation of topological derivatives for this problem are investigated.

In collaboration with B. Su (MPI for Math. in the Sciences, Leipzig, now Iowa State Univ.), the construction of weak solutions for a moving boundary problems based on the level set approach has been investigated, a paper is in preparation.

- **Symmetries**
  N. Bila and P. Kügler continued their work on applying the Landweber method and the derivative-free Landweber method on the reduced similarity spaces associated with a parameter identification problem modeled by a PDE. A new case was studied, namely, when the mathematical model is invariant with respect to scaling transformations (a joint paper is in preparation). Moreover, recent work [1] with Dr. J. Niesen (Herriott Watt University Edinburgh on finding new classes of symmetry reductions related to a parameter identification problem has been continued. By extending the notion of nonclassical symmetries (which is a common approach in the theory of symmetry groups) the aim was to find nonclassical equivalence transformations (paper in preparation).

  Within the SFB-activity concerning symmetries, there has also been an international Workshop on "Symmetries, inverse problems and image processing" (January 2005 in Linz), co-founded by the SFB. The list of plenary speakers included leading experts in the area such as Peter J. Olver (Minnesota), Arieh Iserles (Cambridge) and Peter A. Clarkson (Kent).

- **Technical University of Copenhagen (DTU)**
  R. Stainko continued his cooperation with the *TOPOPT*–group around Prof. Dr. M. Bendsoe and Prof. Dr. O. Sigmund about various aspects of modelling, formulating and solving various topology optimization problems. The fruitful discussions, for instance, have been a useful support for the above cooperation between Project F1308 and Project F1309.

- **SINTEF Applied Mathematics (Norway)**
  Dr. T. Dokken (SINTEF, coordinator) and Prof. B. Jüttler and four other European partners **(University of Cantabria, Spain; University of Nice and INRIA, France; think3, Italy, University of Oslo, Norway)** are involved in a IST–FET research project within the Fifth Framework Programme of the European Commission. After completing the contract negotiations, the projected has started on July 1st, 2002.

- **Seoul National University (Korea)**
  We continued the cooperation on issues of visualization and computer animation with Prof. Myung–Soo Kim (Seoul). This lead to a joint publication "Computing the distance between two surfaces via line geometry" which was presented at the 10th Pacific Conference on Computer Graphics.

- **The University of Hong Kong (China)**
  Prof. Jüttler authored a joint paper with Prof. Wenping Wang on "The shape of spherical quartics".

- **Arizona State University (USA)**
  Prof. Jüttler authored a joint paper with Prof. Wagner on "Kinematics and Animation".

- **Daimler Chrysler Research (Germany)**
  Prof. Jüttler authored a joint paper with Dr. Schwanecke on "Analysis and Design of Hermite subdivision schemes".

- **RICAM**
  Like other parts of the SFB, project F1322 is now conducted over the Radon Institute for Applied and Computational Mathematics (RICAM). E.g., the post-doc M. Rosenkranz (part of the SFB throughout 2004) now is employed by RICAM. The interdisciplinary environment of this instutition provides an additional incentive to cross-group (in particular symbolic-numerical) cooperations. One of these is an ongoing research activity to apply symbolic computation techniques for polynomial decomposition in the convergence analysis of semi-iterative regularization methods.

2 Guests

- **Prof. Jozef KACUR:** University Augsburg, Germany, March 31–April 1, 2004. Talk: "Numerical solution of contaminant transport in dual-well flow"

- **Dr. Teodora MITKOVA:** University Magdeburg, Germany, May 5–7, 2004. Solvability and finite element approximation of a mathematical model for the flow in magnet-fluid-seals

- **Prof. Mirella MANARESI:** University of Bologna, Italy, May 26–27, 2004. Research group in Algebra and Geometry, Lecture on generic projections

- **Prof. Günter BRENN:** TU Graz, Austria, July 14, 2004. "On laminar turbulent behavior in pipe fluid dynamics – a new approach"

- **Mag. Jiri KOSINKA:** University Prag, Czech Republic, July 25–26, 2004. Talk: "On Appollonius problem and the approximation of conics by quadratic splines"

- **Mag. Michael BARTON:** University Prag, Czech Republic, July 25–26, 2004. Talk:

"Computing cylinders from tangent information and applications in robotics"

- **Mag. Jiri SCRUBAR:** University Prag, Czech Republic, July 25–26, 2004. Talk: "Spatial generalizations of the 9 point cirde"

- **Dr. Bo SU:** Max Planck Institut Leipzig, Germany, August 17–19, 2004. Collaboration with Martin Burger concerning the analysis of level set methods and viscosity solutions, completion of a joint paper.

