The Quality of Numerical Software: Assessment and Enhancement

In this chapter we provide some background on the conference which brought together the researchers whose work is described in this volume. Further information, including access to transparencies and audio recordings of some of the talks, are available at the conference World Wide Web site: <http://renoir.csc.ncsu.edu/IFIP/WoCo7/>.

1 CONFERENCE VENUE

The conference entitled *The Quality of Numerical Software: Assessment and Enhancement*, was held 8–12 July 1996 at St. Catherine's College in Oxford, England. This was the seventh working conference organized by the IFIP Working Group on Numerical Software (WG 2.5) on behalf of the IFIP Technical Committee on Software: Theory and Practice (TC 2). The 76 conference attendees heard 26 invited presentations by researchers active in this field*. In addition, nine brief presentations were contributed by attendees in an "Open Session" which was arranged at the meeting itself. Considerable time was allotted for discussions of issues raised in the presentations, and the bulk of this discussion is recorded in this volume.

2 THE PROGRAM

Monday, 8 July 1996

- 9.00-9.30 *Welcome, Administrative Details, Conference Rationale.* Brian Ford (Numerical Algorithms Group, United Kingdom) and John Rice (Purdue University, USA)
- 9.30-10.10 *Testing the Correctness of Linear Algebra Software.* Nick Higham (University of Manchester, United Kingdom)
- 10.10-10.40 Break
- 10.40-11.20 *Matrix Market: A Web Resource of Test Matrix Collections.* Ronald F. Boisvert (National Institute of Standards and Technology, USA)
- 11.20-12.00 *Is Nonnormality a Serious Computational Difficulty in Practice?* Francoise Chatelin (University of Paris IX Dauphine, France)
- 12.00-12.20 Discussion of Morning Papers. Takao Tsuda (Hiroshima City University, Japan)
- 12.20-2.00 Lunch

*This proceedings volume contains two additional invited papers whose authors were unable to be present at the conference.

- 2.00-2.40 *Case Studies on the Development of ScaLAPACK and the NAG Numerical PVM Library.* Sven Hammarling (Numerical Algorithms Group, United Kingdom)
- 2.40-3.20 *Automatic Parallel Program Generation for Finite Element Analysis.* Shun Doi (NEC Corp., Japan)
- 3.20-3.50 Break
- 3.50-4.30 *Improving the Usability of Numerical Software through User-Centered Design.* Cherri Pancake (Oregon State University, USA)
- 4.30-5.10 *Network-based Scientific Computation via Inferno: Solution of Partial Differential Equations.* Bill Coughran, Jr (Bell Laboratories, USA)
- 5.10-5.30 Discussion of Afternoon Papers. Bo Einarsson (University of Linköping, Sweden)

Tuesday, 9 July 1996

- 9.00-9.40 *Quality of Service and Scientific Workflows.* Mladen Vouk (North Carolina State, USA)
- 9.40-10.20 *Organizing a Numerical Software Development Team.* Jeremy Du Croz (Numerical Algorithms Group, United Kingdom)
- 10.20-10.50 Break
- 10.50-11.30 *Assuring the Quality of the Process of Assuring Software Quality.* Lee Osterweil (University of Massachusetts, USA)
- 11.30-12.10 *Real Inferno.* Eric Grosse (Bell Laboratories, USA)
- 12.10-12.30 Discussion of Morning Papers. John Rice (Purdue University, USA)
- 12.30-2.10 Lunch
- 2.10-2.50 *Testing and Evaluating Software for Large-Scale Constrained Optimization.* Philip Gill (University of California at San Diego, USA)
- 2.50-3.30 *Automatic Differentiation and Numerical Software Design.* Chris Bischof (Argonne National Laboratory, USA)
- 3.30-3.50 Break
- 3.50-4.30 *The Impact of Automatic Differentiation and Result Verification Techniques on the Quality of Numerical Software.* Wolfgang Walter (Technical University Dresden, Germany)
- 4.30-5.10 *The Visual Diagnosis on Numerical Calculation of PDE Problems and Experiments.* Yukio Umetani (Hitachi, Japan)
- 5.10-5.30 Discussion of Afternoon Papers. Margaret Wright (Bell Laboratories, USA)

