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Numerical and Symbolic Scientific Computing

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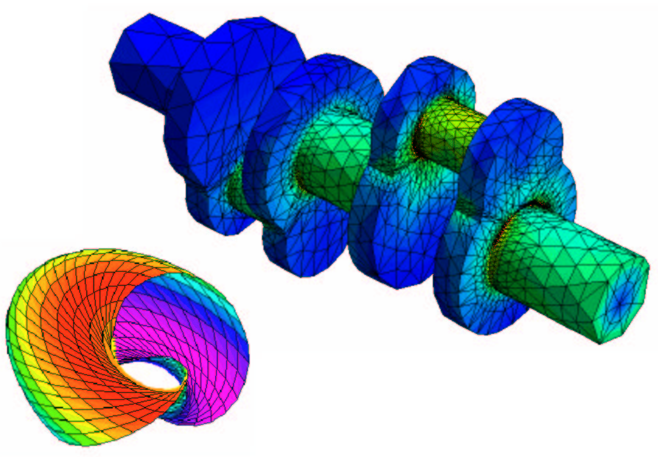

Supported by

Special Research Program SFB F013

"Numerical & Symbolic Scientific Computing"

Speaker: Prof.Dr. U. Langer
Vice Speaker: Prof.Dr.Dr.h.c. B. Buchberger
Office: Dr. M. Kuhn, A. Krennbauer

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

- numerical,
- symbolic, and
- graphical

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

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

The methodological coherence of the SFB can be summarized as follows: In the subprojects F1302 - F1305, new symbolic proving and solving algorithms for various domains of mathematics (integers, real number, complex numbers, general domains defined by functors) have been developed that can be used in connection with numerical methods for treating a benchmark class of direct and inverse problems described by partial differential equations with constraints, which is the subject of a second group of subprojects (F1306, F1308 - F1311). Refined graphical tools are used for the visualization and presentation of the results, which is one of the subjects of subproject F1301.

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

- on the interaction of the methods where this is relatively immediate (e.g. in the preprocessing and postprocessing phase of the application of numerical methods)
- on training the co-workers of the project coming from the symbolic and the numerical side to work closely together and build up a common language and expertise,
- on preparing the methods from symbolic computation (e.g. computer-support in formal proofs, algebraic constraint solving, algebraic analysis of PDE solvability) that should later be seamlessly integrated with the numerical analysis.

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

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

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

- Institute of Analysis and Computational Mathematics,
- Institute of Measurement Technology,
- Institute of Industrial Mathematics,
- Institute of Mechanics and Machine Design,
- Institute of Symbolic Computation,
- Institute of Technical Computer Science and Telematics.

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

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

or contact our office.

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Linz, March 2000 Ulrich Langer

F 1301: Service and Coordination Project

Prof. Dr. U. Langer
Dr. M. Kuhn, Dr. G. Haase
P. Furchtlehner, A. Krennbauer

The scientific part of Project F1301 is concerned with the coordination of scientific software and the graphical pre- and postprocessing. This includes in particular to provide new and to extend existing software concepts. In 1999, we concentrated on the further development of the numerical software package FEPP [6]. In particular, a parallel version of FEPP has been established and the coupling of finite and boundary element discretizations has been introduced.

1 Scientific Computing Tools

The applications considered within the SFB cover a wide range including problems from elasticity and electromagnetics. Most of these applications are based on common principles which can be implemented very efficiently using the advantages of C++. The aim of the development of scientific software is to provide modular tools which allow the fast implementation of new problem classes and new algorithms. In the current state, three tools are provided: the mesh generator NETGEN [5], the simulation code FEPP, and the visualization module VIPP. The close interaction of the modules is essential for the efficient processing of extremely large data sets. So the hierarchical data structures provided by the numerical schemes are used for real-time interactive visualization. The problem solving environment has been applied successfully to advanced problems arising, e.g., in magneto-statics [3]. Figure 1 shows the geometry of a transformer with iron core and 3 coils. The screenshot of the visualization modul VIPP of FEPP in Figure 8 shows the mesh generated by NETGEN. The field is described by $\mathrm{curl}(H) = J$, $\mathrm{div}(B) = 0$, $B = \mu H$ where H, B, J are the magnet field, magnetic induction and prescribed currents, respectively. The numerical model is based on the vector potential $B = \mathrm{curl}(u)$ and a discretization by edge elements. The uniqueness of u is recovered by weak gauging $\mathrm{div}(u) = 0$ resulting in a mixed formulation [3]. A modified, but exact, formulation is solved by multigrid methods.

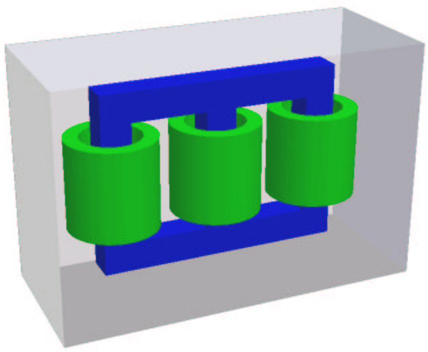

Figure 1: Geometry of the transformer.

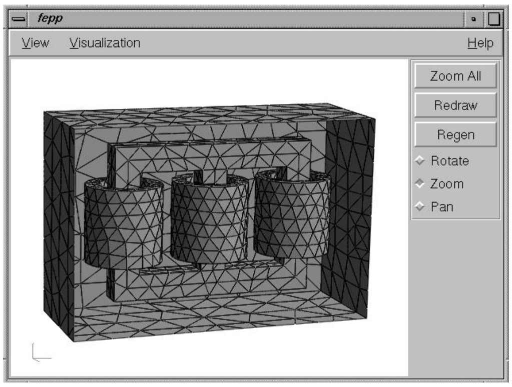

Figure 2: Screenshot: coarse mesh.

2 Parallelization

As mentioned before, FEPP tackles a wide range of problems arising in mathematical physics. Consequently, various numerical schemes have to be provided including Finite and Boundary Element Methods. All these differences cause different needs for the distribution of data as well as for the parallel generation and solution of the discrete systems. We have developed a unifying parallelization concept which minimizes those parts of the code which are specific for some strategy of parallelization, see [2]. Hereby, we observe that all the parallel techniques under consideration lead to one and the same parallel iterative algorithm applied to particular vector types which correspond to the kind of data distribution. Then the most essential operation of the parallel iteration is the type-conversion of such vectors. This conversion is hidden in the preconditioner or, more precisely, in the smoother if multigrid is used as preconditioner. The calculation of scalar products is the only remaining operation which has to be overloaded correctly. Moreover, the concepts of operator overloading and inheritance provided by C++ are exploited. The methods are especially designed for massively parallel computers and workstation clusters. They are based on algorithms described in the book by G. Haase [1]. The speedup which describes

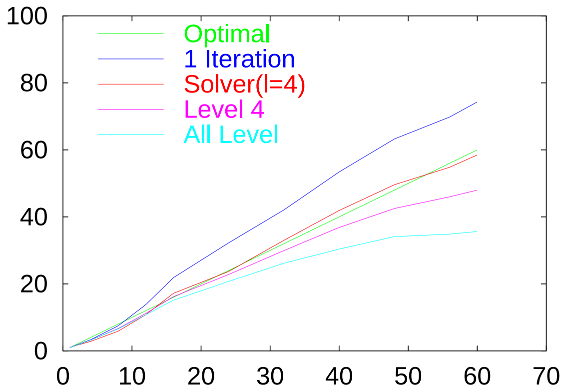

Figure 3: Speedup results for the transformer.

the gain of using several prcessors instead of one, is a measure for evaluating the efficiency of parallel algorithms. Figure 3 shows speedup results for the example from magneto-statics given above. We observe that the speedup for the overall time performs well until $P = 16$ and is no longer optimal for $P = 60$. This loss of efficiency is due to the setup phase for interface unknowns which shows rather bad scalability in the current implementation. Taking the speedup with respect to one iteration on the finest grid, we observe even super-speedups, e.g., a speedup of 74 for 60 processors. The total wall-clock time for solving the system with 1.691.370 unknowns was 54 seconds using 60 300MHz processors of a SGI ORIGIN 2000. Summarizing, we observe an optimal scalability of our iterative solver. In the case of outer iterations, e.g. for nonlinear problems, where the linear solver is called repeatedly on a fixed mesh, the time required for the setup phase can be neglected and the solver which shows optimal efficiencies will dominate.

3 FEM–BEM Coupling

Finite Element Methods (FEM) and Boundary Element Methods (BEM) are the most popular discretization techniques for the numerical solution of partial differential equations. Each method has its own advantages. So, non-linearities can be modelled more easily by FEM whereas exterior problems fit nicely into the framework of BEM since only the boundary has to be discretized. We have derived a formulation for 3D magneto-statics which is based on vector–valued FEM ($B = \mathrm{curl}(u)$) and scalar BEM ($H = \nabla\Phi$). In a joint work [4] with O. Steinbach, University of Stuttgart, the BEM has been implemented in FEPP. The coupled FEM–BEM discretization has been applied to a model of a permanent magnet. Figure 4 shows the resulting magnetic induction. Starting with 144 tetrahedra, 92 surface

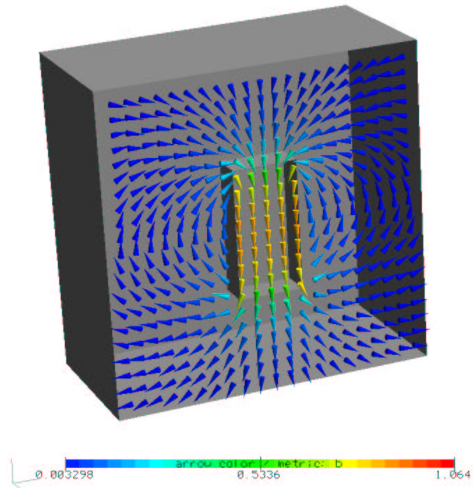

Figure 4: FEM–BEM solution.

elements and 48 nodes at the coupling boundary Γ_+ finer meshes are obtained by adaptive refinement resulting in 175529 tetrahedra, 1350 surface elements and 677 nodes on Γ_+. The overall CPU time on an 250Mhz SGI Octane was about 10 minutes. Hereby optimal preconditioners based on multigrid methods have been used yielding numbers of iterations independent of the number of unknowns. Coupled FEM–BEM discretizations will also be used in F1306 and F1308 for solving exterior magneto-mechanical problems and inverse scattering problems, respectively.

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F 1302: "Solving and Proving in General Domains"

Prof. Dr. B. Buchberger

Dr. Claudio Dupré, D.I. W. Windsteiger

Dr. T. Jebelean, F. Kriftner, D.I. K. Nakagawa, D.I. D. Vasaru

1 "Solving and Proving in General Domains"

The subproject, also called "*Theorema*", aims at integrating computation and deduction in a coherent software system that can be used by the working scientist for building and checking mathematical models, including the design and verification of new algorithms. Currently, the system uses the rewrite engine of the computer algebra system *Mathematica* for building and combining a number of automatic/interactive provers (high-order predicate-logic, induction for lists/tuples and natural numbers, etc.) in natural deduction style and in natural language presentation. These provers can be used for defining and proving properties of mathematical models and algorithms, while a specially provided "computing engine" can execute directly the logical description of these algorithms.

In the previous phases of the development of the system a number of provers were implemented and integrated with each-other and with a common user-interface. During last year, these components have been improved w.r.t: efficiency, scope of application, and user interface. Currently the system already allows to treat complex mathematical knowledge in *complete exploration cycles* - see [1] - both for proving and for computing. Also, new components have been designed and implemented, as well a new general proving strategy *PCS: Proving – Computing – Solving* see [2], the integration in the system of special provers (considered as "black-box" provers) and special simplifiers, the enhancing of existing provers via "failure analysis" and "cascade lemma generation" strategy and "depth simplification extension" strategy, and proof simplification, see [2]. All these new components are currently integrated in the system in a smooth manner, based on the same rewrite engine.

In the current state of the development cycle the following new features are implemented:

- The system provides facilities for composing and manipulating large mathematical text and for structuring, in a hierarchical way, large mathematical knowledge bases, the "Theorema Formal Text"; it provides also a "Command Language" in order to process (proving, computing or solving) knowledge.
- A more general Proving Strategy which integrates the three phases of mathematical activities, namely proving, computing and solving (PCS). This approach to proving is not limited to general predicate logic provers, but it can be easily extended to the design of special provers. These new provers are applied to analysis (see the Example in figure 5 which displays a proof generated completely automatically by *Theorema*) and set theory.
- In the system are now integrated Special provers like the Groebner-Basis Prover and the Gosper-Zeilberger Prover; the Groebner Basis method was invented by Buchberger and developed by Buchberger and his group at RISC.
- Tools for the integration with external simplifiers (QEPCAD, PolynomialSimplifier).
- Tools for enhancing existing provers by meta-strategies; in particular two strategies have been implemented: The "Cascade lemma generation" and the "Extended Simplifier". The Cascade strategy analyzes a failing proof of a proposition and tries to conjecture a lemma; the Cascade strategy is then recursively applied to a new proof situation which includes the new lemma until either a successful proof of the original proposition is found, or it fails and produces a list of the conjectured and proved lemmas. Failure Analyzer and Conjecture Generators have been implemented for natural numbers; experiments are done also with tuples. The "Extended Simplifier" strategy extends the simplifying power of a simplifier for a certain class of terms (defined by a set of function constants), to terms involving new function constants by recursively simplifying the subterms occurring inside a term whose outermost symbol is one of the new constants.
- Proof Simplification, realized by removing superfluous branches and superfluous steps from the proof objects generated by the provers, in particular the predicate logic prover. Certain deduction steps generate alternative branches of proofs; by simplification of a proof, only the branches which are effectively useful for the success are shown. During the search for a

proof, some formulae may be generated which finally are not necessary for proving the goal; by simplification the deduction steps producing these formulae are removed.

The *Theorema* system (as version 1.0) has been distributed to a selected number of users from the international research community which volunteered to beta-test the system: researchers from the European project INTAS 96-760 (Uppsala, Kiev, St.Petersburg) and from the CALCULEMUS consortium (UK, Germany, Italy, France, Netherlands) are evaluating the *Theorema* system. Currently there are 35 registered users of the system and their comments and suggestions are used for improving the system. Additionally, the beta testers and new volunteers have access to the newest version of the system on the Internet at `http://www.theorema.org`.

