Symbolic-Algebraic Methods and Verification Methods - Theory and Applications

21.11.-26.11.1999

organized by

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OVERVIEW

The second Dagstuhl seminar on *Symbolic-Algebraic Methods and Verification Methods - Theory and Applications* brought together 39 participants from 9 countries, with 10 participants coming from overseas. The seminar continuous a first one held in 1992 in Dagstuhl.
The 35 talks covered a wide range of topics of the three areas Computer Algebra, Verification Methods and Real Number Theory. The aim of the seminar was to bring together experts of those different areas to discuss common interests.
All three areas aim on computing correct results on the computer. Here correct is to be understand in a mathematical sense including all model, discretization and rounding errors. The methods may also synergize and use good numerical approximations as a basis for subsequent computation of error bounds.
In the talks we saw some algorithms with result verification for finite dimensional as well as infinite dimensional problems, solutions to classical problems in Computer Algebra and a number of efforts to combine different methods and areas. Such methods mutually benefit from each other and are very promizing. Moreover, we saw a number of practical applications.
Everybody enjoyed the very pleasant atmosphere, the excellent food and the surroundings inviting to intensive discussions and recreational hiking.
We would like to express our thanks to all who contributed to the conference and to the administration of the Dagstuhl center for their excellent job.

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1 Hierarchies of Variables, Types and Controls

by Rudolf F. Albrecht

The concept of controllable variable var V is introduced to describe a family $S = (S_{[p]})_{p \in P}$ of structured objects (relations) $S_{[p]}$ if for all $p \in P$ $S_{[p]}$ is a concatenation $S_{[p]} = K\kappa_{[p]}V_{[p]}$, where object K is the same for all p and $\kappa_{[p]}$ is a concatenation. $K = \emptyset$ is permitted. The object var V is defined on a (structured) domain (type) $D = \{V_{[p]}|p \in P\}$ with respect to structure S, the composite object var $S = K\kappa$ var V is used to represent $S_{[p]}$ by assignment var $S := (p)S_{[p]}$ for any given p, $S_{[p]}$ sometimes called a "state" or "instanciation" of var S. We assume, the selection of var $V := (p)V_{[p]}$ and the concatenation $\kappa_{[p]}$ are the result of a functional assignment- (or "control"-) operator $C(\text{var } S) : p \mapsto K\kappa_{[p]}V_{[p]}$.
Constructive computations are represented by a composition of "primitive" functional operations (algorithm). The primitives as well as the composite function are of form var $y :=$ var $f(\text{var } x)$ with var $f : F \stackrel{=}{\text{def}} \{f_{[p]}|f_{[p]} : X \to Y\}$, var $x : X$, var $y : Y$ depending on var f, var x. Mathematically exact assignment values $f_0, x_0, y_0 = f_0(x_0)$ to var f, var x, var y are in general not available or representable and for contructive computation approximated by $f^* \in F$, $x^* \in X$, $y^* = f^*(x^*) \in Y$. An estimation of the quality of the approximate result y^* in dependency of f^*, x^* can be obtained by introducing topological filter bases $\mathbf{F} \stackrel{=}{\text{def}} \{F_{[q]}|q \in Q \wedge F_{[q]} \subseteq F\}$ with $f_0 \in \cap\mathbf{F}$ and $F \in \mathbf{F}, \mathbf{X} \stackrel{=}{\text{def}} \{X_{[r]}|r \in R \wedge X_{[r]} \in X\}$ with $x_0 \in \cap\mathbf{X}$ and $x \in \mathbf{X}$ as neighborhood systems to f_0 and x_0 and by extension of the functions $f \in F$ to set functions. Generalized distance measures for f^* from any $f \in \cap\mathbf{F}$ and for x^* from any $x \in \cap\mathbf{X}$ are then given by $d(f, f^*) \stackrel{=}{\text{def}} \cap \{B|B \in \mathbf{F} \wedge f^* \in B\}$ and by analogously defined $d(x, x^*)$. We assume $d(f, f^*) \in \mathbf{F}$ and $d(x, x^*) \in \mathbf{X}$. For any $f \in F, f(\mathbf{X})$ is a filter base $\mathbf{Y}(f)$ on pow Y with $y_0 \in \cap\mathbf{Y}(f)$. Given $d(x_0, x^*) \in \mathbf{X}, d(f_0, f^*) \in \mathbf{F}$, then $y_0 \in \cup\{f(d(x_0, x^*))|f \in d(f_0, f^*)\}$.
The topological reasoning can also be applied to parameter sets and control functions and can be extended to hierarchies of functional computations and assignments.
Examples are "fuzzy sets", interval arithmetic, "fuzzy" control.

2 Bounds for Eigenvalues with the Use of Finite Elements

by Henning Behnke

(Joint work with U. Mertins, Clausthal)
For the computation of bounds to eigenvalues of selfadjoint problems the method of Rayleigh - Ritz and Temple - Lehmann - Goerisch for upper and lower bounds, respectively, have proven to be very powerful. The application of the Rayleigh - Ritz method using finite elements for non convex domains is very well understood. Up to now all known applications of the Temple - Lehmann - Goerisch method are using "classical" trial functions on convex or even rectangular domains or finite elements which are restricted to some special cases.
We present general Temple - Lehmann - Goerisch methods, which can be applied to finite elements. These methods require the same regularity as the corresponding Rayleigh - Ritz procedures. Results for partial differential equations of second and fourth order are given.

