SIAM Conference on Optimization, Validated Computing 2002, and the Fields Institute Informal Working Group on Validated Optimization A Personal View<sup>†</sup>

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Validated Computing 2002 took place in Toronto on May 23 to May 25, 2002, immediately after the Seventh SIAM Conference on Optimization and immediately before an informal workshop on validated optimization at the Fields Institute on the University of Toronto Campus. Highlights included

- a tutorial introduction to interval techniques, in the evening immediately following the SIAM Conference on Optimization and immediately preceding Validated Computing 2002 (we thank George Corliss);
- an awarding of the 2002 Moore Prize for the best application of interval computations;
- a banquet honoring Ramon Moore for his ground-breaking work in interval analysis.

Program details for Validated Computing 2002, including a schedule and extended abstracts in both PostScript and PDF format, can be found at

http://www.cs.utep.edu/interval-comp/interval.02/program.html We cordially thank Vladik Kreinovich for setting up this web page. The announcement and explanation for Validated Computing 2002 can still be found at

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http://interval.louisiana.edu/conferences/
Validated_computing_2002/html_notice.html
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Details of the Fields Institute Informal Workshop on Validated Optimization, including a daily schedule, images of most of what was

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written on the blackboards, miscellaneous images, and images of George Corliss' notes can be found at

http://www.fields.utoronto.ca/programs/scientific/01-02/ numerical/optimization/

We thank George Corliss for setting this up, both during and after the workshop.

Information about the SIAM Conference on Optimization can be found at

http://www.siam.org/meetings/op02/index.htm

#### 1. The Moore Prize

The editorial board of *Reliable Computing* received ten excellent nominations for the Moore Prize, including work by C. Camacho and L. H. de Figueiredo, K. Makino, R. L. Muhanna and R. L. Mullen, K. Nagatou, P. S. V. Nataraj and K. Kotecha, N. S. Nedialkov and K. R. Jackson, J. B. S. Oliviera and L. H. de Figueiredo, U. Schäfer, S. Sheela, and W. Tucker. The applications ranged from mathematics (nonlinear dynamics) to physics and astronomy (asteroid orbit prediction, etc.) to mechanics (clever ways of validating finite element models; ordinary and partial differential equations) to computational geometry to validated global optimization. Evaluating full-length papers for each nominee and voting, the *Reliable Computing* editorial board chose Warwick Tucker of Cornell University (and soon to be at the University of Uppsala) as a clear winner.

Dr. Tucker's work, "A Rigorous ODE Solver and Smale's 14<sup>th</sup> Problem," uses interval computations to prove once and for all that a strange attractor exists for the Lorenz equations. This has been a high-profile mathematical question for 35 years. Many others had previously attempted but had failed to answer this question rigorously. Although new to the area, Dr. Tucker resolved the question with innovative techniques for hyperbolic (semi-stable) fixed points for the verified integration of the Lorenz system of ordinary differential equations. The work appears in Tucker's Ph.D. dissertation and in the paper "A Rigorous ODE solver and Smale's 14<sup>th</sup> Problem," to appear in *Foundations of Computational Mathematics*.

The Lorenz equations, proposed by Edward Lorenz in 1963, are a highly simplified set of equations associated with atmospheric dynamics (obtained by ignoring higher-order terms in certain Taylor series):

$$\begin{aligned} x_1' &= -\sigma x_1 + x_2 \\ x_2' &= \rho x_1 - x_2 - x_1 x_3 \end{aligned}$$

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$$x_3' = -\beta x_3 + x_1 x_2,$$

where the parameters corresponding to the question of the strange attractor are  $\sigma = 10$ ,  $\beta = 8/3$ , and  $\rho = 28$ .

Since the Lorenz equations are not presently considered to be a realistic model of atmospheric dynamics, Tucker's success is an application to mathematics, in contrast to engineering, financial, or biological applications that have immediate monetary consequences. However, Tucker's work is related to basic techniques in the validated integration of systems of ordinary differential equations, techniques with wide applicability. Furthermore, Tucker's success has received wide recognition outside our area of specialization, and even outside mathematics. Also, actual atmospheric phenomena sometimes mimic phenomena associated with the Lorenz equations, and it may be possible to rigorously connect the Lorenz equations to more realistic models. Finally, Tucker's techniques are now being applied to traditional engineering and science application areas.