Moreover, the system is in use for teaching purposes:

- **Prof. Buchberger**
  Lectures on "Thinking Speaking Writing" by using *Theorema* as training tool, RISC, Hagenberg.

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

- **Unisoftwareplus**
  Planning to use *Theorema* for commercial educational software.

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Prove:

(l+) $\forall_{f,a,g,b} (\mathrm{limit}[f, a] \wedge \mathrm{limit}[g, b] \Rightarrow \mathrm{limit}[f+g, a+b])$,

under the assumptions:

(l) $\forall_{f,a} \left(\mathrm{limit}[f, a] \Leftrightarrow \forall_{\epsilon>0} \exists_{N} \forall_{n \geq N} (|f[n] - a| < \epsilon) \right)$,

(d+) $\forall_{x,y,z,t,\delta,\epsilon} (|(x+z) - (y+t)| < \delta + \epsilon \Leftarrow (|x-y| < \delta \wedge |z-t| < \epsilon))$,

(f+g) $\forall_{f,g,x} ((f+g)[x] = f[x] + g[x])$,

(max) $\forall_{m,M1,M2} (m \geq M1 \wedge m \geq M2 \Leftrightarrow m \geq \max[M1, M2])$.

We assume

(1) $\mathrm{limit}[f_0, a_0] \wedge \mathrm{limit}[g_0, b_0]$,

and show

(2) $\mathrm{limit}[f_0 + g_0, a_0 + b_0]$.

Formula (1.1), by (l) and by introducing a Skolem function, implies:

(4) $\forall_{\epsilon>0} \forall_{n \geq N_0[\epsilon]} (|f_0[n] - a_0| < \epsilon)$.

Similarly, formula (1.2) implies:

(6) $\forall_{\epsilon>0} \forall_{n \geq N_1[\epsilon]} (|g_0[n] - b_0| < \epsilon)$.

Formula (2), using (l), is implied by:

(7) $\forall_{\epsilon>0} \exists_{N} \forall_{n \geq N} (|(f_0 + g_0)[n] - (a_0 + b_0)| < \epsilon)$.

We assume $\epsilon_0 > 0$ and show

(9) $\exists_{N} \forall_{n \geq N} (|(f_0 + g_0)[n] - (a_0 + b_0)| < \epsilon_0)$.

We have to find $N_2^\star$, such that

(10) $\forall_{n \geq N_2^\star} (|(f_0 + g_0)[n] - (a_0 + b_0)| < \epsilon_0)$.

Formula (10), using (f+g), is implied by:

(11) $\forall_{n \geq N_2^\star} (|(f_0[n] + g_0[n]) - (a_0 + b_0)| < \epsilon_0)$.

Formula (11), using (d+), is implied by:

(12) $\exists_{\delta,\epsilon,\ \delta+\epsilon=\epsilon_0} \forall_{n \geq N_2^\star} (|f_0[n] - a_0| < \delta \wedge |g_0[n] - b_0| < \epsilon)$.

We have to find $\delta_0^\star$, $\epsilon_1^\star$, $N_2^\star$ such that

(13) $\forall_{n \geq N_2^\star} (|f_0[n] - a_0| < \delta_0^\star \wedge |g_0[n] - b_0| < \epsilon_1^\star) \bigwedge (\delta_0^\star + \epsilon_1^\star = \epsilon_0)$.

Formula (13), using (4) and (6), is implied by:

$\forall_{n \geq N_2^\star} (\delta_0^\star > 0 \wedge n \geq N_0[\delta_0^\star] \wedge \epsilon_1^\star > 0 \wedge n \geq N_1[\epsilon_1^\star]) \bigwedge (\delta_0^\star + \epsilon_1^\star = \epsilon_0)$,

which, using (max), is implied by:

(14) $\forall_{n \geq N_2^\star} (n \geq \max[N_0[\delta_0^\star], N_1[\epsilon_1^\star]] \wedge \delta_0^\star > 0 \wedge \epsilon_1^\star > 0) \bigwedge (\delta_0^\star + \epsilon_1^\star = \epsilon_0)$.

Formula (14) is implied by

(15) $\forall_{n \geq N_2^\star} (n \geq \max[N_0[\delta_0^\star], N_1[\epsilon_1^\star]]) \bigwedge (\delta_0^\star + \epsilon_1^\star = \epsilon_0) \bigwedge \delta_0^\star > 0 \bigwedge \epsilon_1^\star > 0$.

Summarizing, we reduced the proof to a solving problem. We have to find $\delta_0^\star$, $\epsilon_1^\star$, $N_2^\star$ such that (15) holds under the current knowledge. The solution of this problem is:

$0 < \delta_0^\star < \epsilon_0$,

$\epsilon_1^\star = \epsilon_0 - \delta_0^\star$,

$N_2^\star = \max[N_0[\delta_0^\star], N_1[\epsilon_1^\star]]$.

Figure 5: Example: Limit of Sum

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

Josef Schicho
Petru Pau, Stefan Ratschan, Mohamed Shalaby

1 Quantifier Elimination for Real Closed Fields

Many problems in mathematics, scientific, engineering and industrial applications can be reduced to the problem of quantifier elimination over real closed fields. One of the most important methods for algorithmic quantifier elimination is Collins' method of cylindrical algebraic decomposition (CAD) [1]. Several results have been obtained in connection with this method.

One of the main steps in the CAD algorithm, the so-called projection phase, is based on resultant techniques for multivariate polynomials. In the project, an effort was made to enrich these polynomials with some additional structure in order to speed up the algorithm. A prototype of this new method has been implemented by Antonin Tesacek [8]. Experiments have shown that one can indeed cut down the number of projected polynomials significantly.

On the other hand, Pau and Schicho [4] generalized the CAD method to the case of trigonometric functions, which occur often in applications in mechanical engineering and control theory. The idea is to use the well-known "tanhalf" transformation, transforming an angle to the tangent of its half. The main problem is to deal with the case where the tangent is infinity, in a systematic way that is compatible with the theory of cylindric algebraic decompositions.

2 Parametrization of Real Algebraic Surfaces

The need to eliminate variables in the presence of equational constraints leads to the problem of parametrization of algebraic varieties. The solution of this problem depends heavily on the dimension of the variety. For surfaces, partial results have already been obtained by Schicho [6]. Based on these results, Schicho considered "proper parametrizations" [7], where the parameters can be expressed by rational functions of the image point. The results were quite satisfactory: the proper parametrization problem for real algebraic surfaces was completely solved.

The most expensive subtask of the parametrization problem is the analysis of singularities. This can be done by Villamayor's algorithm, which was recently implemented by Bodnar and Schicho. Figure 26 shows a parametric surface with a double point of type $\mathbf{A}_2$.

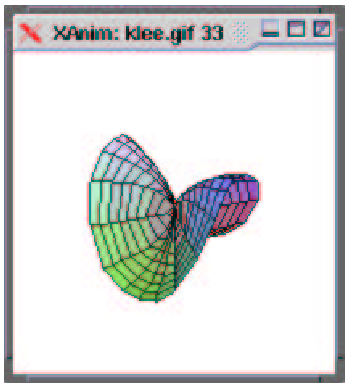

Figure 6: A Surface Singularity.

Another crucial step in the parametrization is to exhibit a pencil of rational curves. Any such pencil can be transformed to a pencil of conics. A special case occurs when the pencil of conics is not unique. For instance, the torus has precisely four such pencils: the rotating circle, the orbits of rotation, and two skew pencils. One of them is displayed in figure 7.

The research in the parametrization problem turned out to be useful for other SFB-projects, especially in the interproject group "Geometry", where applications to problems in CAD/CAM have been investigated [2].

3 Approximate Quantifiers

The theory of approximate quantifiers, which has been developed by Stefan Ratschan in his thesis [5] developed further. It captures now two possible sources of errors, namely an error of uncertainty and an error of irrelevance. This allows to model situations occuring in engineering and industrial applications more adequately. Logically, this distinction is described in terms of set-valued truth functions.

Ratschan also provided a constraint programming language and an implementation for these concepts.

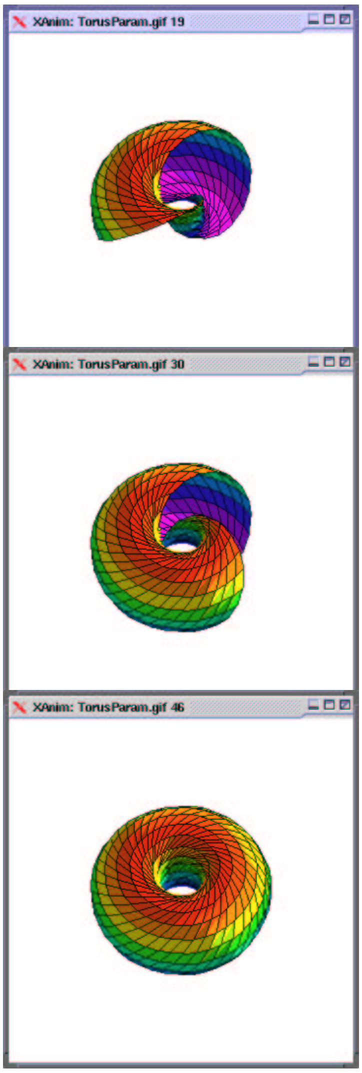

Figure 7: A Skew Pencil of Conics.

4 Numerical Solution of Inequality Constraints

As a case study for the sub-project "Exact Real Number Arithmetic", Kutsia and Schicho [3] devised and implemented an algorithm for the solution of inequality constraints which is purely based on numerical computation.

5 Exact Real Number Arithmetic

The traditional ways of representing numbers symbolically or numerically reach only a small subset of the reals. Many computations cannot be performed exactly within these subsets.

In exact real number arithmetic, real numbers are described by "generators" that can generate arbitrary many digits. Arithmetic is then realized as operations on these generators. This approach goes back to ideas of Brouwer and Bishop and has been suggested by various authors. Pau, Ratschan, and Schicho are currently working on the development of a Maple package for exact real number arithmetic which is especially dedicated to algebraic problems (polynomial factorization, variable elimination, solution of equations). This subproject resides in between symbolic and numerical computation, because one can use ideas from symbolic as well as numerical algorithms.

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

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

1 Results of the Project

In this second year of the project we have made progress in all the main project goals, i.e. in the symbolic parametrization of curves and surfaces, in the development of software for algebraic curves and surfaces, and in the symbolic solution of partial differential equations. A result in universal algebra was achieved in [HeLa99].

1.1 Parametrization of curves and surfaces

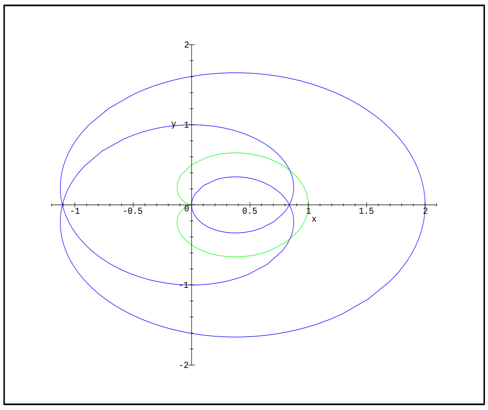

Figure 8: Chinacolcardioid.

Every real algebraic curve which is parametrizable over the complex numbers, is in fact also parame-trizable over the reals. We have investigated how such a real parametrization of a real algebraic curve can actually be determined. This problem seems to be completely solved now [SeWi99]. So, for instance, the cardioid curve (green) defined by

$$f(x,y) = -y^2 + 8x^2y^2 + 4y^4 - 4xy^2 + 4x^4 - 4x^3 = 0,$$

and also its offset curve (blue) with distance 1 can be parametrized with real coefficients. A parametrization of the offset curve is

$$x(t) = \frac{2(t^2-1)(3t^4+10t^2-1)}{(t^2+1)^4},$$

$$y(t) = \frac{2t(t^6-t^4-13t^2+5)}{(t^2+1)^4}.$$

Furthermore we have investigated the symbolic parametrization of pipe and canal surfaces. These are important objects in computer aided geometric design. The symbolic computation of formulas for parametrizations of these surfaces is now understood [HLSW99],[Land99].

Our achievements in this part of the project have been presented at various lectures at conferences and research institutions, compare [Wink99c], [Wink99d], [Wink99e]. They are also described in the overview paper [Wink99a].

1.2 The software system CASA

After having done a thorough analysis of the functionalities and the interrelations of various subpackages in our program system CASA (compare the report for 1998), we have started to implement the findings of this analysis.

All source files of CASA are now under revision control. The documentation does no longer exist in 3 different versions; the CASA help files for Maple as well as the LaTeX form of the functions documentation are generated from one source. The documentation has been converted to an automatically readable format; several Perl scripts have been written to support generation of online help and LaTeX format. A test suite has been added for each user function of CASA.

Soon we will have a new version (CASA 2.4.3), branching out to computation over fields of positive characteristic, applications in algebraic geometric coding theory, and parallel computation in curve plotting and singularity analysis.

Ralf Hemmecke has presented some of these new features in this talk [Hemm99].

1.3 Differential polynomials and symmetries of PDEs

The activity of Erik Hillgarter in the classification of symmetry groups of 2nd order PDEs has been continued [Hill99]. Many of these groups can now be treated algorithmically, and solutions can be determined.

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F 1305: "Symbolic Summation and Combinatorial Identities"

A.Univ.-Prof. Dr. Peter Paule

DI Dr. Axel Riese, Dr. Frederic Chyzak

DI Fabrizio Caruso, DI Carsten Schneider, Burkhard Zimmermann

1 Symbolic Summation and Combinatorial Identities

Scientific results have been achieved in various subareas of the field of interest. Despite the fact that these subareas overlap in several respects (theoretical background, techniques and tools, etc.), for the sake of better transparency of the presentation, the achievements are detailed in separate subsections.

1.1 Indefinite and definite summation

Over the last years the WZ method, in particular Zeilberger's algorithm, has been widely spread and successfully applied to problems involving definite hypergeometric sums. Concerning Mathematica implementations various packages developed at RISC (by Paule and Schorn, and by Riese) have become standard references. Now, within the frame of the SFB project, the first implementation in Macsyma has been carried out by F. Caruso. Macsyma Inc. is planning to incorporate the code into the standard Macsyma library.