3 Towards Algorithm Verification in Theorema

by Bruno Buchberger

Proving correctness is critical in many branches of science and engineering. TH∃OREM∀ is a new mathematical software system that provides support for proving mathematical theorems. The current version of TH∃OREM∀ is programmed in the computer algebra system Mathematica. It retains access to all the underlying computer algebra functions but offers, in addition, a library of general and special provers that generate proofs in a human-readable style with natural language explanations. Provers have two essential arguments: the proposition to be proved and the knowledge base. In TH∃OREM∀, knowledge bases may be built up hierarchically from definitions, axioms, propositions etc. in a form that resembles the usual style in mathematical textbooks. In this context, algorithms are just special propositions, i.e. the TH∃OREM∀ language (a version of higher-order predicate

logic) is both a logic and a programming language.
In the talk we report on the current state of the TH∃OREM∀ project mainly by presenting examples of writing formal texts in various areas of mathematics and generating the proofs of the theorems occurring.

4 Symbolic-Numeric Algorithms for Polynomials: some recent results

by Robert M. Corless

One of the most powerful recent ideas for the solution of systems of multivariate polynomials, namely the conversion of such systems to eigenproblems for families of commuting sparse matrices, will be shown by example.
The facts that the matrices are sparse and commute have theoretical and practical consequences: their sparsity allows efficiency, while their commutativity promotes numerical stability.
Implications for validated computing will be discussed.

5 Global Optimization

by Georg F. Corliss

Baker Kearfott's GlobSol package has been applied to several industrial problems. I have previously reported on some of the successes. Here, I report on some of the failures. A design optimization problem prototypical of a rocket nozzle design used an äll together approach" presenting finite element analysis equations as equality constraints to the optimizer. A differential equations parameter identification problem coming from the control of a magnetic resonance imaging machine used a similar approach. A gene search engine was trained with a neural network. In each of these problems, we were only able to solve VERY small versions of the problem before the tight coupling of the variables in the constraints gave very large over-estimations. Hence, no strategy was able to discard any boxes, and the program appeared to run

forever.
One possible tool to attack the over-estimation is the Taylor model of Martin Berz. He encloses functions of about 10 variables in a polynomial with floating-point coefficients plus a remainder interval. I give one- and two-dimensional examples to show how Berz idea works.

6 Symbolic-Numeric QD-Algorithms with Applications in Function Theory and Linear Algebra

by Annie Cuyt

The qd-algorithm, devised by Rutishauser, is an ingenious way to compute the poles of a meromorphic function from its Taylor series development, or to compute the eigenvalues of certain tridiagonal matrices.
Various authors have studied many variants of the algorithm (progressive, differential, orthogonal, ...). We present

1. a symbolic variant which enables the detection of polar singularities of multivariate functions in closed algebraic form,

2. a symbolic-numeric implementation of the above with the same properties but usable with inexact data,

3. a symbolic multivariate homogeneous variant which solves the solution of the (smallest) eigenvalue problem of certain parameterized tridiagonal matrices.

All procedures are illustrated with numerical examples. More detailed information can be found at http://www.uia.ac.be/u/cuyt/.

7 Verified Bounds for Linear Systems Through the Lanczos process

by Andreas Frommer

Consider a linear system

$$Ax = b \tag{1}$$

with a symmetric positive definite matrix A. Given an approximate solution to the system, it is possible to represent the 2-norm and the energy-norm of the error as a Riemann-Stieltjes integral involving an unknown discrete measure. However, variants of Gaussian quadrature rules can be applied and computed through applying the Lanczos process to the residual of the approximate solution. Moreover, this technique allows to have a priori information on the sign of the integration error. For example, the Gauss-Radau rule yields an upper bound on the error norm, provided one knows a lower bound on the smallest eigenvalue of A. These results have been developped by Golub, Golub and Meurant and others.
The purpose of this talk is to present a version of the Lanczos process with rigorous control of numerical rounding errors. We then apply this version to get numerically guaranteed bounds on the Riemann-Stieltjes integrals. Bounds on the smallest eigenvalues can be obtained by a technique proposed by Rump relying on (sparse) factorizations. In this respect, our approach may be regarded as a computationally cheap way to improve – to a certain extent – the bounds obtained by Rump's method.
We will present several numerical examples with matrices form the Matrix Market collection.

8 Structural Filtering for Geometric Programs

by Stefan Funke

In geometric algorithms, every decision regarding the position of geometric objects can be expressed as the sign of an arithmetic expression. To get reliable results, these sign determinations must be carried out exactly. Naive use of arbitrary precision arithmetic induces a considerable overhead compared

to pure floating-point arithmetic. A very common technique to reduce this overhead is the use of so-called floating-point filters. The idea is to evaluate the expression using floating-point arithmetic first but also compute an error bound for the deviation from the exact value. If the error bound is smaller than the absolute value of the approximation, exact and approximated value have the same sign. This scheme introduces an overhead of a factor about 2 if properly implemented.
We introduce a new filtering technique called *Structural Filtering* which can reduce this overhead even further. Especially for (nearly) degenerate cases which are very difficult for filters at predicate level, our approach pays off. The basic idea is very simple. We divide the algorithms in phases; at the end of each phase we guarantee correctness, but within one phase, we allow imprecisions. Presenting experimental and theoretical results, we show the value of this new technique.
The conference version of this paper appeared in the Proceedings of the 11th Canadian Conference on Computational Geometry and has been submitted to a journal.