- **Dipl.-tech.-math. René SIMON:** TU Berlin, Aug. 30–Sep. 1, 2004. Talk: "Approximation of elliptic optimal control problems"

- **Prof. Martin PETERNELL:** TU Wien, September 14, 2004. The cooperation devoted to parameterization of convolution surfaces, which was started one year ago, has been continued. Meanwhile, a joint paper on this subject has been accepted for publication in Computer Aided Geometric Design.

- **Mr. Yang HUIDONG:** KTH Sweden, October 9–12, 2004. Talk: "Computing GTD-coefficients via direct numerical simulation"

- **Prof. Joris VAN DER HOEVEN:** Université Paris-Sud, Département de Mathématiques, Oct. 24–27, 2004. He worked together with T. Beck and J. Schicho on algorithms for multivariate power series.

- **DI. Ekaterina SHEMYAKOVA:** University Moskau, Russia, April 25–May 3, 2004. Talk: "Topics in involutive bases"

- **DI. Seyed Mohammed AJDANI:** University Zanjan, Iran, May 5–June 9, 2004. Applications of automatic reasoning to graph theory

- **Dr. Mijail Quintana BORGES:** University of Oriente, Cuba, May 17–June 18, 2004. Joint research on Groebner bases and coding theory, lecture "Using Groebner bases for determining the equivalence of linear codes and solving the decoding problem"

- **Prof. Lezek DEMKOWICZ:** University of Texas, USA, June 13–18, 2004. "hp Finite Elements, Maxwell's equations, exact sequences and de rham diagram, projection-based interpolation, automatic hp-adaptivity, and other stories"

- **Dr. Sonia PEREZ-DIAZ:** University Alcal, Spain, June 20–26, 2004. joint research on algebraic curves and surfaces

- **Dr. Ha LE:** Inria- Rocquencourt, August 21–26, 2004. Talk on symbolic summation, research cooperation

- **Prof. George E. ANDREWS:** Penn State University, Sep. 14–Oct. 12, 2004. Talk "Partitions with Short Sequences and Ramanujan's Mock Theta Functions" and joint research on plane partitions

- **Dr. Elmar WINGS:** ProCom Aachen, Oct. 30–Nov. 4, 2004. Talk: "Some new techniques for shape reconstruction from unorganized points", cooperation with Bert Jüttler

- **Dr. Viktor LEVANDOVSKYY:** University Kaiserslautern, November 9–13, 2004. Talks "Recent Developments in Algorithmic Questions of Noncommutative Computational Algebra" and "Gröbner Basics in a Noncommutative Setting: Algorithms and Applications"

- **Dr. Evelyn HUBERT:** INRIA Paris, France, November 14–19, 2004. Joint research on differential characteristic sets, lecture "Triangulation-decomposition algorithms for differential systems"

- **Prof. Dr. Vladimir SOKOLOV:** Landau Inst. for Theoretical Physics, Russia, December 4–15, 2004. Discussion and lectures on common research interests in symmetries and integrability of differential equations

- **Prof. Dr. Wenping WANG:** University of Hongkong, Dept. of Computer Science, December 12–21, 2004. Talk "Some new techniques for shape reconstruction from unorganized points"

3 Lectures at other Universities

- **B. Buchberger:** Waseda Gakuin High School, Japan. October, 2004. Computer Algebra for high school students.

- **B. Buchberger:** Waseda Gakuin High School, Japan. October 2004. Didactic Principles for Using Computer Algebra in Class: lecture for high-school teachers.

- **B. Buchberger:** Kyoto University, Japan. October, 2004. How to Give Talks and Write Papers: lecture for Graduate students.