Around 1980, M. Karr developed an algorithmic summation analogue (in the setting of suitable difference field extensions) to Risch-integration. Despite the fact that its domain of application potentially is very general (e.g., including harmonic numbers that arise in the analysis of algorithms), Karr's method has not achieved the attention it deserves. Now, within the SFB, C. Schneider developed a first Mathematica prototype that implements Karr's machinery in full generality.

In addition, Schneider succeeded to extend Karr's approach also to *definite* summation problems. To this end, he needed to extend linear difference equation solvers to very general domains. This enables to provide a new and sufficiently general algorithmic tool for attacking problems that lie beyond the scope of the methods available so far. For example, with Schneider's package one cannot only prove but also *find* the closed form evaluation of an identity recently used by Fulmek and Krattenthaler for counting tilings of a hexagon; namely, if $H_n := 1 + 1/2 + \cdots + 1/n$ denotes the n-th harmonic number then

$$\sum_{k=1}^{n} \frac{H_k\,(3+k+n)!\,(-1)^{k+n-1}}{(1+k)!\,(2+k)!\,(n-k)!} - \frac{n!}{(3+n)!} \sum_{k=1}^{n} \frac{(3+k+n)!\,(-1)^k\,(1-(2+n)\,(-1)^n)}{k\,(1+k)!^2\,(n-k)!} = (2+n)(-1)^n - 2.$$

1.2 MacMahon's Partition Analysis

In his famous book "Combinatory Analysis" (1916) MacMahon introduced partition analysis as a computational method for solving problems in connection with linear homogeneous diophantine inequalities and equations, respectively. For several decades this method has remained dormant. In recent SFB work, carried out jointly with G.E. Andrews (Penn State, USA), it has been demonstrated that partition analysis is ideally suited for being supplemented by modern computer algebra methods.

A Mathematica package `Omega` has been developed which can be used as a tool for solving problems with constraints in form of linear diophantine inequalities or equations, respectively. As worked out by Andrews and Paule, a variant of partition analysis can be applied also to hypergeometric multisum identities. Applications of `Omega` range from the preprocessing for automatic theorem proving to enumeration problems in statistical physics. For example, consider the generating function for solid partitions on the cube, namely $\sum q^{a_1+\cdots+a_8}$ where the sum runs over all nonnegative integers satisfying inequalities $a_i \geq a_j$ whenever an edge is directed from a_i to a_j on the corresponding cube (see Figure 1).

As pointed out by MacMahon it is extremely hard to compute the closed form expression by hand; now with the `Omega` package this is fully automated and a matter of seconds.

1.3 Additive number theory

The Rogers-Ramanujan identities belong to the most outstanding identities in additive numbers; the first

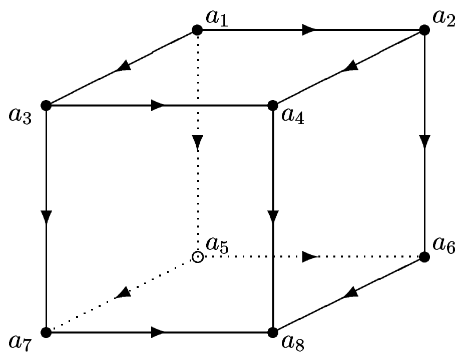

Figure 9: Solid partitions on the cube

one reads as:

$$1+\sum_{k\geq 1}\frac{q^{k^2}}{(1-q)(1-q^2)\cdots(1-q^k)}$$
$$=\prod_{n\geq 0}\frac{1}{(1-q^{5n+1})(1-q^{5n+4})}.$$

In the literature one finds many variations, variants and generalizations; around 1980 some of these formulae found important applications in statistical mechanics, e.g., within the context of R. Baxter's hard hexagon model.

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

In recent years, A. and J. Knopfmacher derived an algorithm, the Extended Engel Expansion, that leads to unique series expansions of Rogers-Ramanujan type if starting from the product side. Various examples related to classical partition theorems, including the Rogers-Ramanujan identities, have been given recently. In joint work with G.E. Andrews and A. Knopfmacher it has been shown that the new and elegant Rogers-Ramanujan generalization found by Garrett, Ismail, and Stanton also fits into this framework. This not only reveals the existence of an infinite, parameterized family of extended Engel expansions, but also provides an alternative proof of the Garrett, Ismail, and Stanton result. A finite version of it, which finds an elementary proof, can be derived as a by-product of the Engel approach.

This achievement can be viewed as the starting point of further investigations, for instance, of the question whether the Extended Engel Expansion can be turned into a proving machinery.

1.4 Holonomic approximation

Holonomic functions form the theoretical basis for many algorithmic investigations in the field. In a co-operation with I. Gutman, a chemist from the university of Kragujevac, this concept in the univariate case has been utilized to predict the number of hexagonal systems consisting of 24 and 25 hexagons with 6 and 5 significant digits, respectively. Informally speaking, a hexagonal system can be viewed as a connected arrangement of hexagonal cells packed in the same way as the typical honeycomb arrangement in a beehive.

After embedding the problem into a suitable setting the prediction has been produced within a few seconds using computer algebra packages such as `gfun` in Maple or `GeneratingFunctions` in Mathematica; the latter has been developed at RISC by C. Mallinger. Remarkably the exact number of hexagonal systems consisting of 23 hexagons, the biggest number that has been computed so far, required 2.4 *years* of CPU time.

1.5 Symbolic methods for wavelet construction

Wavelets are one of the most popular tools in signal- and image processing. These functions are widely used in many practical applications such as data compression, or for the solution of partial differential equations. Wavelets are special functions which often have a fractal character. This makes it relatively difficult to work with them explicitly; for example, point evaluation of a wavelet function may already be a computationally expensive task. To work with wavelets one uses the nice feature that they are defined by a small number of parameters, the so-called filter coefficients. In general, any algorithm relying on wavelets only uses the filter coefficients and not the wavelet function itself.

In cooperation with O. Scherzer and A. Schoisswohl, the project group F1305 carried out a detailed study of the basic equations for the filter equations. In particular, it turned out that Gröbner bases methods enable to compute closed form representations of the wavelet coefficients. To this end a more economic description of the algebraic variety defined by $2N+1$ Daubechies equations in $2N$ unknowns have been found; namely, in terms of N algebraic equations in N unknowns. Remarkably, various combinatorial identities play an important role in this process. One expects that this approach extends to the construction of new wavelets of more general type.

References

The exact references for the papers referred to in this report are to find via the corresponding link on the SFB homepage.

F 1306: Coupled Field Problems: Advanced Numerical Methods and Application to Nonlinear Magnetomechanical Systems

Prof. Dr. U. Langer, Prof. Dr. R. Lerch
DI S. Reitzinger, DI M. Schinnerl, DI J. Schöberl
Dr. G. Haase, Dr. M. Kaltenbacher

This project benefits from the participation of researchers with different scientific background. Modern numerical methods as adaptive multigrid methods have been brought together with challenging applications involving different physical fields.

1 Numerical Methods for 3D Magneto-Mechanical Systems

The physics of magneto-mechanical systems is described by instationary partial differential equations. The Maxwell equations for the magnetic field in the low frequency range reads as

$$\nabla \times (\frac{1}{\mu}\nabla \times \vec{A}) + \gamma\frac{\partial \vec{A}}{\partial t} - \gamma\vec{v} \times (\nabla \times \vec{A}) = \vec{J_e} - \gamma\nabla\Phi. \qquad (1)$$

Here, $\vec{A}$ denotes the magnetic vector potential, μ the magnetic permeability, γ the electric conductivity, $\vec{v}$ the velocity, $\vec{J_e}$ a given current density and Φ an electric potential.

The Lamé equations for a linear isotropic material give a relation between the mechanical displacement $\vec{d}$ and acting forces:

$$\frac{E}{2(1+\nu)}\left((\nabla\cdot\nabla)\vec{d} + \frac{1}{1-2\nu}\nabla(\nabla\cdot\vec{d})\right) + \rho\frac{\partial^2 \vec{d}}{\partial^2 t} = \vec{f_V}. \qquad (2)$$

In (2) $\vec{f_V}$ denotes the volume force, E the Young's modulus, ν the Poisson ratio and ρ the specific density of the material.

Both equations are coupled by several terms, namely the electromotive force, the Lorentz force and variations of the magnetic field caused by mechanical deformations, see [6].

The discretization of the weak forms of (1) and (2) is done by the finite element (FE) method. While standard nodal value elements are used for the mechanical field, edge elements have to be used for the approximation of the magnetic field. The mechanical field is of interest only in the solid parts of the system, but the magnetic field is present also in the surrounding air. Due to different physical effects and the arising smoothness properties (mechanical waves, magnetic boundary layers) also different mesh sizes are used for both fields.

The arising ordinary differential equations are solved by time stepping methods. In each time step the non-linear coupling terms are taken into account. Due to the stiffness implicit schemes leading to a sequence of large scale linear systems of equations are required. For their efficient solution multigrid (MG) methods are required. To obtain good performance and robustness with respect to geometry and parameters several multigrid components have been designed and adapted [5], [4].

2 Application: Magnetically Excited Plate

To verify the developed calculation scheme and to show its advantages compared to standard approaches, the structure in Fig. 25 is considered. It

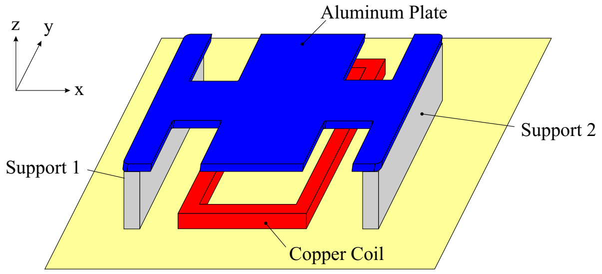

Figure 10: Principal setup of the magnetically excited aluminum plate

consists of an aluminum plate above a copper coil. If a transient electric current flows in the coil, a magnetic field is produced, which induces eddy currents in the plate. The Lorentz force resulting thereof, generates a mechanical displacement $\vec{d}$, which additionally influences the behavior of the plate by electromotive force.

2.1 Numerical Simulation

The transient behavior of the plate is now simulated by the developed MG tool and for comparison with a standard approach. Since the coil is loaded by a capacitor discharge which causes a very strong deformation of the aluminum plate, the displacement of the plate must be considered in the simulation process. The MG simulation model consisted of a magnetic FE mesh with 356,587 edges and a mechanical mesh of 26,580 degrees of freedom. The accumulated calculation time for the necessary 400 time steps was 14 hours on an SGI ORIGIN 300 MHz within the multigrid fe package FEPP. The simulation by means of a conventional unigrid solver needed 137 hours.

2.2 Simulation Results

In order to verify the developed scheme, the simulated results were compared to measurements obtained by a piezoelectric acceleration sensor. The measured and simulated displacement d_z in the center of the plate is displayed in Fig. 11. A very good

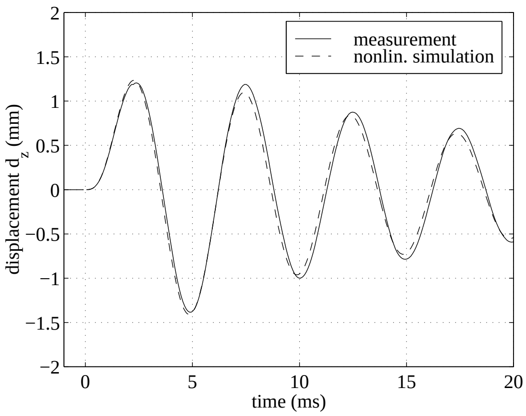

Figure 11: Displacement d_z in the center of the aluminum plate

agreement between numerical simulation and measurement can be observed.

3 Mesh Generation

The development on the automatic mesh generator NETGEN developed by J. Schöberl has been continued. A view highlights are meshing possibilities for thin structures, preprocessing capabilities for coupled field problems and interfaces to available CAD tools, see [http:\\www.sfb013.uni-linz.ac.at\ ~joachim\netgen].

4 Algebraic Multigrid

One of the key issues in this project is the development of Algebraic Multigrid (AMG) solvers. Our motivation is to provide fast solvers for unigrid codes as well as to have fast solvers for problems on complicated geometries with a rather fine coarse-grid, or problems where geometric multigrid fails (e.g. non-aligned anisotropies). S. Reitzinger develops the AMG package PEBBLES meeting these goals, see [http:\\www.sfb013.uni-linz.ac.at\ ~reitz\pebbles.html].

On discretizations with anisotropic elements (e.g. for resolving thin geometries, edge singularities or boundary layers) the M-matrix property gets lost. These causes essential difficulties for standard AMG methods based on the assembled stiffness matrix. For these problems the element preconditioning method has been developed [3].

The AMG code PEBBLES was incorporated into the coupled field finite element code CAPA and used therein as a solver. A lot of real life problems in 2D and 3D have been tested. One coupled field example was a transient simulation of a loudspeaker. Here, the magnetic part (which geometry additionally changes in time) was solved with AMG (see [1]). The overall computation time could be reduced tremendously. Besides 3D nonlinear electrostatic and magnetostatic field problems were under consideration in [2].

Recent developments in the AMG package was the extension to matrix equations arising from systems of partial differential equations (as Lamé equation). A new approach was developed for 3D magnetic field problems, where the underlying discretization is done by edge elements. The parallelization of AMG is in progress together with project F1301.

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F 1308: Large Scale Inverse Problems

Prof. Dr. Heinz W. Engl
Dr. Thorsten Hohage
Dr. Barbara Kaltenbacher

1 Newton-type methods in inverse scattering

Our aim is to solve 3D inverse scattering problems, which consist in reconstructing a scatterer using measurement data of scattered waves. Such problems arise in medical imaging, geophysical explorations, and nondestructive testing. The scatterer may either be an impenetrable obstacle or a local inhomogeneity in the refractive index.