9 Application of Bernstein Expansion to the Solution of Systems of Polynomial Inequalities and Equations

by Jürgen Garloff

We present a new method for computing all solutions of a system of polynomial inequalities or equations in a given box. The approach is based on the expansion of a multivariate polynomial into Bernstein polynomials. This expansion is now a well established tool for bounding the range of a multivariate polynomial over a box. Our method is a typical domain-splitting procedure: Starting with the given box, the algorithm sequentially splits it into subboxes by eliminating unfeasible boxes using bounds for the range of the given polynomials over each of them which are provided by Bernstein expansion. The algorithm ends up with some subboxes of sufficiently small volume. These boxes undergo a test for existence of solutions. On some examples we demonstrate that our approach compares well with methods based on partial cylindrical algebraic decomposition.

10 Symbolic-Algebraic Computations in the Context of a Modeling Language for Mathematical Programming

by David M. Gay

The context of my talk was AMPL, a language and system for expressing, solving, and manipulating mathematical programming programming problems (i.e., finite dimensional algebraically defined constrained optimization problems); much of AMPL is joint work with Robert Fourer (who is a professor at Northwestern University) and Brian Kernighan (a Bell Labs colleague). I described two areas where symbolic-algebraic computations occur with AMPL. The first area is in "presolving" a problem instance, i.e., simplifying it before presenting it to a solver — a separate program that actually solves the problem. So far, AMPL's presolver deals mostly with linear constraints (treating nonlinearities as though they had infinite range, a treatment that clearly admits room for improvement), applying the simplifications described in 1975 by Brearley, Mitra and Williams (Math. Prog. 8, pp. 54-83). Noteworthy is that directed roundings make AMPL's presolver more reliable. Though the details are unfortunately still system-dependent, it is possible to arrange for directed roundings on most of today's platforms. The second area where symbolic-algebraic computations arise in the AMPL context is in arranging for efficient computation of the Hessian (matrix of second partial derivatives) of the Lagrangian function in the AMPL/solver interface library. We use backwards automatic differentiation to compute Hessian-vector products. Many problems exhibit partially separable structure, as pointed out in a series of papers by Griewank and Toint. That is, many problems involve an objective function and constraint that consist of a linear part and the sum of nonlinear functions which, after a linear change of variables, depend on only a few variables. We find this structure by walking expression graphs, then use it to efficiently assemble the whole (sparse) Hessian if desired, or to compute full Hessian-vector products. Pointers to papers giving more detail about the above areas and about AMPL in general appear in the AMPL web site, `http://www.ampl.com/ampl/`.

11 Exact Real Arithmetic by means of Linear Fractional Transformations

by Reinhold Heckmann

In exact real arithmetic, computable real numbers are considered as potentially infinite streams of digits. At each time, a finite prefix of the stream is known, and a rule to compute the remainder. *Linear fractional transformations (LFT's)* can be used both for the representation of the digits and for the implementation of the basic operations on digit streams.
One-dimensional LFT's are functions $x \mapsto \frac{ax+c}{bx+d}$ which can be specified by matrices $\left(\begin{smallmatrix} a & c \\ b & d \end{smallmatrix}\right)$ so that matrix multiplication corresponds to function composition. A digit k in base r can be represented as the digit matrix $\left(\begin{smallmatrix} 1 & k \\ 0 & r \end{smallmatrix}\right)$. Thus, digit streams become infinite products of digit matrices.
Some simple operations such as $3x$, $-x$, or $1/x$ can be immediately obtained as special LFT's. Similarly, addition, multiplication, and division are special instances of two-dimensional LFT's (generalisations of LFT's to two arguments). Square roots can be obtained as fixed points of LFT's, and thus can be computed by feedback loops. Transcendental functions such as cosine or logarithm can be expressed as infinite LFT expansions which can be obtained from Taylor series or continued fraction expansions in a systematic manner.

12 Convex-Concave Extensions

by Christian Jansson

We present a new notion which is called convex-concave extensions. These extensions provide for given nonlinear functions convex lower bound functions and concave upper bound functions, and can be viewed as a generalization of interval extensions. Convex-concave extensions can approximate the shape of a given function in a better way than interval extensions which deliver only constant lower and upper bounds for the range. Therefore, convex-concave extensions can be applied in a more flexible manner. For example, they can be used to construct convex relaxations. Moreover, it is demonstrated that in many cases the overestimation which is due to interval extensions can be drastically reduced. Some numerical examples, including constrained global optimization problems of large scale, are presented.

13 Rewriting and Decision Procedures: A Case Study of Presburger Arithmetic

by Deepak Kapur

For theorem provers to be useful as well as acceptable for use in applications, it is essential that properties considered trivial and obvious by domain experts are proved automatically without any user guidance. This has been the main design goal of Rewrite Rule Laboratory (RRL), a rewrite-based induction prover. Our experience in using RRL for mechanically verifying arithmetic circuits suggests that a theorem prover implementing (i) conditional rewriting, (ii) decision procedures for congruence closure and quantifier-free Presburger arithmetic with uninterpreted function symbols, (iii) heuristics for carefully selecting induction schemes from recursive function definitions given as terminating rewrite rules, and (iv) intermediate lemma speculation, well integrated with (v) backtracking, can be used to automatically verify number-theoretic properties of parameterized and generic adders, multipliers and division circuits (including the SRT division circuit).

