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Numerical Software with Result Verification

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Preface

Reliable computing techniques are essential if the validity of the output of a numerical algorithm is to be guaranteed to be correct. Our society relies more and more on computer systems. Usually, our systems appear to work successfully, but there are sometimes serious, and often minor, errors. Validated computing is one essential technology to achieve increased software reliability. Formal rigor in the definition of data types, the computer arithmetic, in algorithm design, and in program execution allows us to guarantee that the stated problem has (or does not have) a solution in an enclosing interval we compute. If the enclosure is narrow, we are certain that the result can be used. Otherwise, we have a clear warning that the uncertainty of input values might be large and the algorithm and the model have to be improved. The use of interval data types and algorithms with controlled rounding and result verification capture uncertainty in modeling and problem formulation, in model parameter estimation, in algorithm truncation, in operation round-off, and in model interpretation.

The techniques of validated computing have proven their merits in many scientific and engineering applications. They are based on solid and interesting theoretical studies in mathematics and computer science. Contributions from fields including real, complex and functional analysis, semigroups, probability, statistics, fuzzy interval analysis, fuzzy logic, automatic differentiation, computer hardware, operating systems, compiler construction, programming languages, object-oriented modeling, parallel processing, and software engineering are all essential.

This book, which contains the proceedings of the Dagstuhl Seminar 03041 ‘Numerical Software with Result Verification’ held from January 19 to 24, 2003, puts particular emphasis on the most recent developments in the area of validated computing in the important fields of software support and in applications.

We have arranged the contributions in five parts. The first part deals with languages supporting interval computations. The paper by Wolff von Gudenberg studies different object-oriented languages with respect to their abilities and possibilities to efficiently support interval computations. The contribution by Hofschuster and Krämer gives an overview of the C-XSC project, a C++ class library supporting intervals, the precise scalar product, standard functions with intervals, and various class abstractions useful for scientific computation.

The second part is devoted to software systems and tools. In a joint paper, Kearfott, Neher, Oishi and Rico present and compare four such systems: GlobSol, a Fortran-based library for the verified solution of nonlinear algebraic systems of equations and global optimization; ACETAF, an interactive tool for the verified computation of Taylor coefficients; Slab, a complete Matlab-style high-performance interval linear algebra package; and (Fixed) CADNA, a tool for assessing the accuracy and stability of algorithms for embedded systems relying on a fixed-point arithmetic. Whereas the first three software systems

use (machine) interval arithmetic, the latter is based on the CESTAC method and its stochastic arithmetic. Going beyond double precision in machine interval arithmetic is the topic of the paper by Grimmer, Petras and Revol. They describe `intPackX`, a Maple module which, among others, provides correctly rounded multiprecision evaluation of standard functions, and the two C/C++ based libraries GMP-XSC and MPFI. The authors include several examples where multiple precision interval arithmetic is of primary importance, for example to show the existence of Kronrod-Patterson rules for numerical integration or in the numerical solution of ODEs in Asian options pricing. The last paper in this part is by Corliss and Yu who report on their approach and their strategy and experience when testing a preliminary version of an interval software package for its correctness.

As software supporting interval and validated computation becomes more and more popular, we witness an increasing number of new modeling techniques using intervals. The third part of this volume contains five papers on these topics. Kieffer and Walter consider parameter and state estimation in dynamical systems involving uncertain quantities. For cooperative models, they use interval-based set inversion techniques to obtain tight bounds on the parameters and states under the given uncertainties. In an additional paper, together with Braems and Jaulin, they propose a new, interval computation-based technique as an alternative to computer algebra when testing models for identifiability. Auer, Kecskeméthy, Tändl and Traczinski show that interval analysis provides new opportunities to model multibody systems and they present an advanced software system `MOBILE` that includes such interval techniques. Bühler, Dyllong and Luther discuss reliable techniques in computational geometry. They focus on distance and intersection computations, an area where slightly wrong floating-point results may produce a completely wrong view of the geometry. The last paper by Alefeld and Mayer deals with the more fundamental issue of how interval arithmetic iterations behave when applied to solve linear systems with a singular coefficient matrix.

Part four considers various applications of validation techniques in science and engineering. It starts with a contribution by Beelitz, Bischof, Lang and Schulte Althoff on methods that guarantee the absence of singularities in certain models for the analysis and design of chemical processes. This is of primary importance, since otherwise multiple steady states may result in spontaneous fluctuations which may even damage the chemical reactor. Fausten and Haßlinger consider workload distributions of service systems in telecommunications under quality-of-service aspects. They develop a method to determine workload distributions involving a verification step based on interval arithmetic. Three important problems in geodesy are dealt with in the paper by Borovac and Heindl, who present verified methods for the direct and the inverse problem of geodetic surveying and the three-dimensional resection problem. Among others, enclosure methods for ODEs turn out to be very useful here. Schichl describes the `CO-CONUT` project, a large, European, modular software project for constrained global optimization. The paper explains the architecture of this software system,

which uses the FILIB++ library for its components based on interval arithmetic. Finally, the paper by Oussena, Henni and Alt describes an application from medical imaging in which verified computations would be of great help.

The last part is devoted to alternative approaches to the verification of numerical computations. The contribution by Lester shows how one can use the formal specification checker PVS to validate standard functions like arctan and some exact arithmetic algorithms. Granvilliers, Kreinovich and Müller present three alternative or complementary approaches to interval arithmetic in cases where uncertainty goes beyond having bounds on input data: interval consistency techniques, techniques using probabilistic information and techniques for processing exact real numbers. This part closes with the paper by Putot, Goubault and Martel, who propose the use of static code analysis to study the propagation of round-off. They also present a prototype implementation of their approach.

We would like to thank all authors for providing us with their excellent contributions and for their willingness to join in groups to present a coherent description of related research and software. We are also grateful to Springer-Verlag for the fruitful cooperation when preparing this volume and, last but not least, to the referees listed below.

January 2004

René Alt
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