Jack Dongarra
Kaj Madsen
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Applied Parallel Computing

State of the Art in Scientific Computing

7th International Workshop, PARA 2004
Lyngby, Denmark, June 2004
Revised Selected Papers

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Preface

Introduction

The PARA workshops in the past were devoted to parallel computing methods in science and technology. There have been seven PARA meetings to date: PARA'94, PARA'95 and PARA'96 in Lyngby, Denmark, PARA'98 in Umeå, Sweden, PARA 2000 in Bergen, Norway, PARA 2002 in Espoo, Finland, and PARA 2004 again in Lyngby, Denmark. The first six meetings featured lectures in modern numerical algorithms, computer science, engineering, and industrial applications, all in the context of scientific parallel computing.

This meeting in the series, the PARA 2004 Workshop with the title "State of the Art in Scientific Computing", was held in Lyngby, Denmark, June 20–23, 2004. The PARA 2004 Workshop was organized by Jack Dongarra from the University of Tennessee and Oak Ridge National Laboratory, and Kaj Madsen and Jerzy Waśniewski from the Technical University of Denmark. The emphasis here was shifted to high-performance computing (HPC). The ongoing development of ever more advanced computers provides the potential for solving increasingly difficult computational problems. However, given the complexity of modern computer architectures, the task of realizing this potential needs careful attention. For example, the failure to exploit a computer's memory hierarchy can degrade performance badly. A main concern of HPC is the development of software that optimizes the performance of a given computer.

The high cost of state-of-the-art computers can be prohibitive for many workplaces, especially if there is only an occasional need for HPC. A solution to this problem can be network computing, where remote computing facilities are exploited via the Internet.

PARA 2004 featured invited talks, contributed talks, minisymposia, and software and hardware vendors. The first day, June 20, was devoted to two parallel tutorials. The minisymposia and contributed talks during the main part of the workshop, June 21–23, were scheduled in parallel sessions. All invited and contributed talks were noncommercial. The workshop attracted 230 speakers from all over the world.

The PARA 2006 Workshop with the title "State-of-the-Art in Scientific and Parallel Computing" will be held in Umeå (Sweden) on June 17–21, 2006.

Tutorials

Validated Scientific Computing Using Interval Analysis was organized by *George F. Corliss* from Marquette University (USA). This tutorial gave an introduction to concepts and patterns of interval analysis. It was assumed that the participants had had a first course in scientific computation, including floating-point arithmetic, error analysis, automatic differentiation, Gaussian elimination, Newton's method, numerical optimization, and Runge-Kutta methods for ODEs. The tutorial included lectures, with examples in MATLAB and Sun's Fortran 95, and a set of supervised, hands-on exercises.

Automatic Differentiation was organized by *Andrea Walther* from the Technical University of Dresden (Germany). This tutorial gave a detailed introduction to the chain

rule based technique of automatic differentiation (AD) that provides first and higher derivatives without incurring truncation errors. Several examples illustrated the theoretical results. Some AD tools, selected as a reasonably representative sample, were tested in supervised, hands-on exercises.

Key Speakers

Richard P. Brent, Oxford University Computing Laboratory (UK), *Fast and Reliable Random Number Generators for Scientific Computing*. Fast and reliable pseudo-random number generators are required for simulation and other applications in scientific computing. Richard outlined the requirements for good uniform random number generators, and described a class of generators having very fast vector/parallel implementations with excellent statistical properties.

Bernd Dammann and **Henrik Madsen**, the Technical University of Denmark (Denmark), *High Performance Computing and the Importance of Code Tuning—Some Practical Experiences from Program Tuning at the DTU HPC Center*. This talk gave a short overview of the High Performance Computer installation at the Technical University of Denmark (DTU), as well as a summary of some code tuning experiments. It is easy to reduce the run time of an application for a given problem by buying a computer with a faster CPU (higher clock frequency). However, very often the same or even better speed-up of the code can be achieved by analyzing and tuning the code—without the need to invest in new hardware.

Jack Dongarra, the University of Tennessee and Oak Ridge National Laboratory (USA), *High Performance Computing Trends and Self Adapting Numerical Software (SANS)—Effort*. In this talk Jack looked at how high performance computing has changed over the last 10 years and predicted future trends. In addition, he advocated the need for self adapting software.