To solve inverse scattering problems, we apply iterative regularization techniques, in particular regularized Newton methods. These methods require several direct problems to be solved in each iteration step. In our case this is already a quite demanding and time consuming task due to the large size of the direct problems. However, as long as the reconstructions of the unknown scatterer are poor, it does not make sense to waste a lot of computer time to highly accurate solutions of the direct problems. Based on our convergence and convergence rate analysis of regularized Newton methods we have developed theoretical results on 'optimal' coupling of direct solvers and the outer Newton iteration (cf. [1, 2]). These results have been tested on 2D inverse obstacle scattering problems. We observed a reduction of the total computation time roughly by a factor 3 in this case. Moreover, we have extensively tested and compared various kinds of iterative regularization methods on these problems (cf. Fig. 12). Since we have made good progress with the implementation of direct inhomogeneous medium problems using FEM/BEM coupling in cooperation with Project F1306, we expect to be able to solve *inverse* 2D and 3D inhomogeneous medium scattering problems in the next future.

2 Solving ill-posed problems by multigrid methods

Finite-dimensional problems are always well-posed in the sense of stable dependence of a solution on the data, although they may be ill-conditioned. Therefore, discretization itself can be considered as a regularization method. After investigating the stabilizing effect of projecting a possibly nonlinear ill-posed equation onto a finite-dimensional space — e.g. a finite element space (cf. [4]), we considered the efficient solution of the resulting finite-dimensional linear and nonlinear systems of equations by multigrid methods. Here the ill-posedness of the underlying infinite-dimensional problems affects the singular system structure. As a consequence the use of conventional pre- and post-smoothers such as Gauss-Seidel iterations lose their smoothing effect: as opposed to well-posed problems (such as elliptic PDEs or second kind integral equations), small singular values typically correspond to high-frequency eigenfunctions. An alternative smoothing operator that turns out to be appropriate for systems of equations arising from finite-dimensional projection of ill-posed problems, was proposed by King (1991) and further investigated within the present project (cf. [3]). Under certain conditions we could show that the resulting multigrid operator with W- or alternating cycle has a level-independent contraction number and therefore yields an efficient preconditioner for the fast iterative solution of the class of systems of linear equations under consideration. A further possible application of this multigrid operator is to use it in a full multigrid method, together with an appropriate choice of the finest grid level in dependence of the data noise level. It was shown within the present project (cf. [3]), that this yields a regularization method for the original ill-posed problem, i.e., a stable approximation method for its solution, which is convergent as the data noise goes to zero.

As a test example we chose the one-dimensional linearized version of a parameter identification problem in groundwater filtration, where one wants to determine the distributed filtration coefficient from pointwise measurements of the piezometric head. The performance of the proposed method turns out to be quite satisfactory. Whereas the condition number of the resulting system matrix grows rapidly with the dimension of the discretization space, the condition number of the multigrid-preconditioned matrix grows slowly (cf. Figure 13). The total CPU time needed for the solution of the equation system is significantly smaller for the multigrid preconditioned conjugate gradient method than for standard methods such as a direct solver or the diagonally preconditioned conjugate gradient method (cf. Figure 14).

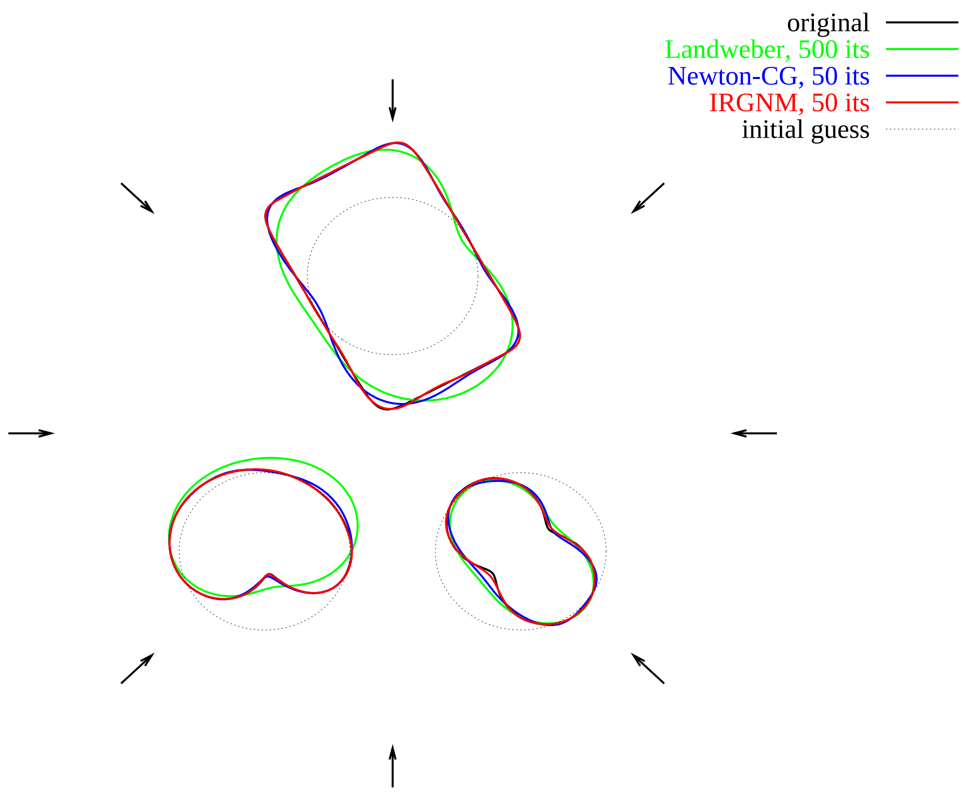

Figure 12: Comparison of iterative regularization methods in inverse scattering

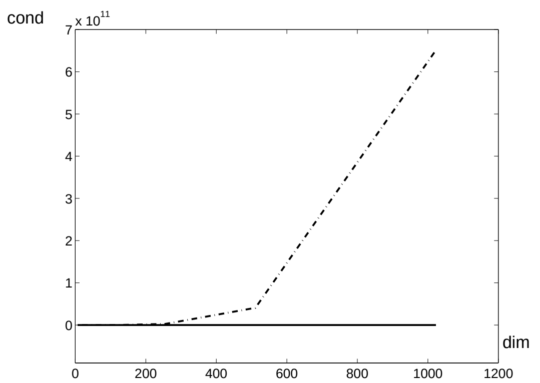

Figure 13: Condition numbers of multigrid preconditioned (solid line) and unpreconditioned (dash-dotted line) system matrix

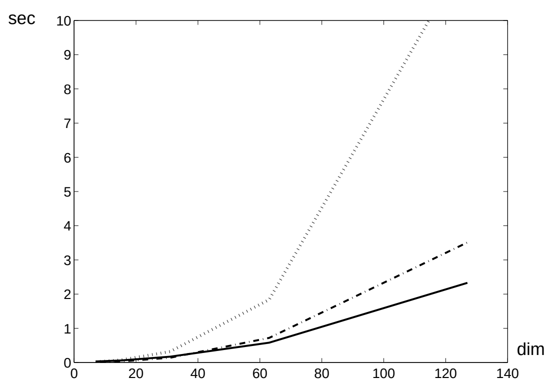

Figure 14: CPU time for multigrid preconditioned CG (solid line), diagonnally preconditioned CG (dash-dotted line) and direct solver (dotted line)

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F 1309: Hierarchical Methods for Simulation and Optimal Design and Applications to Magnetic Field Problems

Prof. Dr. Ulrich Langer, Dr. Ewald Lindner

Dr. Gundolf Haase, Wolfram Mühlhuber

1 Optimal Sizing

In many industrial applications the design of a machine or of mechanical structures has to fulfill various constraints. In most cases even an optimal design with respect to several restrictions is wanted. These requirements are mainly induced directly by requirements of the individual buyer or indirectly by competition on the world market. Unfortunately due to lack of time the engineers designing a machine component have to stop their design process after a few iterations – in most cases only two or three – and take the best design obtained so far because no more time is left for drafts that would possibly meet the requirements to a larger extent.

Tools supporting such a design process have to fulfill mainly two goals:

- They have to be flexible enough to get rid of the various requirements. Nevertheless they also have to be robust to produce reliable results. Especially, it is desirable to spend only little work when the requirements change.
- On the other hand these tools have to be fast. The faster the tool, the more design drafts can be optimized.

In the beginning we focussed our research activities on geometric modeling and multilevel optimal shape design algorithms applied to industrial machine components [2]. Recently we have concentrated on *Optimal Sizing Problems*, the simplest problems in shape optimization. Here the design parameter is the distribution of a quantity over a constant cross section. Our model example is the optimization of a frame for which the thickness is the design parameter. There, the mass of the frame shall be minimized taking into account that the stresses in the frame shall not exceed a certain limit. The thickness distribution is approximated by a piecewise constant function e.g. constant on each finite element of

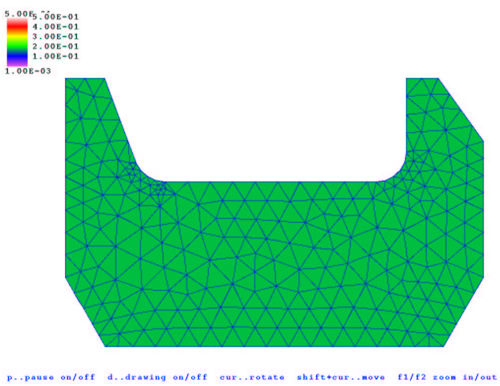

Figure 15: Initial thickness distribution

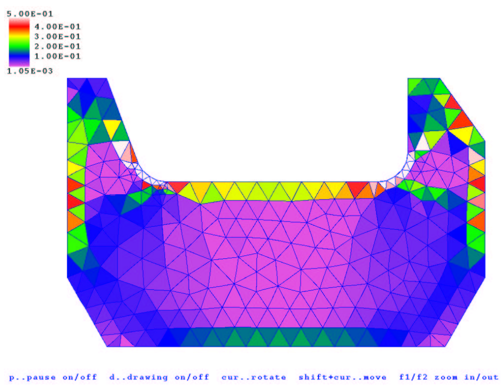

Figure 17: Optimized thickness distribution

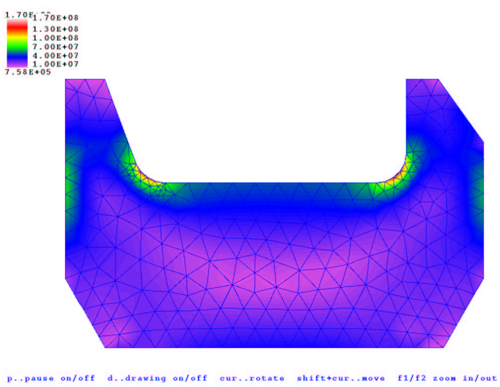

Figure 16: Van Mises stresses, initial configuration

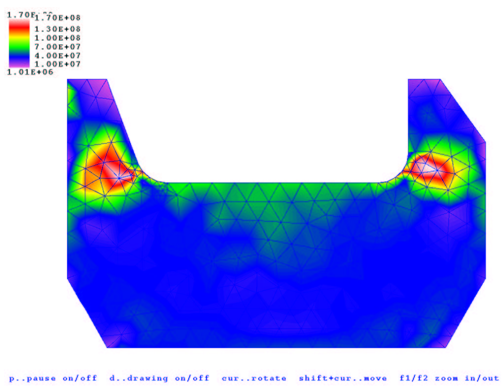

Figure 18: Van Mises stresses, optimized config.

the coarsest grid.

Optimal sizing problems can be formulated as nonlinear optimization problems with constraints includeing PDE constraints. The most typical aspect is the appearance of a state equation, in our case describing the deformation of the frame under load. This state equation can also be interpreted as equality constraints for the optimization problem. Therefore, the solution of the state equation can be eliminated in a formal way which leads to an equivalent optimization problem which is easier manageable by standard optimization procedures. In this transformed optimization problem only the design parameters appear but no more the solution of the state equation.

For solving this transformed optimization problem standard optimization routines can be used, e.g. *Sequential Quadratic Programming* as in our code. This method needs function and gradient evaluations of the objective and the constraints, the need for Hessian information is avoided by using Quasi-Newton update formulas.

The current implementation of our optimizer is based on dense matrix linear algebra and therefore, only well suited for small to medium size optimization problems. But in order to close the gap to topology optimization which is of high practical importance, new optimization methods for large scale problems have to be developed.

2 Calculation of Gradients

The currently used optimization routine is based on an SQP method using a Quasi-Newton update formula for estimating the Hessian of the objective. Therefore, only evaluations of the objective and the constraints and their gradients are required. As these functions may become very complicated, the implementation of analytic derivatives is more or less impossible. Furthermore it would be not well suited for the use in a design process, as one would then loose the flexibility of the code completely.

Four different strategies for calculating gradients have been investigated:

- The use of *Finite Differences* is for most people the first method they think of for getting an approximation to the gradient. In a critical way these depend on the choice of the increment used. In order to increase the stability extrapolation methods for controlling the step length were combined with a finite difference scheme. This works fine, but the computational effort is very high, especially for a large number of design parameters (see also [2]).

- *Automatic Differentiation* (cf. [1]) follows a completely different approach. Here, the starting point is a computer program that calculates numerical values for a function. First a symbolic evaluation graph mapping the design parameters to the functional value is built. Like symbolic differentiation, AD operates on this evaluation graph by systematic application of the chain rule, familiar from elementary differential calculus. However, in the case of AD, the chain rule is applied not to symbolic expressions, but to actual numerical values, which avoids the exponential growth of the evaluation complexity of symbolic differentiation. This approach works fine also for many design parameters, as the computational effort for the gradient is independent of the number of design parameters, but it requires huge memory and disk capabilities for storing the evaluation graph.

- Both previously mentioned methods are black box methods to some extent and do not take into account the special structure of the problem. But this is done by the *Adjoint Method* known from shape optimization. Here, one gets many partial derivatives by solving only one adjoint problem. Unfortunately, one may have to handle and implement huge expressions for the remaining partial derivatives which makes this approach only useful for rather simple functions. More complicated objectives require symbolic methods.

- In order to make the adjoint method more flexible and also better usable for complex objectives, we combined it with automatic differentiation. This new method brings the strengths of both approaches together and results in an *Hybrid Method* which calculates many partial derivatives by solving one adjoint problem and the remaining ones by using automatic differentiation. It also reduces the large memory and disk requirements of automatic differentiation severely. The computational effort for calculating the gradient is comparable to three function evaluations, independent of the number of design parameters.