To make theorem provers such as RRL more effective, it is important that decision procedures for well-known data structures and representations frequently used in many application domains be integrated efficiently with rewriting and induction. Using the example of quantifier-free subtheory of Presburger arithmetic, properties and requirements for integration of rewriting and induction with decision procedures are discussed. It is shown how a decision procedure can be used for deducing implicit equalities, generating appropriate instantiations of definitions and lemmas so that they are applicable, suggesting induction schemes which exploit semantic information, and speculating intermediate lemmas needed to prove theorems.

Sufficient conditions are identified for deciding a priori, the validity of certain simple equational conjectures expressed using function symbols that are recursively defined over the terms of a decidable theory. The concept of a theory-based function definition is introduced. Conditions on conjectures and interaction among the definitions of functions appearing in them that guarantee the simplification of each induction subgoal are identified. It is shown that the cover set method which implements inductive reasoning in RRL can be used as a decision procedure for a subclass of such conjectures.

14 Massively Parallel Isolation of Polynomial Real Roots

by Werner Krandick

Two new scheduling algorithms are presented. They are used to isolate polynomial real roots on massively parallel systems. One algorithm schedules computations modeled by a pyramid **DAG**. This is a **D**irected **A**cyclic **G**raph isomorphic to Pascal's triangle. Pyramid DAGs are scheduled so that the communication overhead is linear in the height of the pyramid. The other algorithm schedules parallelizable independent tasks that have identical computing time functions in the number of processors. The two algorithms are combined to schedule a tree-search for polynomial real roots; the first algorithm schedules the computations associated with each node of the tree; the second algorithm schedules the nodes on each level of the tree.
The search tree is processed using a modified version of the well-known Descartes method. We replaced exact integer arithmetic by software-supported multiprecision floating point arithmetic. Roundoff error is controlled through the use of interval arithmetic.
Using 32 processors on the Cray T3E we isolate the real roots of random polynomials of degree 1000 in less than a second on the average; a mantissa length of 63 bits is sufficient in these computations.

15 Derivative-Based Subdivision in Multi-Dimensional Verified Gaussian Quadrature

by Bruno Lang

When implementing a general-purpose routine for multi-dimensional verified Gaussian quadrature, several decisions must be made.

- Enclosing the remainder terms requires enclosures for the uni-directional Taylor coefficients of the function over the current domain ("box"). Enclosures for these Taylor coefficients may be obtained via automatic differentiation techniques, coupled with standard interval evaluation. Sharper enclosures may be obtained by first subdividing the box or by

using a gradient-based approach, at a higher cost.

- If the error bound cannot be met with the current box then the box must be subdivided. Here we must decide on the direction(s) along which the box is cut and on the number of pieces. We discuss several objective functions on which these decisions may be based.

- The maximum order of Gaussian rules determines the amount of work spent in approximating the integral and the recursion depth of the algorithm.

Based on extensive numerical experiments we give recommendations on how to set the above-mentioned algorithmic parameters in order to achieve good overall performance.

16 Comparison of Three Finite Difference Approximations for Dirichlet Problems

by Nami Matsunaga

We consider the linear Dirichlet problem

$$\begin{aligned} -\Delta u + c(x,y)u &= \varphi(x,y) && \text{in } \Omega, \\ u &= \psi(x,y) && \text{on } \Gamma = \partial\Omega, \end{aligned}$$

and the semilinear Dirichlet problem

$$\begin{aligned} -\Delta u + f(x,y,u) &= \varphi(x,y) && \text{in } \Omega, \\ u &= \psi(x,y) && \text{on } \Gamma, \end{aligned}$$

where $\Omega \subset R^2$ is a bounded domain, c, φ, ψ and f are given functions and $c \geq 0$ and $f_u \geq 0$.
We apply three finite difference approximations, the Shortley-Weller, the Bramble and the Collatz, to the Dirichlet problems. It is shown with the use of graphics that the Shortley-Weller approximation is superior to the others and that the Bramble approximation is generally better than the Collatz.

17 Modifications of the Oettli–Prager Theorem

by Günter Mayer

(Joint work with Götz Alefeld, Universität Karlsruhe, Germany, and Vladik Kreinovich, The University of Texas at El Paso, USA)

Let S be the set of solutions x of linear systems $Ax = b$ whose coefficient matrix A varies in a given real $n \times n$ interval matrix $[A] = [\underline{A}, \overline{A}]$ and whose right–hand side b lies in a given real interval vector $[b] = [\underline{b}, \overline{b}]$ with n components. The Oettli–Prager Theorem

$$x \in S \Longleftrightarrow | \check{A}x - \check{b} | \leq \Delta A \cdot |x| + \Delta b$$

characterizes S using the midpoints $\check{A} := (\underline{A} + \overline{A})/2$, $\check{b} := (\underline{b} + \overline{b})/2$ and the radii $\Delta A := (\overline{A} - \underline{A})/2$, $\Delta b := (\overline{b} - \underline{b})/2$ of $[A]$ and $[b]$, respectively. We list several equivalent formulations of the theorem recalling that the boundary of S consists of finitely many pieces of hyperplanes. By applying the Fourier–Motzkin elimination process of linear programming the theorem is modified in order to describe the symmetric solution set $S_{\rm sym} := \{\, x \mid Ax = b,\ A = A^T \in [A] = [A]^T,\ b \in [b] \,\}$. We show that the boundary of $S_{\rm sym}$ consists of finitely many pieces of hyperplanes and quadrics. We also consider solution sets with $A \in [A]$ being restricted in some other kind (A skew–symmetric, Toeplitz matrix, Hankel matrix, etc.). In addition, we apply the elimination process to the algebraic eigenvalue problem $Ax = \lambda x,\ x \neq 0$, thus characterizing the sets of eigenpairs $E := \{\, (x, \lambda) \mid Ax = \lambda x,\ x \neq 0,\ \lambda \text{ real},\ A \in [A] \,\}$ and $E_{\rm sym} := \{\, (x, \lambda) \mid Ax = \lambda x,\ x \neq 0,\ A = A^T \in [A] = [A]^T \,\}$, respectively.