Iain Duff, the Rutherford Appleton Laboratory (UK) and CERFACS (France), *Partitioning and Parallelism in the Solution of Large Sparse Systems*. Iain first reviewed the various levels of parallelism that are available in the direct solution of large sparse linear systems. He also briefly considered iterative as well as direct methods in this study.

Fred Gustavson, the IBM T.J. Watson Research Center (USA), *Ideas for High Performance Linear Algebra Software*. In this talk Fred presented several ideas for the development of sequential and parallel HPC dense linear algebra software. The main results were obtained from the algorithms and architecture approach.

Per Christian Hansen, the Technical University of Denmark (Denmark), *Large-Scale Methods in Inverse Problems*. Inverse problems arise in geophysics, tomography, image deblurring and many other areas where the goal is to compute interior or hidden information from exterior data. This talk presented a survey of numerical methods and paradigms suited for large-scale inverse problems.

Bo Kågström, the University of Umeå (Sweden), *Recursive Blocked Algorithms and Hybrid Data Structures for Dense Matrix Library Software*. Matrix computations are both fundamental and ubiquitous in computational science and its vast application areas. Along with the development of more advanced computer systems with complex memory

hierarchies, there is a continuing demand for new algorithms and library software that efficiently utilize and adapt to new architecture features.

John K. Reid, the Rutherford Appleton Laboratory (UK), *Fortran Is Getting More and More Powerful*. There is much happening just now with respect to Fortran. The features of Fortran 2003 have been chosen and the standard is very near completion. John is the convener of the ISO Fortran Committee.

Peter Sloot, the University of Amsterdam (The Netherlands). *Scientific Computing in the Grid: A Biophysical Case Study*. Workers at the University of Amsterdam conducted computer simulation experiments in pre-operative planning of vascular reconstruction with a physician in the experimental loop. Peter showed new results from numerical simulations of blood flow with 3D cellular automata.

Zahari Zlatev, National Environmental Research Institute (Denmark), *Large-Scale Computations with the Unified Danish Eulerian Model*. The Unified Danish Eulerian Model (UNI-DEM) is a mathematical model for performing different comprehensive studies related to damaging effects from high pollution levels in Denmark and Europe. The model is described by a system of partial differential equations (PDEs).

Minisymposia

Interval Methods, organized by *Luke Achenie*, University of Connecticut (USA), *Vladik Kreinovich*, University of Texas at El Paso (USA), and *Kaj Madsen*, Technical University of Denmark (Denmark). In many practical problems there is a need to (a) solve systems of equations and inequalities, and/or (b) optimize some performance measure. The results obtained by conventional algorithms are either local or cannot be guaranteed. Interval analysis provides guaranteed approximations of the set of all the actual solutions of the problem. This ensures that no solution is missed. There were 21 speakers in this minisymposium.

Trends in Large Scale Computing, organized by *Scott B. Baden*, University of California at San Diego (USA). Software infrastructures for large scale computation often fail to realize the full potential afforded by technological advances, and the result is lost opportunities for making scientific discoveries. This minisymposium examined two important issues in software infrastructure for large scale computation: achieving scalability, and optimization through specialization. There were 5 speakers in this minisymposium.

High Performance Linear Algebra Algorithms, organized by *Fred G. Gustavson*, IBM T.J. Watson Research Center (USA), and *Jerzy Waśniewski*, Technical University of Denmark (Denmark). The algorithms of Linpack and Eispack and later LAPACK and ScaLAPACK have stood the test of time in terms of robustness and accuracy. The focus of this minisymposium was on explaining high performance versions of these algorithms. There were 7 speakers in this minisymposium.

Substructuring, Dimension Reduction and Applications, organized by *Zhaojun Bai*, University of California (USA) and *Rencang Li*, University of Kentucky USA. There are a variety of reasons to go for substructuring and dimension reduction in scientific computations and applications. Substructuring makes it possible to solve large and seemingly intractable computational problems by some kind of divide-and-conquer technique. It

also offers a general methodology for parallelization. There were 12 speakers in this minisymposium.

Parallel Processing in Science and Engineering, organized by *Adam W. Bojańczyk*, Cornell University (USA). This minisymposium concerned selected aspects of parallel and distributing computing as they arise in engineering. Both non-traditional applications as well as relevant software tools were presented. There were 9 speakers in this minisymposium.