In the future the hybrid method shall be generalized from optimal sizing problem to shape optimization problems which have an even more complex structure of the objective.

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F 1310: Estimation of Discontinuous Parameters in Differential Equations

Walter Hinterberger, Esther Radmoser, Luca Rondi, Otmar Scherzer, Armin Schoisswohl

1 Denoising of Images

Esther Radmoser, Otmar Scherzer (Institut für Industriemathematik), Joachim Weickert (Lehrstuhl für Bildverarbeitung, Univ. Mannheim)

One of the most active fields of research in modern image analysis is modeling and application of partial differential equations. For image processing we have developed connections between regularization theory and partial differential equations [14, 12, 13]. These coherence allow to exchange ideas from different mathematical areas. A joint paper of E. Radmoser, O. Scherzer, J. Weickert [12] (University of Mannheim, Germany), presented at the Scale Space Conference' 99, was selected for an extended version in a special issue of the ten most important contribution to this conference [13].

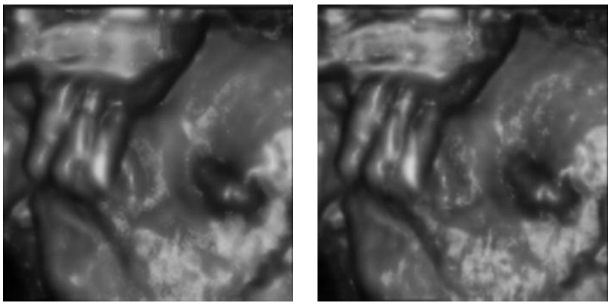

Figure 19: 3D Ultrasound data (left),denoised (right)

The expertise obtained in this part of the project is transferable to many problems in inverse problems.

2 Recovery of discontinuous conductivities: a variational approach

Luca Rondi (Institut für Industriemathematik)

We propose a variational approach for the *inverse problem* of impedance tomography with discontinuous conductivities. The problem is highly unstable. To stabilize the computations of the conductivity we propose a new technique that originates from image segmentation. This is joint work with Fadil Santosa (University of Minessota, USA).

3 Optical Flow and Image Interpolation

Walter Hinterberger, Otmar Scherzer (Institut für Industriemathematik)

Optical flow is the motion field in a video sequence. It is used for video compression as well as in computer vision. The knowlege of the motion helps to reduce the amount of data and thus is useful for compressing video sequences.

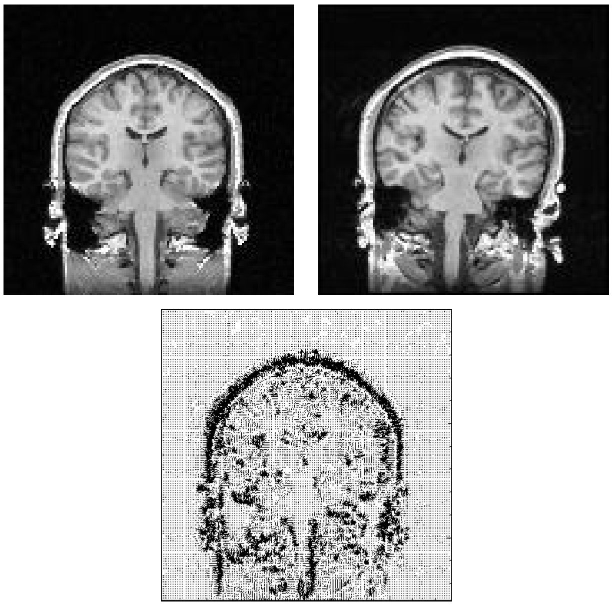

Figure 20: Slices of MR data of two different brains (top) and the optical flow field (bottom).

We use the optical flow for image interpolation, to generate visually attractive video sequences between two given images. Problems of this type occur when the image acquisition is slow or expensive. We developed appropriate interpolation models based on systems of partial differential equations [10].

4 Construction of wavelets using computer algebra methods

Frédéric Chyzak (INRIA Rocquencourt, France), Peter Paule, Burkhart Zimmermann (RISC), Otmar Scherzer, Armin

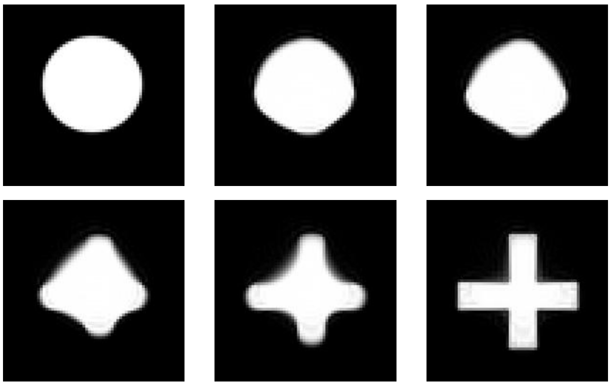

Figure 21: Interpolated sequence between a circle and a cross.

Schoisswohl (Institut für Industriemathematik)

Many problems in signal and image processing and in partial differential equations can be handled efficiently with wavelet-functions.

Wavelets are typically defined by a small number of coefficients. We are concerned with the symbolic calculation of the coefficients of the *Daubechies wavelets* on the real line [7, 8, 3]. The constitutive equations for the filter coefficients can be transformed into an algebraic system that can be solved symbolically using Gröbner basis elimination.

Starting from the analytically known filter coefficients for the wavelets on the real line we developed a matrix analytical approach for the construction of (bi)orthogonal wavelets on intervals that puts the constructions in the literature [4, 11, 5, 6] in a unified framework. Our approach can be implemented with computer algebra methods, thus avoiding numerical instabilities in usual implementations.

A paper describing this work has been accepted for publication in *Experimental Mathematics* (cf. [2]).

5 Inverse Problems

Moreover, there have been successful collaborations within the group of Prof. Engl (Project 1308). We mention the publications Burger and Scherzer [1] and Engl and Scherzer [9].

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F 1311: "Structural Dynamics of Elasto-Plastic Multi-Body Systems: Integrated Symbolic and Numerical Computations"

H. Irschik

J. Gerstmayr, W. Brunner, A.K. Belyaev

H. Holl, U. Pichler

1 Virtual Virials

The project started in October 1998.
Since we intend to develop a unified approach for problems of multi-body dynamics and of nonlinear continuum mechanics, a preliminary study has been performed with respect to the material description of the nonlinear field theories of mechanics. Referring to an undistorted reference configuration, a generalization of the principle of virtual work and of the Betti reciprocal theorem has been developed, first for static problems. In this study, performed by H. Irschik and A. K. Belyaev, Finger's virial has been introduced into a tensorial formulation utilizing Da Silva's astatic tensors of deformable bodies. The virial theorem then has been extended to a formulation termed the Principle of Virtual Virials. In order to obtain a better understanding of the foundations of the structural theories to be implemented in the multi-body system, the Principle of Virtual Virials has been used to derive beam type equations of motion from the three-dimensional field equations without using any approximation. The virial formulation presently is extended to kinetic equations, and its connections to inelastic problems are studied.

2 Elastic-Inelastic Analogy

We include plasticity into the multi-body system by means of an analogy between plastic strains and thermal expansion strains. In order to consider geometric nonlinearities, we developed an extension of Maysel's formula of thermoelasticity to the nonlinear material description mentioned above. In these studies, performed by W. Brunner, J. Gerstmayr, H.J. Holl, H. Irschik, U. Pichler, we made use of the previously developed generalisation of the Principle of Virtual Virial. Both, isotropic and anisotropic bodies have been studied, and thermally loaded beams with a v. Kármán type of nonlinearity have been considered as example problems. As a further result of these considerations, we performed a symbolic and numerical computational study on bifurcation and jump phenomena in thermally loaded beams.

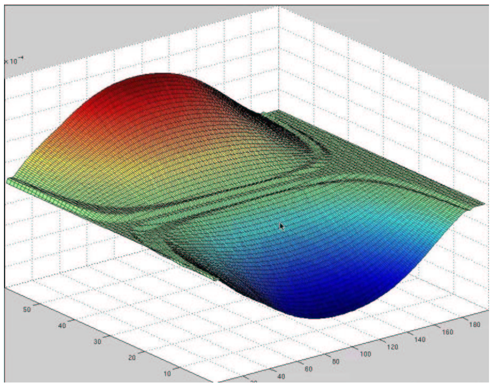

Figure 22: Visualisation of the Plastic Zones in the Pendulum.

3 Elasto-Plastic Pendulum

In the next step of our investigations, such structural elements have been subjected to large rigid body movements, additionally to their deformation from the undistorted reference configuration. We used the elasto-plastic pendulum with distributed mass and stiffness as a benchmark problem. A shadow reference configuration has been considered, co-rotating with the pendulum and oriented towards the tip of the pendulum. Only small deformations or second-order nonlinearities then need to be introduced for practical purposes. Within this formulation, a non-linear system of differential-algebraic equations (DAE) has been derived by the above Principle of Virtual Virials for the case of a beam-type pendulum. Linear eigenfunctions have been used first as virtual deflections. Special emphasis has been given to the convergence of the solution by splitting a quasi-static drift and enforcing also dynamic boundary conditions to be solved exactly. This turned out to be of special importance for an accurate calculation of stresses and plastic parts of strain. The latter act as driving sources (in the sense of the above mentioned thermal analogy) and enter the system of DAEs for the flexible and rigid-body co-ordinates as disturbances, to be calculated from the non-linear constitutive equations of plasticity. In these investigations performed by J. Gerstmayr, H. Irschik, A.K. Belyaev and H. Holl, we first studied the case of a crank-slider-type pendulum with a guided rigid-body motion. Additionally to plasticity, we introduced ductile damage in order to study low-cycle fatigue and rupture in the machine element. We then extended the formulation to the case of an elasto-plastic pendulum which is released from rest and is driven by its own weight, the stiffness and yield stress being weakened by a high-temperature environment. The rigid-body rotation of the pendulum now represents an additional generalized coordinate of the problem. It extends the system of ordinary differential equations for the flexible coordinates to a system of DAEs. An implicit scheme, based on a Runge-Kutta method and including the iterative calculation of plastic sources, has been developed and successfully applied. It turned out that in our formulation only a low number of generalized coordinates is necessary to obtain an accurate result for the time-varying distribution of stresses and plastic zones. It is emphasized that this advanced problem of dynamic plasticity has not been studied in the open literature so far. In order to obtain comparative results, W. Brunner and J. Gerstmayr therefore extended an algorithm for rigid multi-body systems with respect to elasto-plastic massless springs. A large amount of rigid elements is necessary to model the elasto-plastic pendulum, and a high numerical effort has to be used in this formulation. Nevertheless, the results of the above formulation could be well reproduced by the latter method, which also represents a genuine formulation of our group.

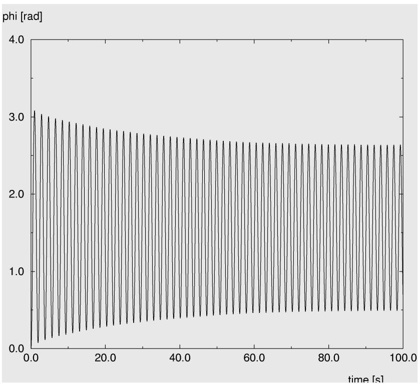

Figure 23: Decay of Vibrations due to Plasticity.

4 Multi-Body Systems

In our present investigations, we recently succeeded to extend the system of DAEs for the elasto-plastic pendulum to a multi-body system made of elasto-plastic beam type elements. In this formulation, the flexible beams are connected by rigid or hinge-type joints. The system of nonlinear DAEs is automatically generated from the single beam-equations and transformed into a system of nonlinear equations, with the use of some optional implicit time integration formula. These equations are suitable to our self-developed Modified-Newton-Algorithm. Additionally some control algorithms are implemented for an active damping of the vibrations of the elasto-plastic multi-body system. So far, our formulation is restricted to systems moving in a single plane. We are just now studying improvements of the formulation, e.g. by using Hermitian polynoms instead of eigenfunctions, thus omitting the numerically tedious splitting of the quasi-static parts.

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SFB F013: Numerical and Symbolic Scientific Computing

Cooperation within the SFB

1 Project F1301

The work within the Project F1301 was concerned with the further enhancement of parallel solvers and their implementation in the FE package FEPP. The Projects F1306, F1308, F1308 which require fast direct field solvers will benifit from these developments.

Furthermore, the implementation of the Boundary Element Methods offers new perspectives for the discretization of field problems. In particular exterior field problems can be treated very efficiently using boundary elements or coupled finite element – boundary element discretizations. In particular the Projects F1306 and F1308 will benefit from this development. Together with F1308, inverse scattering problems will be considered which give rise to problems on unbounded domains.

2 Project F1302

Cooperation with the Project F1305 (symbolic summation and combinatoric identities): In several meetings were identified specific proof techniques and computation methods which are now fully integrated in the *Theorema* software system in relation to the treatment of the domains of natural numbers. In particular, the implementation of the Gosper-Zeilberger Summation Algorithm (Project F1305) is now integrated in the *Theorema* software system, and, in cooperation with the other components of the system, are already capable to produce reasoning about summation formulae.

Cooperation with the Project F1303 (proving and solving over reals) and with the Project F1306 (advanced numerical methods): A set of problems about the characterization of multidimensional system of equations using quantifier elimination in real closed fields and proving/computing by rewriting were chosen. An experimental link between the *Theorema* system and the Quantifier Elimination via Partial Cylindrical Algebraic Decomposition (QEPCAD) Algorithm has been realized and it is currently under a test phase. Cooperation with Project F1308 (large scale inverse problems): We started to develop coherent and formally consistent text in the *Theorema* system for the mathematical foundations of the methods used by this subproject. The contents follows the models used in the "Lecture notes on partial differential equations" (Prof. Engl).

3 Project F1303

Multigrid methods and domain decomposition algorithms are of major importance in the solution of large scale numerical field problems. The analysis of convergence involves Hilbert space techniques. It is interesting to observe that many existing proofs in this theory can be given in a formalization of the theory of Hilbert spaces, using only a small number of axioms.