18 The Exact Computation Paradigm in Computational Geometry

by Kurt Mehlhorn

Geometric Computations maintain symbolic information, e.g., a planar graph, and numerical information, e.g., the positions of the nodes of the graph. In the presence of rounding errors, symbolic and numerical information may

contradict each other. Program crashes may result from this. The obvious solution to this problem is to use exact arithmetic. The evaluation of tests in geometric programs is tantamount to evaluating signs of arithmetic expressions. I discuss methods for exact sign computation of rational expressions and of expressions involving roots.

19 Numerical Verification Method for Solutions of Nonlinear Hyperbolic Equations

by Teruya Minamoto

We consider a numerical method to verify the existence and uniqueness of the solutions of the following nonlinear hyperbolic problem with guaranteed error bounds:

$$\begin{cases} u_{tt} - \triangle u &= -f(x,t,u) & (x,t) \in \Omega \times J, \\ u(x,t) &= 0 & (x,t) \in \partial\Omega \times J, \\ u(x,0) &= 0 & x \in \Omega, \\ \frac{\partial u}{\partial t}(x,0) &= 0 & x \in \Omega, \end{cases}$$

where Ω is a bounded open interval on $\mathbf{R}$ or a bounded rectangular domain in $\mathbf{R^2}$. Let $J = (0,T)$ with $T > 0$, and let $Q = \Omega \times J$. For two Banach spaces $L^p(Q)$ and $L^2(Q)$, $f : L^p(Q) \to L^2(Q)$ is a continuous map and Fréchet differentiable.
Using a C^1 finite element solution and an inequality constituting a bound on the norm of the inverse operator of the linearized operator, we numerically construct a set of functions which satisfies the hypothesis of Banach's fixed point theorem for a map on a suitable Banach space $L^p(Q)$ in a computer. We present detailed verification procedures and show some numerical examples.

20 H-bases and Gröbner bases

by Michael Möller

H-bases and Gröbner bases are both based on the concept of graded rings. Both allow a splitting of problems for multivariate polynomials into a sequence of problems in finite dimensional linear subspaces of this ring. H-bases were originally introduced by Macaulay 1916. The concept of Gröbner bases was introduced by Buchberger in 1965. We compare properties of Gröbner and H-bases, characterize H-bases, give reasons, why we can expect better numerical performance compared to Gröbner bases, show the normal forms concept for H-bases, and present finally a method for computing H-bases for arbitrary zero-dimensional ideals given by a basis.

References

[1] Möller, H. Michael, and T. Sauer: H-bases for polynomial interpolation and system solving, Advances in Computational Mathematics, in print

21 A Numerical Verification of Bifurcated Solutions for the Heat Convection Problem

by Mitsuhiro T. Nakao

We consider the Rayleigh-Bénard problem for the heat convection using the Boussinesq equations for the velocity, pressure and temperature in the two dimensional strip domain $(x, z) \in R \times (0, \pi)$, which includes two parameters, Prandtl and Rayleigh number. We assume the stress free boundary condition for the velocity on the both boundaries $z = 0 and \pi$ and the Dirichlet boundary condition for the temperature T = 1 on the lower boundary and T = 0 on the upper boundary. The bifurcated periodic solutions of the equilibrium state are computed with guaranteed error bounds. By these validated computational results, we can calrify several facts which could not be proved by using any kind of theoretical approaches up to now. Therefore, our work should be a significant example of the computer assisted proof in analysis.

22 Geometric Series Bounds for the Local Errors of Taylor Methods for ODEs

by Markus Neher

Interval Taylor methods for the validated solution of ODEs often consist of two parts. First, a coarse enclosure of the solution is calculated. The coarse enclosure is then used in the second part of the algorithm to obtain refined bounds for the local discretization errors. To compute the coarse enclosure usually a fixed point iteration is used, which can result in rather small step sizes in the integration of the ode.
We present an alternative enclosure method that uses geometric series to bound the local discretization errors in the Taylor series method. The solution of an IVP is represented as a power series, and a high–order Taylor polynomial is used as approximate numerical solution. By analyzing the recurrence relation for the Taylor coefficients, we construct a geometric series that is a convergent majorant to the Taylor remainder series. Thus, the computation of a coarse enclosure becomes obsolete.
In [2], the method was presented for linear ODEs with polynomial coefficient functions. It is also applicable to linear ODEs with analytic coefficient functions and to some nonlinear ODEs. Extensive numerical simulations have shown that sometimes very large step sizes can be used in practical calculations, with the side effect of reducing overall wrapping operations.
The critical step with regard to roundoff errors is the evaluation of the Taylor polynomial. When large step sizes are used, the summands of the polynomial often cancel out each other. If such a cancellation occurs, a multiple precision arithmetic is required to procure tight enclosures.
To demonstrate the applicability of our method, a PASCAL–XSC program has been written for linear n–th order ODEs. Its practical performance is compared with numerical examples with the well–known program AWA by Rudolf Lohner [1].