Warwick Tucker received his certificate from G. William Walster of Sun Microsystems, with congratulations from Ramon E. Moore.

### 2. The Banquet Honoring Ramon Moore

Most, if not all, of the work involving interval analysis during the past forty years can be traced to Ramon E. Moore, from his dissertation at Stanford in 1962 to his book *Interval Analysis* (Prentice–Hall, 1966), to his book *Methods and Applications of Interval Analysis* (SIAM, 1979), as well as other scholarly papers and books. To honor Ray, we held a banquet on Friday evening.

Friday afternoon, in a plenary session leading up to the banquet, we heard talks on the history of interval analysis from prominent participants in that history. This included Bill Walster (filling in for Eldon Hansen, who was indisposed), K. Madsen and Stig Skelboe (representing the Danish school, including the well-known "Moore–Skelboe" algorithm), Louis B. Rall (an early proponent of both interval methods and automatic differentiation), Annie Cuyt (a former student of Rall), and Ullrich Kulisch (director emeritus of the well-known Karlsruhe group, producers of the "SC" computer languages).

Friday evening, during a very nice banquet at the Westin Harbour Castle Hotel (the conference venue), Bill Walster presented Ramon Moore with a fancy bound volume of his early papers on interval analysis. Ray, in turn, presented each conference participant individually with a lapel pin stamped with the "Reliable Computing" logo<sup>1</sup>. Everyone, including Ramon Moore, was thoroughly pleased.

Sun Microsystems has purchased permission to post Moore's early papers (in the bound set he received) on the World Wide Web. They can be found at

http://interval.louisiana.edu/Moores\_early\_papers/ bibliography.html

# 3. Relationships to the Seventh SIAM Conference on Optimization

Immediately following the Seventh SIAM Conference on Optimization in the same venue, Validated Computing 2002 and the SIAM Conference on Optimization shared both topics and participants. In two minisymposia on "Interval Methods in Optimization," various experts among us presented our techniques to the optimization community at large. Perhaps more importantly, there was informal interaction, especially between experts in interval branch and bound methods and experts in deterministic global optimization methods that do not use interval arithmetic.

For example, a minisymposium on the DIRECT (as in "direct search") algorithm for global optimization, as well as in several poster sessions, people presented variants of a direct search algorithm extremely similar to a simple interval algorithm. In the DIRECT algorithm, upper and lower bounds on the range of a function are obtained from estimates for Lipschitz constants. A list, ordered, for example, on the basis of the lowest lower bound, is kept, as in interval techniques. Various heuristics are used to decide which box to subdivide next. In contrast to interval techniques similar to interval Newton methods are not used; a significant amount of the research focuses on handling the large list efficiently.

The DIRECT algorithm seems primitive to researchers in interval techniques for global optimization. However, proponents of the DIRECT algorithm counter that interval methods cannot be used for black-box objective functions. (A "black-box" objective function is one given by a very large computer program that represents years of effort in development.) Interval experts counter that validated computing should be in mind from the start of the modeling process. However, that is not always practical if the work has already been done, and the practicality

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<sup>&</sup>lt;sup>1</sup> This logo, designed by V. M. Nesterov and A. G. Yakovlev in the late 1980's, represents an arbitrary nonlinear curve completely enclosed in interval brackets.

of the intervals-at-the-beginning approach has not yet been thoroughly tried.

In an invited talk, C. T. Kelly highlighted such black-box problems in which gradient-based methods fail, and in which cruder "sampling methods" must be used. Although Kelly did not mention such methods, interval methods would also be impractical for such problems, if we are not allowed to examine the "black box."

A wealth of other traditional techniques were also presented at the SIAM Conference on Optimization. Traditional techniques are far ahead of validation in certain areas, particularly in large-scale problems and in problems for specialized classes, such as linear or quadratic programming. Also, not only can interval methods borrow basic approximation ideas from point methods, but "approximate" solutions can often be used to accelerate global algorithms.