For a particular class of subspace correction methods, Schicho and Schöberl reduced the convergence analysis to a quantifier elimination problem over the theory of real closed fields. This problem was indeed tractable with existing software (QEPCAD, which was written by H. Hong). Thus, the convergence rate could be deduced in a semi-automatic way. This was done in the interproject working group "Computer Supported Proving".

The determination of a general symbolic solution of an equational constraint—which has been studied intensively in project 1303—is equivalent to the problem of parametrization of algebraic varieties, which is studied in the subproject 1304. Applications to problems in CAD/CAM have been investigated in the interproject working group "Geometry".

As one of the most promising activities of the project 1303, Ratschan, Schicho, and Pau started to devise and implement algorithms for algebraic problems in the frame of exact real number arithmetic. This is a computational model of the reals, where a number is represented by a "generator" which can produce arbitrary many digits. It turned out that we could utilize ideas from symbolic as well as from numerical algorithms for the solution of various problems.

4 Project F1304

The main activity for advancing the coherence of the SFB was the organization of the workshop SNSC'99. Prof. Winkler has organized the SFB-Workshop on "Symbolic and Numerical Scientific Computation" (SNSC'99), August 18–20, 1999, in Hagenberg.

In this workshop renowned scientists presented their views of the interaction of symbolic and numerical computation for the solution of scientific problems, namely Chandrajit Bajaj (University of Texas, Austin TX, USA), Keith O. Geddes (University of Waterloo, Kanada), Vladimir Gerdt (Joint Institute for Nuclear Research, Dubna, Russland), Erich Kaltofen (North Carolina State University, Raleigh NC, USA), Anders Lennartson (Königliche Technische Hochschule, Stockholm, Schweden), Fritz Schwarz (Gesellschaft für Mathematik und Datenverarbeitung, Bonn/St.Augustin, Deutschland), Wenda Wu (Beijing Municipal Computing Center, Beijing, China) and Franz Ziegler (Technische Universität Wien).

In addition to these overview lectures, researchers from the SFB and also from other institutions presented talks on their new results.

60 scientists participated in SNSC'99. The abstracts of the talks are collected in [Wink99b].

5 Project F1305

Many of the results achieved with respect to summation methods are directly related to Project F1302 "Proving and Solving in General Domains". For example, the Paule/Schorn package (an extended version of Zeilberger's algorithm implemented in Mathematica) has already been incorporated as a prover and solver into the Theorema package.

F. Caruso's PhD work, namely the study of possible combinations of numeric and symbolic approaches to solving linear systems of equations over multivariate rational functions is globally related to the numerics groups of the SFB.

Significant collaboration (a first joint paper meanwhile has been accepted by Experimental Mathematics) has been carried out between O. Scherzer (project F1310) and his student A. Schoisswohl, and the group of Paule (F. Chyzak and B. Zimmermann; the latter will be employed by the SFB after completing his diploma thesis in spring 2000). Namely, as described in the general presentation of the 1999 results, it turned out that certain parameters that are needed for the construction of wavelets can be computed in a purely symbolic fashion. This enables to generalize wavelet construction mechanisms; further developments involving also the group of U. Langer (project F1306) are envisioned.

Another aspect that reflects the coherence within the SFB is the "Special Function Interest Group" (leader: Paule). For instance, the four lectures on holonomic functions given by F. Chyzak were attended by SFB workers from different projects such as F1302, F1304, F1305, F1306, F1308, F1309, F1310, and F1311.

6 Project F1306

The cooperations with Project F1301 and Project F1309 are naturally strong and include numerical analysis as well as implementation of finite element software.

A joint goal with **project 3** is the development of automatic proving techniques for problems in Hilbert spaces as occur in the analysis of multigrid and domain decomposition methods. The key idea is to reduce the variational problem in the infinite dimensional Hilbert space to a space of small, fixed dimension where quantifier elimination algorithms developed in project 3 are applicable. We have already recovered the theorem estimating the convergence rate of the multiplicative Schwarz method involving two subspaces.

Successful joint research with **project 8** is the design and analysis of a mixed variational formulations for the inverse problem of parameter identification. A technique for analyzing the total error consisting of the data error, regularization error and the finite element discretization error with low order elements was developed. Numerical experiments has been carried out within the finite element package FEPP.

For a nonlinear problem arising from image recovering a multigrid algorithm was developed together with **project 10**. It was implemented into the package FEPP.

The relation to **project 11** is based on one hand side on the formulation and discretization of nonlinear problems arising in computational mechanics. On the other hand side, we strongly work together on the development of the finite element mesh generation code NETGEN which is used in several projects.

7 Project F1308

Continuing our cooperation with project F1306 we use a reformulation of the projection-regularized Newton method for the inverse groundwater filtration problem in two dimensions as a mixed variational problem, which allowed us to achieve a significant reduction of the requirements on the discretization (cf. [2]). Some first numerical experiments with the finite element package FEPP confirm our theoretical results.

Further progress was also made in implementing a coupled FEM/BEM method within FEPP. This will be used as a direct solver for the inverse inhomogeneous medium scattering problem.

In another cooperation with project F1306 we considered a nonlinear inverse problem for the heat equation, namely the problem of finding a cooling function to be applied to the boundary of some body (e.g., some steel billet) such that a prescribed temperature distribution is achieved inside the body (e.g., for fulfilling certain quality requirements in steel making). An implementation of a regularized Newton method for this inverse problem in the finite element package CAPA yielded quite interesting results (cf. [1]).

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8 Project F1309

The intensive cooperation with the Projects F1301 and F1306 concerning the development of FEPP was continued. This led to a native integration of the routines needed for the optimization into our finite element code. Also the cooperation with the Projects F1303 and F1304 concerning the handling of constrained geometry was continued.

9 Project F1310

Cooperations with Prof. Peter Paule (Project 1305: Symbolic Summation and Combinatorial Identities) and Prof. Heinz Engl (Project 1308: Large Scale Inverse Problems). Both cooperations led to joint publications.

10 Project F1311

In order to numerically solve the differential algebraic equations (DAEs) which are gained from the field equations of a flexible multibody system, expert-knowledge has been transfered from projects F1306 and F1309. The introduction of p-version finite elements into the existing formulation has been discussed with J. Schöberl (project F1306) and was sucessfully implemented.
The existing automatic 3D mesh-generator NETGEN (written by J. Schöberl) was extended in cowork by J. Gerstmayr and J. Schöberl with an interface to STL-format files, which opens the possibility to use more complex models in the FE calculations, and has various interfaces to CAM programs like Pro-Engineer and ABAQUS. Objects simply described by surface-triangles (STL-format), not useable for a FE calculation but easily gained from 3D-primitives, can be handled by the mesh-generator. A modeller for this STL-format objects is in development, which could be used to test the 3D-FE programs of different projects. With the use of these tools, we will be able to extend the existing multibody system code to a three dimensional formulation.

Coherence within the SFB

- **Visualization Library:**
  Any project using the field simualtion of FEPP can make use of the visualization library developed by G. Kurka in Project F1301. These are, in particular, Projects F1306 and F1309.

- **Parallelization Library:**
  Any project using the field simualtion of FEPP can make use of parallel implementations of the algorithms developed by M. Kuhn in Project F1301. These are, in particular, Projects F1306, F1308 and F1309.

- **Theorema Software:**
  At the SFB–Workshop in Strobl all the SFB groups had the possibility to inspect the functionality of the *Theorema* software in live interactive presentations on the computer and to discuss various ways of interaction with the other sub-groups. The main conclusion was that the software will evolve into a version which should be useful for the current work of the mathematicians from the other disciplines in order to investigate mathematical models (e.g. by automating parts of the proofs, by direct execution of algorithm specifications, and by providing an intelligent environment for creating mathematica texts). Moreover, the work in this subproject will be directed towards analysing and integrating the proof techniques specific to the models which are currently used by the other subgroups: natural numbers, sets, real numbers, algebraic domains.

  Additionally, several meetings were organized with the participation of only few groups, in order to facilitate a proper focus on the concrete research cooperation opportunities:

  - Meetings with Project F1305: We identified several proof techniques and computation methods which will be integrated in the *Theorema* software in relation to the treatment of the domains of natural numbers. Currently our induction provers are already capable to produce reasoning about simple summation formulae.
  - Meetings with Project F1303 and F1306: We selected a set of problems about the characterization of multidimensional system of equations using quantifier elimination in real closed fields and proving/computing by rewriting.

- **Proving Techniques:**
  In project 1306, multigrid methods and domain decomposition methods are considered. The convergency analysis requires Hilbert space techniques. It was observed that many existing proofs in this theory can be given by a formalization of the theory of Hilbert spaces using only small number of axioms. In some cases, one can further reduce to a problem in the theory of real closed fields, which is investigated in project 1303. Using software developed by the proposer of the project, we could in one particular example automatically produce the precise convergency rate.

  Actually, quantifier elimination techniques have been used in the analysis of numerical algorithms in other contexts. We want to continue this joint approach in order to find more such applications.

- **Geometry:**
  Initiated by Project F1304, a discussion on geometric problems has started with other Projects (F1306, F1309). In particular we are discussing topologically correct numerical traces of curves, so-called α-shapes of curves, and also transformation problems in constructive solid geometry.

- **Construction of Wavelets:**
  About half of the results achieved with respect to summation methods in Project F1305 are directly related to Project F1302 "Proving and Solving in General Domains". F. Caruso's work, namely the study of possible combinations of numeric and symbolic approaches to solving linear systems of equations over multivariate rational functions is globally related to the numerics groups of the SFB. - Substantial collaboration (see SFB-Report 99–14) was carried out between O. Scherzer (Project F1310) and his student A. Schoisswohl, and the group of Paule. Namely, it turned out that certain parameters that are needed for the construction of wavelets can be computed in a purely symbolic fashion. This enables to generalize wavelet construction mechanisms; further developments involving also the group of

U. Langer (Project F1301 and F1306) are envisioned.

- **Inhomogeneous Medium Problem:**
In cooperation between Project F1301, F1306 and F1308, we are working on the inhomogeneous medium problem. The direct problem and its derivative will be implemented using a FEM-BEM coupling (in 2 and later in 3 space dimensions). To effectively compute the solution for many directions of the incident wave, we plan to investigate an extrapolation method.

- **Parameter Identification Problem:**
Currently the projection regularized Newton method for the parameter identification problem is being implemented in the finite element package FEPP in a cooperation between Projects F1306 and F1308. To this end several algorithmic aspects have been considered, especially the solution of the the finite-dimensional linearized problem $P_{Y_n}F'(a_n)s_n = P_{Y_n}(u^\delta - F(a_n))$ in each Newton step. Here the question of the choice of the ansatz functions for s_n is of major relevance. The theory suggests the use of basis functions that lie in the range of $F'(a_n)^*$ and are therefore quite smooth (H^3, in our example). It turned out (and could also be theoretically supported) that the reformulation of the Newton step equation as a mixed variational equation makes it possible to release these smoothness conditions so that hat functions can be used to approximate s_n.

- **Handling of Constraints:**
In a cooperation between the projects F1303, F1304 and F1309 a concept for parameterizing geometrical shapes was developed. This approach is based on recording the generation steps. Each primitive operation has several parameters. How the individual primitives are related to each other is included using constraints. Using symbolic methods, it is possible to eliminate constraints and reduce the number of parameters considerably.

  There are, however, good reasons not to realize this approach within the SFB. First, there are already similar implementations available in modern CAD systems. Second, a new implementation must not use the existing software because these are proprietary and quite expensive. Third, one would have to write a layer of a CAD-system from the scratch, which is a big effort. Finally, the problem which arose in F1309 and motivated this approach could be solved by ad hoc methods. Thus, we decided to retain from a realization of this approach after a thorough investigation.

- **Bounded Variation Regularization:**
Cooperation between F1310 and J. Schöberl from Project 1306: Development of analytical results for bounded variation regularization in a multi-grid setting.

- **Blind Deconvolution:**
Cooperation between F1310 and M. Burger from project F1308: Analysis of regularization methods for blind deconvolution and blind separation problems arising in image and signal processing. Convergence analysis of the alternating minimization method for the iterative solution of the regularized problems, and development of a network-based discretization method using ideas from Project F1308.

- **Symbolic Summation and Combinatorial Identities:**
Cooperation between F1310 and P. Paule from Project F1305.

SFB F013: Numerical and Symbolic Scientific Computing

National and International Cooperations

1 Cooperations with other Research Institutions

- **University of Stuttgart:** Dr. O. Steinbach has an expertice in the field of Boundary Element Methods. As a result of the cooperation, Boundary Element discretizations have been implemented in the package FEPP (see Project F1301).

- **University of Chemnitz (SFB 393):** The SFB F013 has strong cooperations with the SFB 393 "Numerische Simulation auf massiv parallelen Rechnern" at the University of Chemnitz, especially to the research groups of Prof. A. Meyer, Dr. M. Jung, Dr. T. Apel, Prof. R. Schneider, Prof. B. Heinrich.

  So the cooperation with Prof. R. Schneider will be intensified. The aim of this cooperation is the development of advanced Finite Element – Boundary Element solvers based on wavelet discretizations for integral operators.

  Doz. Thomas Apel (Univ. Chemnitz) and Dr. J. Schöberl work together on mixed finite element methods on anisotropic meshes. A joint paper (with Prof. S. Nicaise) is submitted.

- **University of Kentucky (Lexington, USA):** There are a close cooperation on parallelization issues between Prof. C. Douglas (Lexingtion) and the working group of Prof.U. Langer. Dr. G. Haase and Prof. U. Langer visited the University of Lexington in September 1999, and, together with Prof. C. Douglas, they have been working on a joint book project about parallel algorithms (F1301).

- **Lawrence Livermore National Laboratory (Livermore, USA):** Prof. U. Langer and Dr. G. Haase (F1301, F1306) spent one week at the LLNL and worked with P. Vassilevski and his colleagues on algebraic multigrid methods, parallelization techniques and scientific computing tools.

- **SFB F011 "AURORA" (Vienna):** There are a cooperation on parallelization issues between Prof. Überhuber (TU Vienna) and the working group of Prof.U. Langer.

- **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).

