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Symbolic and Numerical Scientific Computation

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Preface

Scientific computation has a long history, dating back to the astronomical tables of the Babylonians, the geometrical achievements of the Egyptians, the calendars of the Mayans, and the number theory of the ancient Chinese. The success of these activities led in many parts of the world to the development of mathematical theories trying to explain the surprising applicability of pure thought to physical phenomena. Probably the most important such development took place in ancient Greece, where mathematics, as we know it today, was created.

Just as practical advances in scientific computation have stimulated the development of theory, so also new theoretical breakthroughs have led to whole new ways of mathematizing science. A prominent example is the development of calculus by Newton and Leibnitz and its application in all areas of science. Mathematical theory, however, became more and more abstract and removed from possible applications.

The twentieth century witnessed the advent of computing devices in the modern sense. Right from the beginning these machines were used for facilitating scientific computations. The early achievements of space exploration in the 1950s and 1960s would have been impossible without computers and scientific computation.

Despite this success, it also became clear that different branches of scientific computation were taking shape and developing apart from each other. Numerical computation saw itself mainly as a computational offspring of calculus, with approximations, convergence, and error analysis forming its core. On the other hand, computer algebra or symbolic computation derived its inspiration from algebra, with its emphasis on solving equations in closed form, i.e., with exact-solution formulae. Both of these branches were very successful in their own right, but barely interacted with each other.

However, this split of scientific computation into numerical and symbolic branches was felt more and more to be a problem. Numerical methods in solving differential equations might make use of an analysis of integrability conditions or symmetries, which can be provided by symbolic methods. Symbolic methods, on the other hand, rely on exact inputs, which are often hard to come by. So they need to be extended to cover certain neighborhoods of their input data. Problems such as these require a well-balanced integration of symbolic and numerical techniques.

In 1998 the Austrian Science Fund (Fonds zur Förderung der wissenschaftlichen Forschung) established the Special Research Program (Spezialforschungsbereich, SFB) "Numerical and Symbolic Scientific Computing" at the Johannes Kepler Universität, Linz, Austria. The speaker of this SFB is Ulrich Langer, and the current co-speaker is Franz Winkler. In this SFB various research groups with backgrounds in numerical analysis and in symbolic computation join forces to bridge the gap between these two approaches to scientific computation. For more detail, please check out the Web page of the SFB: `http://www.sfb013.uni-linz.ac.at`. Besides bringing local researchers together to work on numerical and symbolic problems, this SFB also sees itself as an international forum. Over the years we have organized several conferences and workshops on scientific computation. In particular, in August 1999 the workshop "Symbolic and Numerical Scientific Computation (SNSC '99)" took place in Hagenberg near Linz, the home of the Research Institute for Symbolic Computation (RISC-Linz). SNSC '99 was quite a success. So in September 2001 we held the second such conference, "Symbolic and Numerical Scientific Computation (SNSC '01)", again in Hagenberg.

As for SNSC '99, Franz Winkler served as the organizer and general chair of the conference. SNSC '01 was designed as an open conference of the SFB. The goal was to further the integration of methods in symbolic and numerical scientific computation. Topics of interest for the conference included all aspects of symbolic-numerical scientific computation, in particular: construction of algebraic multigrid methods for solving large-scale finite element equations, computer-aided geometric design, computer-supported derivation of mathematical knowledge, constraint solving, regularization techniques, combinatorics and special functions, symmetry analysis of differential equations, differential geometry, visualization in scientific computation, and symbolic and numerical methods in engineering sciences. The following invited speakers addressed these topics in their presentations:

J. Apel, "Passive Complete Orthonomic Systems of PDEs and Riquier Bases of Polynomial Modules,"
M. Dellnitz, "Set-Oriented Numerical Methods for Dynamical Systems,"
E. Hubert, "Differential Equations from an Algebraic Standpoint,"
F. Schwarz, "Algorithmic Lie Theory for Solving Ordinary Differential Equations,"
H.J. Stetter, "Algebraic Predicates for Empirical Data,"
R. Walentyński, "Solving Symbolic and Numerical Problems in the Theory of Shells with *MATHEMATICA*."

In addition to these invited presentations, 25 contributed talks were given at the conference.

This book contains the proceedings of the conference SNSC '01. The participants were encouraged to submit revised and elaborated papers on their presentations, and many of them did so. These submissions were then carefully refereed by at least two independent referees each, under the supervision of the editors.

The papers in this proceedings volume fall into three categories:

I. Symbolics and Numerics of Differential Equations,
II. Symbolics and Numerics in Algebra and Geometry,
III. Applications in Physics and Engineering.

In the following we briefly describe the various contributions and their interrelations.