In any case, both interval (validated) and unvalidated ("traditional") approaches to optimization will have their place for quite some time. More interaction between the groups of researchers is warranted, both to avoid duplication of effort and to share the best of both group's tools.

Another source of interaction and overlap between the two conferences centered on common interests between experts in interval computations and experts in automatic differentiation.

#### 4. Validated Computing 2002 Highlights

Aside from the historical and honorary content, numerous research advances were presented at Validated Computing 2002. Many of these were incremental, rather than monumental. However, taken all-together they represent continued satisfactory progress. We are particularly impressed with the rate at which sophisticated real problems are being successfully solved. Most of the tools have been around for some time. However, combining these tools in new and novel ways has resulted in more success in applications and in better algorithms (such as for global optimization). We foresee continued progress along these lines.

An applications panel discussion took place on Thursday evening. Linda Petzold, a renowned expert in the numerical solution of differential-algebraic systems, was invited to Validated Computing 2002 to stimulate interaction between experts in validation and other experts in numerical computations. During the panel discussion, she recommended we "reach out" across disciplines and find "killer applications", as a formula for professional success. Examples of excellent applications presented at the conference were Tucker's prize-winning paper "A Rigorous ODE Solver and Smale's 14<sup>th</sup> Problem", P. S. V. Nataraj and J. J. Barve's paper on "Generation of Bode and Nyquist Plots to a Prescribed Accuracy for Non-Rational Transfer Functions," and the range of applications reviewed in Mark Stadtherr's survey "Reliable Modeling Using Interval Analysis: Chemical Engineering Applications." Nataraj and Barve report interval run times that are much faster than those of existing point routines. Stadtherr, who has won prizes within the chemical engineering community for this work, reports discovery of previously unknown, yet more physically meaningful solutions to various models. Arnold Neumaier's excellent survey "Solving Real-Life Robotics Problems with Interval Techniques" provided guidance for future important applications.

Reaching out to other communities is occurring on several fronts, such as optimization, differential equations, and fuzzy set theory. These efforts include special sessions at conferences and special *Reliable Computing* issues on the interfaces between interval analysis and other disciplines. These efforts should continue.

During the applications panel discussion Andreas Griewank, a leader in automatic differentiation, voiced a contrasting opinion to the value of "killer applications." Reviewing his efforts at promoting automatic differentiation, he surmised that recognition of a field depends not only on one or two important applications, but also on continuing exposure of the scientific community as a whole to the techniques, and on many consistent small successes over time. To do this, we need to continue to "reach out" as we have mentioned. Where we have the power, we should provide incentives and encouragement for this type of interdisciplinary participation and collaboration.

In summary, a common thread was the need for collaboration of every kind.

#### 5. Informal Workshop on Validated Optimization

Touted as "informal," we were not even sure of all participants until the first day of the workshop. However, with George Corliss' expert organizational skills, we ended up with both a full schedule and effective interaction from Monday, May 27 through Saturday morning, June 1. The talks ranged from more-or-less traditional preparation to computer demonstrations to simple question-and-answer sessions. However, participants were free to interject and initiate discussion at any point in any presentation. This very effectively sharpened the ideas and increased the understanding of all the participants. Due to mutual interest, participants spent much of the time on the Martin Berz / Kyoko Makino Taylor models and associated software in COSY-Infinity. This was somewhat reminiscent of a dissertation defense, except that it lasted for days. In any case, it productively increased collective understanding of Taylor models, and will result in increased accessibility to the research community at large.

Other highlights were Mihály Markot's explanation of the circle packing problem, and Jeff Tupper's explanation of GraphEq, a highquality graphing package for instructional use<sup>2</sup>; GraphEq's power is directly due to the interval technology underlying it.

## 6. Acknowledgements

We wish to acknowledge the other members of the scientific committee, especially Dan Berleant and Weldon Lodwick, for proofreading this report and supplying material.

<sup>&</sup>lt;sup>2</sup> available at www.peda.com

VC02\_report.tex; 20/06/2002; 12:40; p.8