- **The CALCULEMUS Consortium**
  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. 3 Rome Italy, Univ. Saarbrücken Germany, INRIA Lorrain France. The consortium organizes yearly a scientific meeting - see [?], and last year applied successfully for an European TMR research network and for a grant from the European Science Foundation.

- **The INTAS Consortium 96-760**
  Consists of a net of Universities and Research Institutes with the common goal of integrating rewrite techniques and efficient theorem proving: RISC-Linz, Univ. Uppsala, Univ. Kiev, Glushkov Institute of Cybernetics Kiev, Steklov Institute of Mathematics St.Petersburg.

- **University of Vienna**
  Cooperation with the working group of Prof. Mathias Baaz on analysis and simplification of automatically generated proofs.

- **University of North Carolina:** Prof. H. Hong (Univ. North Carolina) and J. Schicho (F1303) have been working together on problem of quantifier elimination and on the generalization of resultants. Dr. J. Schicho visited the University of North Carolina in April 1999.

- **University of Passau:** In the winter term 99/2000, Prof. Volker Weispfenning (Univ. Passau) and J. Schicho (F1303) organized a joint seminar on computer algebra and quantifier elimination, taking place in Passau and in Hagenberg. The participants are: Prof. Volker Weispfenning (Univ. Passau), Dr.

Isolde Mazucco (Univ. Passau), Hirokazu Anai (Univ. Passau), Andreas Dolzmann (Univ. Passau), Thomas Sturm (Univ. Passau), Dr. J. Schicho (SFB 1303), Dr. Stefan Ratschan (SFB 1303), Petru Pau (SFB 1303), Mohamed Shalaby (SFB 1303).

- **Genova and Leipzig:** Ralf Hemmecke traveled to Genova and Leipzig for discussing involutive bases with Robbiano, Sturmfels, and Apel.
- **GMD in Bonn:** Erik Hillgarter spent a few days at GMD in Bonn and worked with Schwarz on the symmetry analysis of pdes.
- **Madrid:** Franz Winkler continued his joint work with Sendra (Madrid) on the parametrization problem.
- **University of Witwatersrand:** Following an invitation of Prof. Arnold Knopfmacher, Prof. Paule was visiting researcher from 1.–24.3.99 at the "Centre for Applicable Analysis and Number Theory", University of Witwatersrand, Johannesburg, South Africa. A joint paper, described in the annual report 1999, was produced.
- **University of Erlangen-Nürnberg:** From October 1999 to February 2000 Prof. V. Strehl visited the group of Prof. Paule for a sabbatical. Despite the fact that his visit was sponsored by the Auslandsbüro of the J. Kepler University, several topics relevant to the SFB work have been investigated. Detailed results will be reported in the annual report 2000.
- **Technical University of Vienna:** Ao. Prof. Helmut Böhm (TU Vienna), Dr. J. Schöberl (F1306) and Dipl.-Ing. H. Gerstmayr (F1311) work together on Finite Element Mesh Generation for Microstructures.
- **Christian Albrechts University Kiel:** Prof. Carsten Carstensen (University Kiel) and Dr. J. Schöberl (F1306) work together on a posteriori error estimates for plate problems. A joint paper is in preparation.
- **University Innsbruck/Technical University Tampere:** Prof. Rolf Stenberg (University Innsbruck) and Dr. J. Schöberl (F1306) (F1306) work together on multigrid methods for plate problems. A joint paper is in preparation.
- **Technical University of Dresden:** Prof. Dr. A. Griewank and Olaf Vogel worked together with Wolfram Mühlhuber (F1309) on the efficient use of AD for optimal sizing problems. Both visited the group of Prof. Langer in June 1999 and gave a 3 weeks course on AD. Wolfram Mühlhuber visited the Technical University of Dresden in November 1999.
- **University of Mannheim:** W. Hinterberger (F1310), J. Weickert (Univ. Mannheim), and O. Scherzer (F1310) have been working on optical flow problems.

  Dipl.-Ing. E. Radmoser (F1310), J. Weickert (Univ. Mannheim), and O. Scherzer (F1310) worked on coherences between regularization methods and diffusion filtering in image processing.

2 Guests

- **Prof. Dr. John WHITEMAN,**
  Brunel University of West London, 13.01. - 14.01.1999, Talk on "Adaptive finite element methods for problems of viscoelastic solid deformation, with applications to polymer processing".
- **Prof. Dr. Craig C. DOUGLAS,**
  University of Kentucky, 29.01. - 01.02.1999, Discussion on Parallelization.
- **Dr. Olaf STEINBACH,**
  Universitt Stuttgart, 12.03. - 24.03.1999, Talks on "BEM fr Randwertprobleme mit nichtlinearen Randbedingungen", "A posteriori Fehlerschtzer fr direkte Randelementmethoden".
- **Prof. Dr. Dietrich BRAESS,**
  Universitt Bochum, 22.03. - 26.03.1999, Talk on "Ein Mehrgitterverfahren fr Mortar-Elemente".
- **Prof. BERHUBER,**
  Dipl. Ing. GANSTERER,
  Dipl. Ing. HAUNSCHMID,
  Universitt Wien, 22.03.99, Seminar on Parallelization.
- **Dipl. Ing. Pavel SOLIN,**
  Universitt Prag, 19.04. - 24.04.1999, Talk on "On the Finite Volume Semi-Discretization of Compressible Euler Equations".
- **Prof. Dr. Hans-Georg ROOS,**
  Universitt Dresden, 7.06. - 11.06.1999, Talk on "Grenzschichtangepate Gitter: Charakterisierung, gleichmige Fehlerabschtzungen, Superkonvergenz"
- **Prof. Dr. Rolf STENBERG,**
  Universitt Innsbruck, 19.05. - 22.05.1999, Talk on "Stabilized finite element methods for Reissner-Mindlin Plates".

- **Prof. Sergej NEPOMNYASCHIKH,**
TU Chemnitz, 09.08. - 15.08.1999.

- **Dr. Ralf HIPTMAIR,**
Universitt Tbingen, 21.09. - 22.09.1999, Talk on "Diskretisierung der Maxwell Gleichungen"

- **Dipl. Ing. Pavel SOLIN,**
Universitt Prag, 01.10. - 31.10.1999, Visualisation for instationary field computations.

- **Dr. Maxim A OLSHANSKII,**
Moscov State University, 04.10. - 18.10.1999, Talk on "A Preconditioned Iterative Technique for the Linearized Incompressible Navier-Stokes Problem".

- **Prof. Carsten CARSTENSEN,**
Universitt Kiel, 21.10. - 22.10.1999, 11.12. - 12.12.1999, Cooperations on error estimators.

- **Prof. Dr. Markus GROSS,**
ETH Zrich, 30.11. - 02.12.1999, Talk on "Modellierungsmethoden in der Chirugiesimulation".

- **Prof. Mathias Baaz**,
University of Vienna, March 24, 1999, Prof. Baaz gave the talk "Logical Tools for the Analysis of Proofs" within the weekly "Theorema Seminars", RISC, Hagenberg.

- **N. Preining**,
University of Vienna, March 24, 1999, Preining gave the talk "Sketches as Proofs" within the weekly "Theorema Seminars", RISC, Hagenberg.

- **Dr. G. Moser**,
University of Vienna, March 24, 1999, Dr. Moser gave the talk "Cut Elimination" within the weekly "Theorema Seminars", RISC, Hagenberg.

- **Prof. J. Millan and Dr. G. Millan**,
University of Caracas, Venezuela. Visit from June to Aug. 1999, using *Theorema* for representing mathematical models for linear control systems.

- **D.I. Mijail Borges-Quintana**,
University of Havana, Cuba, from May 6 to June 24, 1999 and from October 5, 1999 to September 30, 2000, D.I. Borges is PhD student in Cuba and he participates in the *Theorema* project with the purpose of formalizing mathematical models for integer programming.

- **Prof. Doina Tatar**,
University of Cluj, Romania, from May 18 to May 24, 1999, Predicate logic proving (resolution, semantic tableaux).

- **Prof. Alexander Letichevsky**,
Glushkov Inst. of Cybernetics, Kiev, Ukraine, from September 22 to September 24, 1999, Rewrite based predicate proving, natural deduction.

- **Vladimir Orevkov**,
Steklov Inst. of Mathematics, St.Petersburg, Russia, from November 21 to November 23, 1999, Complexity of predicate logic proving (esp. sequent calculus).

- **Dr. Boris Konev**,
Steklov Inst. of Mathematics, St.Petersburg, Russia, from May to June 1999, Predicate logic proving (meta-variables).

- **Dipl.-Ing. Talal Salame:** University Bonn, 14.1. - 16.1.1999. Dipl.-Ing. Talal Salame visited Dr. Josef Schicho and applied for a position.

- **Prof. Hoon Hong:** University of North Carolina, 15.3. - 17.3.1999. Prof. Hoon Hong discussed with Dr. J. Schicho (1303) about generalizations of results.

- **Prof. Jaime Gutierrez:** University of Cantabria, 23.9. - 30.9.1999. Prof. Jaime Gutierrez and J. Schicho (1303) worked together on the problem of algebraic simplification of sine-cosine equations. Prof. Jaime Gutierrez also gave a talk on this topic.

- **Dr. Thomas Breuer:** Universität Aachen, 10.10. - 13.10.1999. Dr. Thomas Breuer applied for a position. He gave a talk on the Computeralgebra-System GAP.

- **Prof. Rob Corless:** University of Western Ontario, 16.10. - 20.10.1999. Prof. Rob Corless gave a talk on symbolic-numeric algorithms for polynomials.

- **Dr. I. Kotsireas:** University of Western Ontario, 27.11. - 30.11.1999. Dr. I. Kotsireas and J. Schicho worked together on a problem of celestial mechanics. Dr. I. Kotsireas also gave a talk on a numerical algorithm for multivariate factorization.

- **R. Liska:** (Technical University of Prague, symbolic/ numerical computation in finite difference modelling in fluid flows),

- **H. Pottmann :** (Technical University of Vienna, computer-oriented geometry),

- **M. Borges:** (Universidad de Oriente, Cuba, Gröbner basis techniques in coding theory),

- **F. Pauer:** (Universität Innsbruck, Gröbner bases in rings of differential operators),

- **Z. Li :** (GMD Bonn, rational solutions of Riccati-like pdes).
- **Dr. F. Chyzak:** INRIA-Paris, 20.11.–4.12.99. After the period of SFB work (October 1998–February 1999) Dr. Chyzak visited Prof. Paule's group in order to continue joint research. It is planned to intensify the contacts to Dr. Chyzak's home institution, the "Algorithms" group at INRIA-Paris (Prof. Ph. Flajolet and Prof. B. Salvy).
- **Prof. M.Z. Nashed:** (University of Delaware) 8.6. – 18.6.1999
- **Dr. L. Rondi:** (University of Trieste) 9.6. – 10.6.1999
- **Dr. J. Weickert:** (University of Mannheim) 2.3. – 4.3.1999
- **Dr. A.K. Belyaev:** State Technical University of St. Petersburg, 7.3.1999 - 15.3.1999 and 16.11.1999 - 1.12.1999. Dr. A.K. Belyaev gave a talk on "Thermodynamic Rationale for Heat Conduction Equation and Dynamic Boundary Value Problem for Piezothermoelastic Materials" and gave special courses on "Modellbildung in der Mechatronik" and on "Dynamik Komplexer Konstruktionen".

3 Lectures at other Universities

- **Dr. J. Schicho:** Lecture on "Exact Real Number Arithmetic" given at the University of Innsbruck, 22.11.99.
- **Prof. Buchberger**
Lectures on "*Theorema*: A New Kind of Mathematical System", given at the University of Timisoara, Romania, April 14, 1999.
- **Prof. Buchberger**
Lectures on "Groebner Bases: Theory and Applications", given at the University of Timisoara, Romania, April 16, 1999.
- **Prof. Buchberger**
Lectures on "*Theorema*: A New Kind of Mathematical System", given at the University of Cluj-Napoca, Romania, April 19, 1999.
- **Prof. Buchberger**
Lectures on "Can Computer Replace Mathematicians?", given at the Symposium "Symbolic Computation", TU Wien, April 28, 1999.
- **Prof. Buchberger**
Lectures on "*Theorema*: A New Kind of Mathematical System", given at the University of Debrecen, Hungary, May 20, 1999.
- **Prof. Buchberger**
Lectures on "Groebner Basen: Die ersten Jahren", given at the Colloquium "100. Geburtstag von Wolfgang Groebner", Universitaet Innsbruck, May 28, 1999.
- **Prof. Buchberger**
Lectures on "*Theorema*: A Progress Report", given at the GMD Bonn, Institut fuer Algorithmen, Bonn, Germany, June 15, 1999.
- **Prof. Buchberger**
Lectures on "Moeglichkeiten und Grenzen mathematischer Modellierung", given at the Sommerakademie der Pro Scientia ueber "Modell und Wirklichkeit", Tainach, Kaernten, September 2, 1999.
- **Prof. Buchberger**
Lectures on "Mathematik am Computer: Die Naechste Ueberforderung?", given at the Lehrerfortbildungsseminar bei der ÖMG-Tagung, Graz, September 24, 1999.
- **Prof. Buchberger**
Lectures on "Mathematik: Altes Eisen oder Schluesseltechnologie?", given at the Fortbildungsseminar fuer "European Women in Management", Hagenberg, October 6, 1999.
- **Prof. Buchberger**
Lectures on "*Theorema*: A System for Supporting Mathematical Proving", given at the North Carolina State University, Department of Mathematics, USA, October 22, 1999.
- **Prof. Buchberger**
Lectures on "*Theorema*: A System for Supporting Mathematical Proving", given at the University of Illinois at Urbana-Champaign, Department of Mathematics, USA, October 22, 1999.
- **Prof. Buchberger**
Lectures on The "*Theorema* Project: The Current State", given at the Mathematica Developer's Conference, Wolfram Research International, Urbana-Champaign, USA, October 23, 1999.
- **Prof. Buchberger**
Lectures on "*Theorema* A System for Supporting Mathematical Proving", given at the Canergie Mellon University, Department of Mathematics, Pittsburgh, USA, October 22, 1999.
- **Prof. Buchberger**
Lectures on "Computer-Mathematik in der Schule", given at the Schulung fuer AHS-Lehrer (6 Stunden), RISC, Hagenberg, December 13, 1999.

