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Computer Algebra in Scientific Computing

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Sadly, Andreas Weber passed away on March 15, 2020. Andreas studied mathematics and computer science at the Universities of Tübingen, Germany, and Boulder, Colorado, USA. He then worked as a postdoc at the Institute for Computer Science at Cornell University, New York, USA; the University of Tübingen, Germany; and the Fraunhofer Institute for Computer Graphics Research, Germany. Since 2001, he was a professor at the University of Bonn, Germany.

Scientifically, he was considered an authority in the fields of physics-based modeling and simulation, as well as applications of computer algebra in the natural sciences and particularly biology. He was incredibly well-read, possessed an immense wealth of knowledge across different disciplines, and was highly committed to international and interdisciplinary networking. Due to his great hospitality and openness, his group in Bonn developed into a permanent lively meeting place of scientists from different fields from all over the world, where science could take place at its best.

Andreas made many contributions to CASC, attending almost all conferences in its history. He contributed many papers, hosted CASC in Bonn in 2007, was an invited speaker in 2010, a PC member during 2000–2013, and most recently served as publicity chair in 2014–2019. We will always remember his good-natured humor and his boundless compassion for science and for others. We will miss his presence very much.

Preface

The International Workshop on Computer Algebra in Scientific Computing (CASC), held annually since 1998, has established itself as a leading forum for presenting recent developments in the area of computer algebra and on pioneering applications of computer algebra methods in sciences such as physics, chemistry, celestial mechanics, life sciences, engineering, etc. The CASC 2020 International Workshop featured a balanced mix of high-level keynote speeches and concurrent oral sessions.

CASC 2020 Venue

It was initially decided, in the autumn of 2019, that the 22nd CASC International Workshop would be held at Johannes Kepler University (JKU), Linz, Austria, in September 2020. The choice of this university was particularly fitting since research in computer algebra has been conducted therein for many years.

The city of Linz, and maybe even more the little village of Hagenberg 25 km north of Linz, is well known in the computer algebra community, since the RISC (Research Institute for Symbolic Computation) is located in a medieval castle in Hagenberg. RISC was founded in 1987 by Bruno Buchberger as an institute of JKU and moved to Hagenberg in 1989. Since its foundation RISC has developed into one of the world's leading institutes in the area of symbolic computation. Buchberger's vision encloses the entire range from pioneering mathematical research to industry proven software engineering. The RISC Software Company was founded in 1992 as part of RISC and it embodies the duality of basic research and applications.

To mathematicians, Bruno Buchberger is known as the inventor of Gröbner bases theory and Buchberger's algorithm, which he developed in his PhD thesis in 1965. Nowadays, Gröbner bases are one of the fundamental pillars of symbolic computation and the applications range from algebraic geometry or applied mathematics to science and engineering. Every major computer algebra system has its implementation of Gröbner bases.

Presently, symbolic computation has a strong basis in Linz. RISC is currently directed by Peter Paule and consists of the following research groups: automated reasoning, computer algebra for combinatorics, computer algebra for differential equations, computer algebra for geometry, formal methods, rewriting-related techniques and applications, and symbolic methods in kinematics. The JKU Institute for Algebra, led by Manuel Kauers, also puts a strong emphasis on research in computer algebra. The main research areas covered are symbolic summation and integration, operator algebras, special functions identities and inequalities, and applications of computer algebra in combinatorics, experimental mathematics, and systems biology. Furthermore, there is a group on symbolic computation under the guidance of Josef Schicho at the Radon Institute for Computational and Applied Mathematics (RICAM),

an institute of the Austrian Academy of Sciences (OeAW). Its focus is on computer algebra, algebraic geometry, differential algebra, holonomic functions, and kinematics.

The research activity of the mathematical departments of Linz actively promote the significant impact of computer algebra in scientific computing. For over 20 years they have been showing a strong commitment to interdisciplinary research. In 1998 the Special Research Program (SFB) "Numerical and Symbolic Scientific Computing" was launched with the participating institutes of Applied Geometry, Computational Mathematics, Industrial Mathematics, and RISC. This enterprise became a role model for interdisciplinary research and doctoral education. At the end of its runtime in 2008, it was succeeded by the doctoral program (DK) "Computational Mathematics: Numerical Analysis and Symbolic Computation." In addition to the four institutes of the SFB, currently the participating institutes are the institute for Algebra, Stochastics, and RICAM. One of the general goals of the doctoral education in the DK is to gain expertise in algorithmic mathematics. Two decades of interdisciplinary cooperation have also shaped the curriculum of the undergraduate education at JKU. There is a basic understanding that scientific computing and computer algebra go well together, which makes Linz a great place to meet for CASC, even if it is only virtually this year.

The Organizing Committee of CASC 2020 monitored the development of the COVID-19 pandemic. The safety and well-being of all conference participants was our priority. After studying and evaluating the announcements, guidance, and news released by relevant national departments, the decision was made to host CASC 2020 as an online event.

Overview of the Volume

This year, CASC 2020 had two categories of participation: (1) talks with accompanying papers to appear in the proceedings, and (2) talks with accompanying extended abstracts for distribution locally at the conference only. The latter was for work either already published, or not yet ready for publication, but in either case still new and of interest to the CASC audience. The former was strictly for new and original research results, ready for publication.