Wednesday, 10 July 1996

- 9.00-9.40 *Developing ODE Software in New Computing Environments.* Larry Shampine (Southern Methodist University, USA)
- 9.40-10.20 *The Reliability of Standard Local Error Control Algorithms for Initial Value Ordinary Differential Equations.* Des Higham (University of Dundee, United Kingdom)
- 10.20-10.50 Break

- 10.50-11.30 *The Evaluation of Numerical Software for Delay Differential Equations.* Wayne Enright (University of Toronto, Canada)
- 11.30-12.10 *Development of Efficient General Purpose Monte Carlo Codes Used in Nuclear Engineering.* Masayuki Nakagawa (Japan Atomic Energy Research Institute)
- 12.10-12.30 Discussion of Morning Papers. Ian Gladwell (Southern Methodist University, USA)

Thursday, 11 July 1996

- 9.00-9.40 *Testing Functions of One or Two Arguments.* Van Snyder (Jet Propulsion Laboratory, USA)
- 9.40-10.20 *The T-Experiments: Errors in Scientific Software.* Les Hatton (Programming Research Limited, United Kingdom)
- 10.20-10.50 Break
- 10.50-11.15 *Visualisation Benchmarking.* Jeremy Walton (Numerical Algorithms Group, United Kingdom)
- 11.15-11.55 *A Methodology for Testing the Numerical Correctness of Approximation and Optimisation Software and Examples of Its Application.* Maurice Cox (National Physical Laboratory, United Kingdom)
- 11.55-12.15 Discussion of Morning Papers. Eric Grosse (Bell Laboratories, USA)
- 12.15-2.00 Lunch

OPEN SESSION

- 2.00-2.20 *Performance Profile for Optimization.* James Lyness (Argonne National Laboratory, USA)
- 2.20-2.40 *Godess — A Platform to Compare ODE-methods.* Per Grove Thomsen (Danish Technical University)
- 2.40-3.00 *Godess — A Generic ODE Solving System.* Gustaf Soederlind (Lund University, Sweden)
- 3.00-3.20 *Computing Space-Time Curvature Using Higher Order Spatial Approximations.* William Schiesser (Lehigh University, USA)
- 3.20-3.40 Break
- 3.40-4.00 *Software Test System for Special Functions.* Dan Lozier (National Institute of Standards and Technology, USA)
- 4.00-4.20 *Parallel Globally Adaptive Integration.* Ian Gladwell (Southern Methodist University, USA)
- 4.20-4.40 *Superconductor Simulation.* Mo Mu (Hong Kong University of Science and Technology)
- 4.40-5.00 *A Programming Environment for Scientific Computing.* Siegfried Rump (Technical University of Harburg, Germany)
- 5.00-5.20 *Why We Couldn't Use Numerical Libraries for PETSc.* Bill Gropp (Argonne National Laboratory, USA)
- 5.20-5.40 Discussion of Afternoon Presentations. Mladen Vouk (North Carolina State University, USA)

Friday, 12 July 1996

- 9.00-9.40 *Two Approaches to Exception Handling in Fortran*. John Reid (Rutherford Appleton Laboratory, United Kingdom)
- 9.40-10.20 *The XSC-Tools for Extended Scientific Computing*. Ulrich Kulisch (University of Karlsruhe, Germany)
- 10.20-10.50 Break
- 10.50-11.30 *Is Numerical Software Relevant? -Is it too late to worry about quality?* James C.T. Pool (California Institute of Technology, USA)
- 11.30-12.10 *If Software Quality is a Perception, How do we Measure It?* Morven Gentleman (National Research Council, Canada)
- 12.10-12.30 Discussion of Morning Papers. Brian Smith (University of New Mexico, USA)

3 ORGANIZATION

Program Committee

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Jeremy DuCroz (Oxford, United Kingdom)
Bo Einarsson (Linkping, Sweden)
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Mladen Vouk (Raleigh, North Carolina, USA)

Local Arrangements

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