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23 Generalized Lyapunov-Schmidt Reduction for Parametrized Equations at Near Singular Points

by Arnold Neumaier

Underdetermined systems of equations with one free parameter are often described by bifurcation diagrams. However, their topology is unstable under perturbation. We show that it is possible to rigorously enclose bifurcation diagrams for systems with imperfections (rounding errors or data uncertainties) in a way that preserves the stable part of the information in a bifurcation diagram.
This is done by generalizing the Lyapunov-Schmidt reduction to the case of imperfect singularities. The results presented neither need very precise information about the location of (near) singularities nor a precise knowledge of (near) null spaces.
Details can be found at the following WWW-site:
`http://solon.cma.univie.ac.at/~neum/papers.html#ly`

24 Fast Verified Numerical Computation

by Shin'ichi Oishi

It is shown that verified error bound for a matrix equation

$$Ax = b, \quad A : n \times n \text{ real matrix} \tag{2}$$

can be computed $n^3/3$ flops computational cost. In this method Higham's backward error analysis is utilized. It is demontrated that computational time for obtaining an approximate solution $\tilde{\chi}$ of equation (2) and that for calculating a verified error bound $\|\tilde{\chi} \cdot \chi_{\text{true}}\|_\infty$ are the same 5 [sec] and 5 [sec], respectively, provided Intel celeron 333MHz CPU is used.

25 Validated Numerical Integration of Piecewise Analytic Functions

by Knut Petras

For many problems in numerical analysis, we need global information about a function f under consideration. If f is a combination of 'standard functions', two types of such information that can be generated automatically by a computer are

- Bounds for higher derivatives (using automatic differentiation and real interval arithmetic)
- Analyticity and bounds in a certain region of the complex plane (using complex interval arithmetic)

It is argued, why the latter method has some advantages upon the first one. We present an algorithm that has optimal order of convergence for piecewise analytic functions. Numerical tests compare its speed with that of the non-validating QUADPACK-routines. Applicability of the used techniques to further problems in numerical analysis is discussed.

26 Verification Methods for Elliptic Differential Equations

by Michael Plum

For nonlinear elliptic boundary value problems of the form

$$-\Delta u + F(x, u, \nabla u) = 0 \text{ on } \Omega, \quad u = 0 \text{ on } \partial\Omega$$

(with Ω denoting a bounded Lipschitz domain), a method for computing tight *enclosures* for solutions, simultaneously providing *existence* statements, is established. It is based on a suitable fixed-point formulation of problem (1), allowing the application of Schauder's Fixed-Point Theorem. The essential numerical subtasks consist in the computation of an *approximate* solution ω, and of appropriate bounds for its defect $-\Delta\omega + F(\cdot, \omega, \nabla\omega)$ and for the

inverse of the linearization L of problem (1) at ω; the latter are obtained via eigenvalue enclosures for L or for L^*L.

The method is used in particular to give a partial positive answer to a conjecture which is under consideration since almost 20 years and could apparently not be proved by purely analytical means; it states that the problem

$$\Delta u + u^2 = \lambda \sin(\pi x) \sin(\pi y) \text{ on } \Omega := (0,1)^2, \quad u = 0 \text{ on } \partial\Omega$$

has at least four solutions for λ sufficiently large. Using our enclosure method - in combination with a numerical mountain pass method established by J. McKenna - we could give a positive answer for the specific value $\lambda = 800$.

To point out the importance of verification methods, it is furthermore shown that for Emden's equation $-\Delta u = u^2$ on Ω, $u = 0$ on $\partial\Omega$, with Ω denoting a long and narrow rectangle, spurious approximate solutions arise which do not correspond to real solutions, although they have a small defect, and although they are indeed solutions of the discretized equation, as has been proved by S. M. Rump. This also indicates the importance of verification methods for the complete differential equation problem, and not only for its discretized version.

27 Self-Validating Methods

by Siegfried M. Rump

A basic property of interval arithmetic is inclusion isotonicity. This implies a remarkable property, the ability to estimate the range of a function over a domain without further knowlegde of the function. However, this comes with a significant drawback, namely frequently a severe overestimation of the range.
Self-validating methods take advantage of the ability to estimate the range of a function but formulate algorithms in such a way that overestimation is diminished. Some examples to that are given.
The fast implementation of interval arithmetic operations is discussed and an approach is presented being faster by more than an order of magnitude compared to previous methods.
For interval standard functions a simple method is presented to calculate inclusions accurate to 3 ulp for all elementary functions and all possible

arguments. Finally, a new algorithm for computation of error bounds of multiple or clustered eigenvalues of a matrix is presented. Computational results show applicability to ill-conditioned problems.
Everything is implemented in INTLAB, more details and free downloading at our homepage.

28 The Linear Complementarity Problem with Interval Data

by Uwe Schäfer

Let M be an $n \times n$ matrix and q an nth order vector. Then the linear complementarity problem $LCP(M, q)$ is defined as follows: Determine (or conclude that there is no) $z \in R^n$ with

$$q + Mz \geq 0, \quad z \geq 0, \quad (q + Mz)^{\mathrm{T}} z = 0.$$

Let $[M]$ be an $n \times n$ interval matrix and $[q]$ an nth order interval vector. Then we consider the linear complementarity problems

$$\left.\begin{array}{rcl} q + Mz & \geq & 0, \\ z & \geq & 0, \\ (q + Mz)^{\mathrm{T}} z & = & 0, \end{array}\right\} M \in [M],\ q \in [q].$$

According to the solution set concerning linear interval equation systems we define the solution set concerning an LCP with interval data.

$$\begin{array}{rcl} \Sigma([M], [q]) & := & \{z \in R^n : \text{There exist } M \in [M],\ q \in [q] \text{ with} \\ & & q + Mz \geq 0,\ z \geq 0,\ (q + Mz)^{\mathrm{T}} z = 0.\} \end{array}$$

I.e. for every fixed $M \in [M]$ and for every fixed $q \in [q]$ every solution of $LCP(M, q)$ is an element of $\Sigma([M], [q])$.