I. Symbolics and Numerics of Differential Equations:

Several invited presentations focused on algebraic methods for the investigation of differential systems. The first paper by E. Hubert, "Notes on Triangular Sets and Triangulation-Decomposition Algorithms I: Polynomial Systems," reviews the constructive algebraic theory of the solution of systems of polynomial equations. The core of any such solution method is the elimination of some variables from some of the given equations. In the optimal case we arrive at a triangular system of equations, which can then be solved "one variable at a time." In her second paper, "Notes on Triangular Sets and Triangulation-Decomposition Algorithms II: Differential Systems," E. Hubert describes the extension of the polynomial elimination theory to differential algebra. Differential polynomials are associated with differential equations, and radical differential ideals with differential systems. Hubert investigates questions about the solution sets of differential systems by viewing them in terms of the corresponding radical differential ideals. In his paper "Passive Complete Orthonomic Systems of PDEs and Riquier Bases of Polynomial Modules," J. Apel relates passive complete orthonomic systems of PDEs and Gröbner bases of finitely generated modules, which can be seen as Riquier bases or so-called involutive bases of these differential systems. This correspondence opens the way for an algebraic analysis of differential systems. Lie's symmetry theory allows us to classify differential systems, determine canonical forms of such systems, derive qualitative properties and in certain cases also solve such systems. F. Schwarz investigates "Symmetries of Second- and Third-Order Ordinary Differential Equations" in his contribution.

In the contributed papers in this category K. Schlacher et al. deal with "Symbolic Methods for the Equivalence Problem of Systems of Implicit Ordinary Differential Equations." The goal in this investigation is to identify solutions of an original set of differential equations as solutions of a given normal form. M. Hausdorf and W.M. Seiler are able to generalize ideas from differential algebraic equations to partial differential equations in their paper "On the Numerical Analysis of Overdetermined Linear Partial Differential Systems." Involutive systems provide important normal forms for differential systems. Some of their algebraic and computational aspects are investigated by R. Hemmecke in "Dynamical Aspects of Involutive Bases Computations."

II. Symbolics and Numerics in Algebra and Geometry:

In their invited paper "Congestion and Almost Invariant Sets in Dynamical Systems," M. Dellnitz and R. Preis propose a new combination of numerical and graph theoretic tools for both the identification of the number and the location of almost invariant sets of a dynamical system which are subsets of the state space where typical trajectories stay for a long period of time before entering other parts of the state space. The algorithms derived find interesting applications in the analysis of the dynamics of molecules.

The contributed papers in this category cover a wide range of different symbolic and numeric techniques and also interactions between these techniques. G. Brown proposes certain combinatorial graphs, so-called datagraphs, as a means for classifying and storing information on algebraic varieties. V. Marotta elaborates Stetter's approach of neighborhoods, i.e., inexactly given symbolic objects, in her paper on "Resultants and Neighborhoods of a Polynomial." The issue here is that in practical applications polynomials are given with inexact coefficients. Given such an inexact object, one tries to identify a neighboring object exhibiting a certain structure. "Multi-variate Polynomials and Newton-Puiseux Expansions" are investigated by F. Beringer and F. Richard-Jung. This provides a generalization of local resolution from the classical curve case to the case of hypersurfaces. P. Paule et al. use algebraic methods for constructing wavelets that satisfy alternatives to the vanishing moments conditions in their paper "Wavelets with Scale-Dependent Properties." N. Beaudoin and S.S. Beauchemin propose a numerical Fourier transform in d dimensions that provides an accurate approximation of the corresponding continuous Fourier transform with similar time complexity as the discrete Fourier transform usually realized by Fast Fourier Transform (FFT) algorithms. The paper by G. Bodnár et al. deals with the method of exact real computations that seems to provide a reasonable and effective alternative to the usual symbolic techniques of handling exact computations. In particular, the authors consider some real linear algebra and real polynomial problems such as inversion of nonsingular matrices, computation of pseudoinverses, greatest common divisor computations, and roots computations. Some of these problems are ill-posed and require regularization techniques like the Tikhonov regularization technique. U. Langer et al. develop a new symbolic method for constructing a symmetric, positive definite M-matrix that is as close as possible to some given symmetric, positive definite matrix in the spectral sense. This technique is then directly used for deriving efficient algebraic multigrid preconditioners for large-scale finite element stiffness matrices.

III. Applications in Physics and Engineering:

Applications of both symbolic and numerical techniques in the theory of shells, i.e., thin layers of physical bodies, are exhibited in the invited paper "Solving Symbolic and Numerical Problems in the Theory of Shells with *MATHEMATICA*" by R.A. Walentyński. The author demonstrates the applicability of a typical computer algebra system, in this case *MATHEMATICA*, to mechanical problems.

Several contributed papers describe hybrid symbolic-numerical techniques for practical problems. A.R. Baghai-Wadji makes a conjecture about the diagonalizability of linearized PDEs as models of physically realizable systems and gives a variety of examples of his conjecture in "A Symbolic Procedure for the Diagonalization of Linear PDEs in Accelerated Computational Engineering." The computer algebra system *Maple* is used by V.L. Kalashnikov in his paper "Generation of the Quasi-solitons in the Lasers: Computer Algebra Approach to an Analysis." A. Shermenev investigates the two-dimensional shallow water equation describing the propagation of surface gravity waves in polar coordinates. He presents some solutions to this equation in the form of analytic representations.

The organizers express their thanks to the Austrian Science Fund (FWF), the University of Linz, the Government of Upper Austria, and the City of Linz for moral and financial support. The organizers would like to thank the institute RISC-Linz for its hospitality during the conference. Last, but not least, we thank Rahul Athale for his work in collecting all these contributions and preparing them for printing.

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