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

- **M. Kuhn** "Parallel Iterative Solvers based on Distributed Data", Talk at the Fachgebiet Theorie Elektromagnetischer Felder, University Darmstadt, June, 1999.

- **M. Kuhn** "Parallel Iterative Solvers for 3D Magnetic Field Problems", Talk at the Oberseminar Numerik, University Stuttgart, November 1999.

- **M. Kuhn** "Highly Efficient Parallel Iterative Solvers based on Distributed Data", Talk at the University of Tübingen, November 1999.

- **M. Kuhn** "Parallel Iterative Solvers for 3D Magnetic Field Problems", Talk at the MPI Leipzig, December 7, 1999.

- **M. Kuhn** "Coupling of FEM and BEM for 3D Magnetic Field Problems", Talk at the University of Chemnitz, December 10, 1999.

- **Dr. G. Haase, Prof. U. Langer:** Lecture on "Scientific Computing Tools for 3D Magnetomechanical Field Problems" given at the Lawrence Livermore National Laboratory, Livermore, USA, September 7, 1999.

- **Dr. G. Haase, Prof. U. Langer:** Lecture on "Scientific Computing Tools for 3D Magnetomechanical Field Problems" given at the University of Kentucky, Lexington, USA, September 15, 1999.

- **Prof. U. Langer:** Lecture on "Mathematische Werkzeuge des Wissenschaftlichen Rechnens" given at the Max-Planck-institute for Mathematics in the Sciences, Leipzig, Germany, January 12, 1999.

- **Prof. U. Langer:** Lecture on "Mathematische Werkzeuge des Wissenschaftlichen Rechnens" given at the University of Salzburg, Austria, January 18, 1999.

- **Prof. U. Langer:** Lecture on "Parallele numerische Verfahren für stationäre Magnetfeldprobleme" given at the ETH Zürich, Switzerland, May 12, 1999.

- **Prof. U. Langer:** Lecture on "Parallele numerische Verfahren für partielle Differentialgleichungen mit Anwendungen in der Magnetfeldrechnung" given at the Karl-Franzens-University of Graz, Austria, June 7, 1999.

- **Prof. U. Langer:** Lecture on "Scientific Computing Tools for 3D Magnetomechanical Field Problems" given at the University of Houston, USA, September 16, 1999.

- **Prof. U. Langer:** Lecture on "Scientific Computing Tools for 3D Magnetomechanical Field Problems" given at the Texas A&M University, College Station, USA, September 17, 1999.

- **R. Hemmecke:** Talk "CASA — A Maple Package to Investigate Algebraic Curves" given at the Univ. Duisburg (Dec. 1999)

- **F. Winkler:** Invited Talk "Advances and Problems in Algebraic Computation" at AAA'58 (58. Arbeitstagung über Allgemeine Algebra), TU-Wien (June 1999)

- **F. Winkler:** Talk "Algebraisches Rechnen - Resultate und Probleme" at Inst. f. Computerwissenschaften, Univ. Salzburg (June 1999)

- **Prof. P. Paule:** "Symbolic Summation: Recent Progress", SFB Workshop in Hagenberg, Symbolic and Numerical Scientific Computation (SNSC'99), 18.–20.8.99 [report on new results of SFB Project F1305 "Symbolic Summation and Combinatorial Identities"];

- **Prof. P. Paule:** "The Renaissance of MacMahon's Partition Analysis", Euroconference: Algebraic Combinatorics and Applications, 12.–19.9.99, Goessweinstein, Germany [invited key note];

- **Prof. P. Paule:** "The Renaissance of MacMahon's Partition Analysis", The Renaissance of Combinatorics'99, 12.–14.10.99, Nankai University, China [invited key note];

- **Prof. P. Paule:** "Algorithmic aspects of q-hypergeometric summation", Symbolic Computation, Number Theory, Special Functions, Physics and Combinatorics, 11.–13.11.99, University of Florida, USA [invited talk];

- **A. Riese**, "Treating q-identities with the computer", Symbolic Computation, Number Theory, Special Functions, Physics and Combinatorics, 11.–13.11.99, University of Florida, USA [invited computer algebra demo];

- **C. Schneider:** "A Mathematica implementation of Karr's Summation Algorithm", Conference: Seminaire Lotharingien de Combinatoire, Schoenthal, Germany, March 1999 [contributed talk].
- **Prof. Irschik:** was the organizer of the special session "Coupled Field Problems" at the 1999 ASME Mechanics and Materials Conference at Virginia Institute of Technology, Blacksburg, VA
- Prof. Irschik served as the organizer of the GAMM-Minisymposium "Hyperbolic Equations with Source Terms" at the GAMM-Tagung in Metz, 1999

SFB F013: Numerical and Symbolic Scientific Computing

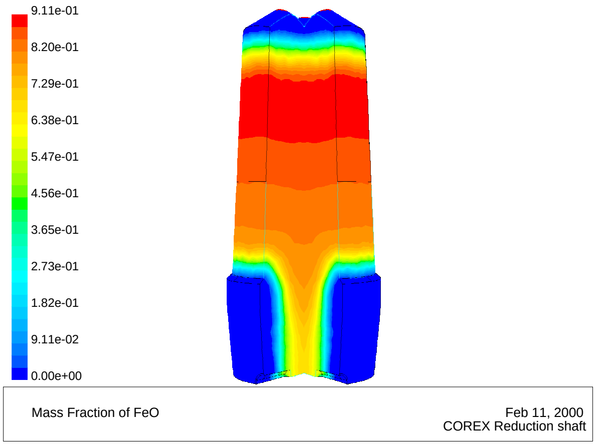
Transfer of Knowledge and Technologies

1 Software Competence Center Hagenberg

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

2 Industrial Mathematics Competence Center

In addition to the Software Competence Center Hagenberg, which is a competence center in the sense of the Kplus program of the Austrian Federal Government and created by the cooperation of groups that are involved with the SFB (RISC Hagenberg, Industrial Mathematics Institute), a new Industrial Mathematics Competence Center has been initiated by Prof. Heinz Engl (Industrial Mathematics Institute Linz, MathConsult GmbH) and Prof. Manfred Deistler (Institute of Econometrics, Operations Research, and System Theory Vienna). Being financially supported by the Ministry of Economic Affairs, the government of Upper Austria and the city government of Linz, its pilot phase started in July 1999. Currently it is building up personnel and infrastructure for a successful application to a full competence center to be co-funded by government and industry. Within this framework we will continue and further develop the extensive cooperation with industry on a growing number of projects with industry partners from a variety of branches. Among them is a joint project of VOEST Alpine Industrieanlagenbau, the Industrial Mathematics Institute and MathConsult on COREX, an ecologically beneficial process for iron production, which has been developed by VAI. This project, which started in the framework of the Christian Doppler Laboratory for Mathematical Modeling and Numerical Simulation in Linz in 1997, could be successfully completed at the end of 1999. In a 3D process simulation model of the COREX reduction shaft, the gas and solid flow, the energy balances, the chemical reactions and the dust deposition can be calculated (the figure below shows the mass fraction of FeO in iron ore (0 - 89%)).



3 Competence Center in Mechatronics

In the field of the pilot-project for the Competence Center in Mechatronics two projects were successfully finished in coherence with SFB-project F 1311, namely "Mechatronic Approach for the Quality Insurance of a New Edge Forming Machine" and "Bindefestigkeitsprüfung von Lagerschalenverbundmaterial mittels nichtlinearer FE". In both projects large plastic deformation has been treated.

In coorperation with the industry further research was done by H. Holl, J. Gerstmayr and H. Irschik in the simulation of a hot-strip mill. A numerical simulation was performed with use of an implicit Runge-Kutta time-integration library, which was developed in SFB-project F1311.

Due to a positive evaluation of the pilot-project a proposal for the Linz Competence Center in Mechatronics (K+) was prepared. In this Competence Center project Prof. Irschik serves as Area Coordinator for the project DYNACON. Contents of the

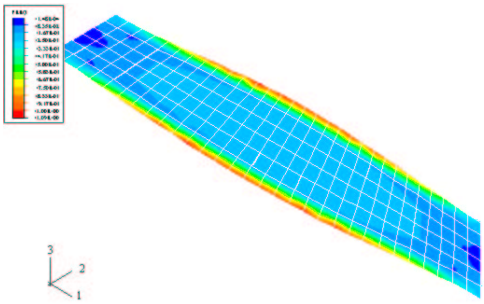


Figure 24: Stress in the Bearing Brass Specimen.

K+-Area DYNACON are shortly described in the following. Modern methods of Advanced Dynamics and Control in Mechanical Systems encompass modeling, simulation and control of mechanical structures and machines in the framework of the modern theory of dynamic systems, with special emphasis on flexible structures and machines, especially in problems of automotive engineering, robotics and in rotating machinery. The classical modeling of structures and machines by rigid body dynamics is combined with continuum mechanics based investigations by finite element methods. Thus, problems of strength and fatigue of materials are treated simultaneously, together with the dynamic analysis. Both, symbolic and numerical computations are involved to derive problem and application oriented models by substructure techniques and order reduction. Based on these lower order models, control of motion, vibrations, structure-born noise and temperature is treated. The application of advanced dynamics to the derived models is promoted by computing techniques employing powerful nonlinear dynamics concepts. The complete models are used for the purpose of simulation and for the validation and stability analysis of the active and passive controller design. The K+ proposal has been accepted in January 2000, the financial support is still lacking.

4 Wolfram Research

Through close contact our group is influencing the development of the Mathematica software in order to include facilities which are useful for automatic reasoning, improved graphical interface, mathematical training, etc. Prof. B. Buchberger and D.I. K. Nakagawa visited the headquarters of Wolfram Research and started a new sub-project of *Theorema* in cooperation with Wolfram Research for implementing the new concept of "logicographic symbols" in *Theorema* based on new interactive graphics tools of Wolfram. We are official beta testers of versions 3 an 4 and also accredited Mathematica developers (access to the Mathematica Developers Kit). We integrated the *Theorema* manual in the *Mathematica* help browser.

5 Unisoftware Plus

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

6 Coaster

The European project Coaster (IVth Frame Telematics Programme, no. F0425), 1998-1999, aims at building commercial software for students. In this project *Theorema* provided the educational content for study in mathematical logic. The partners come from France, Belgium, Spain, and Greece.

7 Theorema

The subproject, also called "*Theorema*", aims at integrating computation and deduction in a coherent software system that can be used by the working scientist for building and checking mathematical models, including the design and verification of new algorithms. Currently, the system uses the rewrite engine of the computer algebra system *Mathematica* for building and combining a number of automatic/interactive provers (high-order predicate-logic, induction for lists/tuples and natural numbers, etc.) in natural deduction style and in natural language presentation. These provers can be used for defining and proving properties of mathematical models and algorithms, while a specially provided "computing engine" can execute directly the logical description of these algorithms.

The *Theorema* system (as version 1.0) has been distributed to a selected number of users from the international research community which volunteered to beta-test the system: researchers from the European project INTAS 96-760 (Uppsala, Kiev, St.Petersburg) and from the CALCULEMUS consortium (UK, Germany, Italy, France, Netherlands) are evaluating the *Theorema* system. Currently there are 35 registered users of the system and their comments and suggestions are used for improving the system. Additionally, the beta testers and new volunteers have access to the newest version of the system on the Internet at `http://www.theorema.org`.

8 Loudspeaker Simulation

The numerical simulation code *CAPA* has been extended within the work of Project F1306. *CAPA* has been used successfully for industrial applications.

For example, the dynamical behaviour of electrodynamical loudspeakers has been fully simulated based on the underlying partial differential equations. Numerical results and measured data matched very well. The optimization process resulted in an improved tone quality of the electrodynamical loudspeaker. (Cooperation with Harmann Audio Electronic Systems GmbH.)

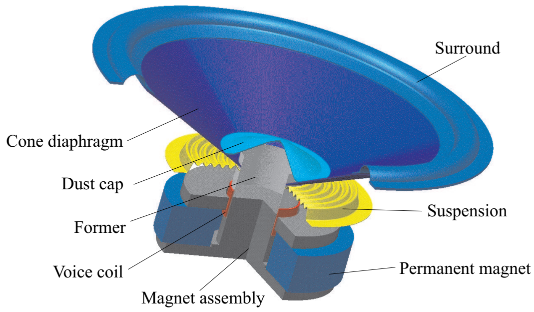


Figure 25: Principal setup of the magnetically excited aluminum plate

9 Optimal Sizing of Injection Moulding Machines

The optimization project F1309 achieved a new quality by directly combining the optimization algorithms with the solvers developed in project F1306. The resulting optimization software is so fast that we

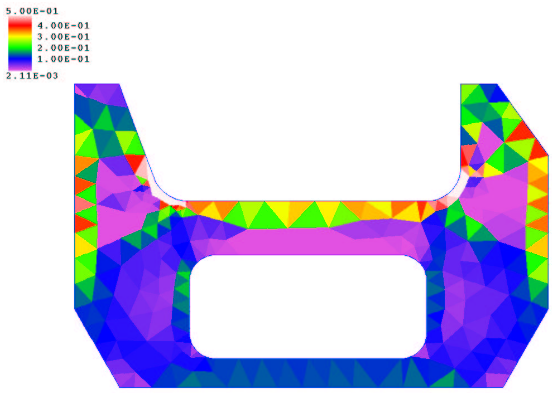


Figure 26: Thickness distribution of a frame.

can use hundreds of design parameters making it realistic to minimize the weight of an injection moulding machine by changing the thicknesses in its supporting parts. The resulting mass reduction is considerable and, therefore, our industrial partner, the ENGEL Group Schwertberg, will use these results to produce new machines by means of a different technology. This cooperation will be continued.

10 Image Compression

Wavelets on the interval are very useful for data compression of image data. The use of such wavelets significantly reduces artifacts of compressed images near the boundaries. The use of computer algebra offers new possibilities in the construction of wavelets.

Some of the results obtained in this SFB-project F1310, in particular wavelets on the interval, are of interest for data compression to reduce so-called edge artifacts and gain higher compression rates. We suggested the company Kretztechnik AG to implement wavelets on the interval into the 3D data compression algorithms which were developed in a former cooperation with the Industrial Mathematics Institute.