We present a theorem that says that the solution set $\Sigma([M], [q])$ is compact and nonempty for every $[q]$, if $[M]$ is an H-matrix with positive diagonal entries. Via an example we show that $\Sigma([M], [q])$ is not necessarily convex.

We emphasis the application of an LCP with interval data in a free boundary problem.

At the end we present some ideas how to include $\Sigma([M], [q])$ and we give some examples.

29 Efficient Exact Computation using the Number Type `leda_real` – Theory and Geometric Applications

by Stefan Schirra

joint work with Christoph Burnikel, Rudolf Fleischer, and Kurt Mehlhorn.
We present the number type `leda_real` which provides exact computation for a subset of real algebraic numbers: Every integer is a `leda_real`, and `leda_real`s are closed under the basic arithmetic operations $+, -, *, /$ and k-th root operations. The number type is available as part of the LEDA library (http://www.mpi-sb.mpg.de/LEDA). `leda_real`s guarantee correct results in all comparison operations.
The `leda_real`s record computation history in an expression dag (i.e., a directed acyclic graph) in order to allow for adaptive evaluation. Moreover they use interval arithmetic as a floating-point filter. Approximations are computed as `leda_bigfloat`s, a software floating-point number type that allows you to choose the mantissa length. If, in a sign computation, the current approximation by a `leda_bigfloat`s is not sufficient to verify the sign, the expression dag is used to re-compute better approximations. Checking for zero involves separation-bounds for expressions. A separation bound for an arithmetic expression of non-zero value is a lower bound on its absolute value. We prove the separation bound that is use in the `leda_real`s.
`leda_real`s provide user-friendly exact computation. All the internals described above are hidden to the user. A user can use `leda_real`s just like any built-in number type. We finally describe some difficult geometric applications of the `leda_real`s.

30 On Some Numerical Methods for Nonlinear Least Squares Problems

by Stepan M. Shakhno

Nonlinear least-square problems appear while estimating parameters and while checking the hypotheses of mathematical statistics, in estimating physics

process parameters using the results from measurement, and in managing of different objects, processes etc. In this work we propose methods for solving nonlinear least-squares problems. These methods are constructed as a combination of known iterative methods with the aim of obtaining greater efficiency in regards to the number of iterations and the number of calculations and to the robustness. The theorems about conditions and speed of iteration convergence for this method are formulated and proved. A comparison is made between these methods and the Gauss-Newton method. We are proposing concrete possibilities of choosing operators. The results of extensive numeric experiments are demonstrated on the basis of tested problems, which are widely known though rather complex. Conclusions have been made on the basis of these experimental results.

31 Pseudozero Domains near Singularities of Polynomial Systems

by Hans J. Stetter

Problems from real-life have some *uncertain data and/or relations*; hence the concept of *true results* must be replaced by that of *valid results* relative to the *tolerance* in the given problem. A result is valid or a *pseudoresult* it if is an *exact* result of a problem within the tolerance neighborhood of the specified problem. A *pseudoresult domain* contains the valid results for a specified tolerance. To solve such problems in a reliable fashion, we need
- a procedure to compute the *backward error* of an approximate result;
- a procedure to *improve* the result if it is not valid;
- a procedure to *analyze the local result sensitivity.*

This last step is necessary to judge which aspects of the result are *meaningful* under the given tolerance.

A property or situation is *singular* it it is non-generic and *disappears with arbitrarily small changes of the data.* At and *near* singularities, computational difficulties arise. It is important to know which result properties remain well-conditioned in the transition between a regular and a singular situation. To analyze such transitions, we introduce a parameter ϵ such that the problem is singular for $\epsilon = 0$.

As an introduction, we consider the *linear* system

$$(A_0 + \epsilon\, A_1)\; x + (b_0 + \epsilon\, b_1) = 0\,,$$

with A_0 singular and $b_0 \in$ range A_0. The solution manifold M_0 for $\epsilon = 0$ *disappears* for $\epsilon > 0$. In the expansion of the zero $z(\epsilon) = z_0 + \epsilon\, z_1 + \mathrm{O}(\epsilon^2)$, the component of z_1 *orthogonal to* M_0 is *well-conditioned* while the component *parallel to* M_0 is increasingly *ill-conditioned* as $\epsilon \to 0$. Accordingly, with the assumption of a tolerance in the problem, the pseudozero sets stretch like $\mathrm{O}(1/\epsilon)$ parallel to M_0 as $z(\epsilon)$ approaches M_0 for $\epsilon \to 0$.

In *multivariate polynomial systems*, there are more possibilities of a singular behavior: Multiple zeros, zeros diverging to infinity, zero manifolds, and combinations of these. We consider only the case where P_0 in the system $P(x;\epsilon) = P_0(x) + \epsilon\, P_1(x) = 0$ has a zero manifold M_0, and we observe – as in the linear system – the behavior of a zero $z(\epsilon) = z_0 + \epsilon\, z_1 + \mathrm{O}(\epsilon^2)$ with $z_0 \in M_0$ which requires that $P_1(z_0) \in$ range $P_0'(z_0)$. With a SVD of $P_0'(z_0)$, the situation is found to be locally analogous to the linear case: For $\epsilon \approx 0$, the *distance* of $z(\epsilon)$ from M_0 remains well-conditioned while its position *along* M_0 is very ill-conditioned; the pseudozero domains extend further and further along M_0.