- **B. Buchberger:** Kyoto University, Japan. October, 2004. How to Work With the Literature: lecture for Graduate students.

- **Tudor Jebelean:** University of Timisoara, Romania. September 2004. Blocked lecture (8 hours) on automated reasoning techniques and their implementation in Theorema.

- **Tudor Jebelean:** University of Cluj, Romania. July 2004. Blocked lecture (8 hours) on automated reasoning techniques and their implementation in Theorema.

- **J. Pílniková** gave a talk on diophantine problems and Lie algebras at the University of Sydney.

- **I. Szilágyi** gave a talk on algorithms for cubic surfaces at the University of Debrecen.

- **J. Schicho** gave a talk on diophantine problems and Lie algebras at the University of Innsbruck.

- **T. Beck** gave a talk on effective manipulation of algebraic power series at the University of Western Ontario.

- In relation to the project **F. Winkler** has visited Charles University in Prague and given a lecture on symbolic geometric algorithms [6].

- **E. Kartashova** has given an invited lecture [7] at the workshop on Integrable Systems in Guernavaca, Mexico.

- **M. Kauers:** "Algorithmische Beweise für neue Klassen von kombinatorischen Identitäten", Invited colloquium talk at Universität Kassel, Germany, November 2004.

- **Dr. M.Burger:** Course "Applied Mathematics Seminar: Infinite-
Dimensional Optimization and Optimal Design",
UCLA, Fall 2003/2004.

- **Dr. M.Burger:** Course "Aspects of Scientific Computing: Numerical Methods for Incompressible Flows", UCLA, Winter 2004. Identification of parameters in polymer crystallization, semiconductor models and elasticity via iterative regularization methods. Lomonossov University Moskow, Russia, Juli/Augusust 2002.

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[6] F. Winkler. Algebraic geometric computation, May 2004. Talk at the Math.Dept., Charles Univ. Prague.

[7] E. Kartashova. Elements of integrability in nonlinear evolution pdes with wave-type solutions, November 2004. Talk at the workshop "Integrable Systems" in Guernavaca, Mexico.

SFB F013: Numerical and Symbolic Scientific Computing

Transfer of Knowledge and Technologies

1 Wolfram Research

Developer of the mathematical software system *Mathematica*. We are in close contact by providing them with the results of our research and with suggestions about the existing and possible facilities of the Mathematica system (see also the section on technology transfer). In particular, the following aspects have been investigated: unification with sequence variables, logico-graphic symbols.

2 The CALCULEMUS Training Network

This network consists of a net of universities and research institutes with the common goal of integrating the functionalities of existing mathematical software and theorem proving systems: IRST Trento Italy, Univ. Edinburgh UK, Univ. Karlsruhe Germany, RISC-Linz Austria, Univ. Nijmegen Netherlands, Univ. Eindhoven Netherlands, Univ. Genova Italy, Univ. Birmingham UK, Univ. Saarbrücken Germany, Univ. Bialystok Poland. The network was supported by the European Union in the frame of the Calculemus Training Network Project HPRN–CT–2000–00102, which ended on Aug.31, 2004, however the cooperation between the groups is continuing, in particular new proposals for EU projects are planned. Within the EU project, the most important role of our group was in two tasks *(a) enhancing computer algebra systems with reasoning power* and *(b) computer aided editing of mathematical texts.* In the frame of task *(a)* we enhanced our existing provers and added new ones to the *Theorema* system (see section describing the subproject F1302), which is implemented on top of the computer algebra system *Mathematica*. In the frame of task *(b)* we continued to include in the *Theorema* system the appropriate capabilities concerning: display of mathematical formulae in natural style (including two dimensional notations and even the possibility of defining new logico-graphic symbols), organization of mathematical knowledge, display of mathematical proofs in natural style and in natural language.