All papers submitted for the LNCS proceedings received a minimum of three reviews, and some received more, with the average number of reviews being 3.2 per paper. In addition, the whole Program Committee (PC) was invited to comment and debate on all papers. At the end of the review process, the PC chose to accept 28 papers. A further 6 papers were accepted later through a conditional path (the authors had to first provide a revised version to meet specific requirements set by the PC). Hence in total this volume contains 34 contributed papers, along with 2 papers to accompany our keynote talks.

The invited talk of Ovidiu Radulescu is devoted to the application of tropical geometry for the mathematical modeling of biological systems. Tropical geometry methods exploit a property of biological systems called **multiscaleness**, summarized by two properties: i) the orders of magnitude of variables and timescales are widely distributed, and ii) at a given timescale, only a small number of variables or

components play a driving role, whereas large parts of the system have passive roles and can be reduced. Several models of biological systems and their reductions are presented. The change of variables is used to "tropicalize" biochemical networks. It is shown how to find the appropriate scalings for parameters with the aid of tropical geometry approaches. The conclusion is made that tropical geometry methods are possible ways to symbolic characterization of dynamics in high dimension, also to synthesize dynamical systems with desired features.

The other invited talk by Werner Seiler is accompanied by a joint paper with Matthias Seiß which gives an overview of their recent works on singularities of implicit ordinary or partial differential equations. This includes firstly the development of a general framework combining algebraic and geometric methods for dealing with general systems of ordinary or partial differential equations, and for defining the type of singularities considered here. An algorithm is also presented for detecting all singularities of an algebraic differential equation over the complex numbers. The adaptions required for the analysis over the real numbers are then discussed. The authors further outline, for a class of singular initial value problems, for a second-order ordinary differential equation, how geometric methods allow them to determine the local solution behavior in the neighborhood of a singularity, including the regularity of the solution. Finally, it is shown for some simple cases of algebraic singularities how such an analysis can be performed there.

Polynomial algebra, which is at the core of computer algebra, is represented by contributions devoted to establishing intrinsic complexity bounds for constructing zero-dimensional Gröbner bases, the implementation of power series arithmetic in the Basic Polynomial Algebra Subprograms (BPAS) Library, the investigation of the relations between the Galois group and the triviality of the exponent lattice of a univariate polynomial, multiplier verification with the aid of Nullstellensatz-proofs, the complexity analysis of sparse multivariate Hensel lifting algorithms for polynomial factorization, the new approximate GCD algorithm with the Bezout matrix, the computation of logarithmic vector fields along an isolated complete intersection singularity, the computation of parametric standard bases for semi-weighted homogeneous isolated hypersurface singularities with the aid of the CAS SINGULAR, acceleration of subdivision root-finders for real and complex univariate polynomials, the optimization of multiplying univariate dense polynomials with long integer unbalanced coefficients with the aid of Tom–Crook approach, the investigation of the Routh–Hurwitz stability of a polynomial matrix family under real perturbations, symbolic-numeric computation of the Bernstein coefficients of a polynomial from those of one of its partial derivatives, and the derivation with the aid of Gröbner bases of new optimal symplectic higher-order Runge–Kutta–Nyström methods for the numerical solution of molecular dynamics problems.

Several papers are devoted to linear algebra and its applications: finding good pivots for small sparse matrices, the presentation of a new linear algebra approach for detecting binomiality of steady state ideals of reversible chemical reaction networks, and parametric linear system solving by using the comprehensive triangular Smith normal form.

Two papers deal with applications of symbolic-numerical computations for: computing orthonormal bases of the Bohr–Mottelson collective model, implemented in the

CAS MATHEMATICA, and a symbolic-numeric study of geometric properties of adiabatic waveguide modes.

Two papers are devoted to the application of symbolic computations for investigating and solving ordinary differential equations (ODEs): contact linearizability of scalar ODEs of arbitrary order and the investigation of the invariance of Laurent solutions of linear ODEs under possible prolongations of the truncated series which represent the coefficients of the given equation.

Three papers deal with the investigation and solution of celestial mechanics problems: applications of the CAS MATHEMATICA, to the study of stationary motions of a system of two connected rigid bodies in a constant gravity field with the aid of Gröbner bases and to the analytic investigation of the translational-rotational motion of a non-stationary triaxial body in the central gravity field; the obtaining of periodic approximate solutions of the three-body problem with the aid of conservative difference schemes and the free open-source mathematics software system SAGE (www.sagemath.org).

The remaining topics include the new complexity estimates of computing integral bases of function fields, first-order tests for toric varieties, which arise, in particular, in chemical reaction networks, Hermite interpolation of a rational function with error correction, the improved balanced NUCOMP algorithm for the arithmetic in the divisor class group of a hyperelliptic curve, algebraic complexity estimates for an efficient method of removing all redundant inequalities in the input system, a multithreaded version of the robust tracking of one path of a polynomial homotopy, the improvement of the Lazard's method for constructing the cylindrical algebraic decomposition, new extensions implemented in the SCALA algebra system, a new MAPLE package that allows obtaining compatible routes in an overtaking railway station of any number of tracks, and the use of the LEGO digital designer for teaching algebraic curves in mathematical education via LEGO linkages.

August 2020

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Organization

CASC 2020 was organized by the Johannes Kepler University (JKU), Linz, Austria.

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