A polynomial system from biomolecular modelling (cyclo-hexane) was used as a realistic example. Since singular phenomena are widespread in multivariate polynomial systems, it is important to be able to *recognize* and *analyze* them. Ideally, the codes for solving such systems should do that automatically.

32 Guaranteed Parameter Estimation for Characterization of Microdevices

by Bernd Tibken

The problem of parameter estimation under noisy measurements is adressed. We assume that a model of the system under investigation is given and that the real measurements which can be made are corrupted by noise. The only knowledge about the noise is an upper bound on the magnitude. Under these assumptions the set of guaranteed parameter estimates is the set of all parameters which are compatible with the real measurements, the model

equations, and the upper bound on the noise. This set is in general a complicated subset of R^n and it is very difficult to obtain an exact representation. Thus, we discuss an interval algorithm which enables us to approximate this set of guaranteed parameters from the inside and the outside. This algorithm is applied to the parameter estimation for a microrelay and leads to an important new characterization of the dynamical behaviour of this microrelay. Some conclusions and an outlook will be given at the end of the talk.

33 A Verification Method for Indices of Eigenvalues of Symmetric Matrices

by Nobito Yamamoto

We propose a simple method for validated computing of eigenvalues of symmetric matrices. The method is based on $L\,D\,L^T$ decomposition and its error estimation. The indeces of eigenvalues with respect to magnitude also can be obtained by the method.
The method has the following features.

1. It is based on elementary theories and easy to understand.
2. Coding and implementation are also easy.
3. As well as bounds of an eigenvalue, the index of the eigenvalue in order of magnitude can be obtained.
4. It can be applied to a multiple eigenvalue or a cluster of eigenvalues.
5. It is also applicable to generalized eigenvalue problems.
6. One can easily extend this method to deal with interval valued matrices, if the widths of the intervals are not so large.
7. For band matrices, we can reduce memories being used.

A defect is that the precision of this method is sometimes not so high because of numerical instability of $L\,D\,L^T$ decomposition. In spite of this defect, we believe through our numerical experiments that this method can be put into practical use.

34 On the Accuracy of the Shortley-Weller Approximation for Dirichlet Problems

by Tetsuro Yamamoto

It is recently known (Yamamoto (1998), Matsunaga-Yamamoto (1999)) that the Shortley-Weller (S-W) finite-difference approximation U applied to the Dirichlet problem

$$\begin{cases} \Delta u = f(x,y,u) & \text{in } \Omega, \quad f_u \geq 0, \\ u = g(x,y) & \text{on } \Gamma = \partial\Omega \end{cases} \tag{$*$}$$

has the following property: If the solution u of $(*)$ belongs to $C^{l+2,\alpha}(\overline{\Omega})$, $l = 0$ or 1 and $0 < \alpha \leq 1$, then

$$|u(P_{ij}) - U(P_{ij})| \leq \begin{cases} O(h^{l+1+\alpha} + k^{l+1+\alpha}) & \text{at } P_{ij} \text{ near } \Gamma \\ O(h^{l+\alpha} + k^{l+\alpha}) & \text{otherwise,} \end{cases}$$

where P_{ij} denote grid points with mesh sizes $\Delta x = h$, $\Delta y = k$. In particular, if $u \in C^{3,1}(\overline{\Omega})$, then the S-W approximation has $O(h^3 + k^3)$ accuracy at grid points near Γ and $O(h^2 + k^2)$ at other grid points, even if the local truncation error is $O(h + k)$ near Γ. It is already shown by Matsunaga (1998) that the Bramble approximation and the Collatz approximation do not have such a property.

In this talk, after reviewing this result, we discuss the behavior of the S-W approximation for $(*)$ in the case where $u \notin C^{l+2,\alpha}(\overline{\Omega})$. Superconvergence and nonsuperconvergence theorems are given as well as numerical examples illustrating the theorems.

This is a joint work with Fang of Ehime University and Chen of Shimane University.

35 How Orthogonality is Lost in Krylov Methods

by Jens–Peter M. Zemke

The fastest known verification methods for the solution of sparse eigenproblems $Av = v\lambda$ and the solution of sparse linear systems $Ax = b$ for a given matrix $A \in \mathbb{K}^{n\times n}$ involve $O(n^3)$ operations and $O(n^2)$ storage.
All known verification methods are direct methods. Krylov methods are direct methods, but due to numerical instability they are only used as iterative methods. The question is whether they can serve as a building block for a purely iterative verification method with lower complexity.
To answer this question a unified framework for perturbed Krylov eigensolvers is presented. Examination results in a relation between convergence, the residuals and loss of orthogonality. A numerical example is used to show the impacts of the obtained relation.
In infinite precision every Krylov linear system solver corresponds to some Krylov eigensolver. In finite precision a linear system solver corresponds to some perturbed eigensolver.
As a consequence, Krylov methods can neither be used to compute guaranteed lower bounds to the smallest eigenvalue nor to compute inclusions of the solution of linear systems. This holds true even if the obtained approximations are close to the exact solution.

Dagstuhl Seminar 99471

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