3 Mathematical Knowledge Management

This is a new field in mathematics with high potential of becoming one of the crucial prerequisites for the further development of mathematics: A significant amount of effort and money is spent for the invention of new mathematical facts and methods but it becomes harder and harder to organize and retrieve what had been invented and, thus, lots of efforts and funds are spent in vain. Our research group was actually the founder of this field, and organized the first international workshop on Mathematical Knowledge Management (a term coined by B. Buchberger at the occasion of organizing this workshop) at RISC, Hagenberg, Austria, in September 2001. During 2004, the *Theorema* group continued to be one of the key research groups in the international community, actively cooperating with the the most important research groups in the field in the frame of the MKM network, and also actively participating at the organization and the proceedings of the MKM conference (MKM 2004, Sep. 2004, Bialowieza, Poland). Currently a new EU project proposal on MKM was submitted, in which the *Theorema* group is involved.

4 Inverse Problems in Electrocardiology

In cooperation with R. Celorrio (University of Zaragoza) an inverse problem in electrocardiology was investigated by A.Hofinger. This problem is concerned with the reconstruction of electric potentials on the cardiac surface via remote measurements. In particular we considered a new approach, where the electrodes are not placed on the patient (e.g. his or her chest), but where a balloon with electrodes on its surface is inserted into the heart using a catheter, and the measurements are taken in the interior. In [1] a fast method has been developed, which allows to solve this severely ill-posed problem in real-time, i.e. a physician could watch the resulting solutions during the examination.

5 Thickness Optimization of Industrial Frames

Using mathematical techniques good initial design models for various production processes are created. These initial designs turn out to be very valueable since faster and faster changing demands and selling conditions are longing for short developement times. Since these optimization processes are simulated with computers instead of costly experiments with prototypes, they help to save expensive develepement times and costs. In this project the

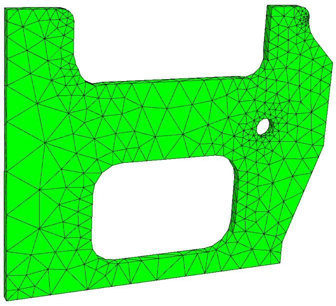

Figure 15: Original design.

mass of a frame is reduced by means of saving material such that the modified and mass reduced frame still endures the forces of a clamping process. In other words, the weight-reduced frame still endures the occurring von–Mises stresses as the original frame. In Fig. 15 we see the original design of

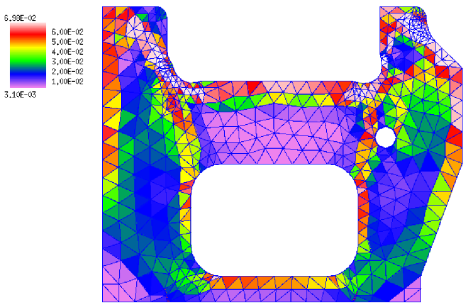

Figure 16: Optimal thickness distribution.

the frame. For the thickness optimization aiming for minimal mass w.r.t. some constraints (e.g. bounded von–Mises stress) just the cross-section of the frame is used. The optimal material distribution is then shown in Fig. 16. Based on this information a 3D

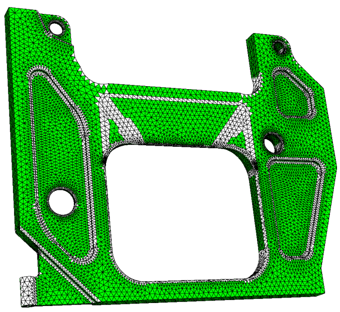

Figure 17: Optimized 3D design.

CAD-design for a prototype is created. We see this prototype in Fig. 17. Here it is already meshed, the first step for the direct computation to verify the von–Mises condition.
Company: ENGEL AUSTRIA GmbH,
A-4311 Schwertberg, Austria.

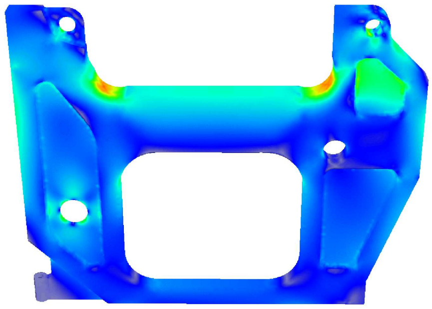

Figure 18: Von–Mises stress distribution.

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