Distributed Computing: Tools, Paradigms and Infrastructures, organized by *Beniamino Di Martino*, *Rocco Aversa*, Second University of Naples (Italy), and *Laurence Tianruo Yang*, Francis Xavier University (Canada). The minisymposium presented recent advances in distributed computing technology, methodology and tools. The presentations featured a variety of topics ranging from mobile and location-aware computing to skeletons and high-level parallel languages, from programming environments and tools for Grid applications development and tuning, to distributed monitoring and security issues. There were 9 speakers in this minisymposium.

High-Performance Computing in Earth and Space Science, organized by *Peter Messmer*, Tech-X Corporation at Boulder (USA). High-performance computing facilities enable simulations of physical phenomena with ever increasing fidelity and accuracy. The range of resolved scales in a single simulation, as well as the number of physical processes included, yield results that can be directly compared with observational data. There were 7 speakers in this minisymposium.

Advanced Algorithms and Software Components for Scientific Computing, organized by *Padma Raghavan*, Pennsylvania State University (USA). This minisymposium concerned algorithms for sparse linear systems solution and function approximation and their implementation using advanced software architectures. Discussions emphasized the role of such techniques for improving the performance of long-running PDE-based simulations. There were 7 speakers in this minisymposium.

Software Engineering and Problem Solving Environments for Scientific Computing, organized by *José C. Cunha*, Universidade Nova de Lisboa (Portugal) and *Omer F. Rana*, Cardiff University (UK). The emergence of computational grids in the last few years provides new opportunities for the scientific community to undertake collaborative and multi-disciplinary research. The aim of this minisymposium was to bring together experts who have experience in developing software tools to support application scientists, and those who make use of these tools. There were 5 speakers in this minisymposium.

Runtime Software Techniques for Enabling High-Performance Applications, organized by *Masha Sosonkina*, Iowa State University (USA). Parallel computing platforms are advancing rapidly, both in speed and size. However, often only a fraction of the peak hardware performance is achieved by high-performance scientific applications. One way to cope with the changeability of hardware is to start creating applications able to adapt themselves "on-the-fly". The talks of the minisymposium discussed this issue from both the application-centric and system-centric viewpoints. There were 6 speakers in this minisymposium.

Sparse Direct Linear Solvers, organized by *Sivan Toledo*, Tel Aviv University (Israel). The matrices of most of the systems of linear algebraic equations arising from scientific and engineering applications are sparse. This minisymposium dealt with some modern algorithms for sparse direct linear solvers. There were 12 speakers in this minisymposium.

Treatment of Large Scientific Models, organized by *Krassimir Georgiev*, Bulgarian Academy of Science (Bulgaria) and *Zahari Zlatev*, National Environmental Research Institute (Denmark). The exploitation of new fast computers in the effort to avoid non-physical assumptions and, thus, to develop and run more reliable and robust large scientific models was the major topic of this minisymposium. There were 9 speakers in this minisymposium.

Performance Evaluation and Design of Hardware-Aware PDE Solvers, organized by *Markus Kowarschik* and *Frank Hülsemann*, University of Erlangen-Nuremberg (Germany). In an ideal situation, all performance optimization of computationally intensive software would take place automatically, allowing the researchers to concentrate on the development of more efficient methods rather than having to worry about performance. However, for the time being, the need to identify and remove the performance bottlenecks of computationally intensive codes remains. As an example of a class of computationally intensive problems, this minisymposium concentrated on the numerical solution of PDEs. There were 7 speakers in this minisymposium.

Computationally Expensive Methods in Statistics, organized by *Wolfgang Hartmann*, SAS Institute Inc. (USA) and *Paul Somerville*, University of Central Florida (USA). A two-dimensional data set with N observations (rows) and n variables (columns) and large scale data requires intensive computational work. Of course there may be even more dimensions of the data set. There were 5 speakers in this minisymposium.

Approaches or Methods of Security Engineering (AMSE), organized by *Taihoon Kim* and *Ho Yeol Kwon*, Kangwon National University (Korea). Security engineering software is needed for reducing security holes. The talks presented a number of methods for designing such software. There were 16 speakers in this minisymposium.

Contributed Talks

Some contributed talks were added to the minisymposium sessions. The others were organized in the following independent sessions: two sessions of "Grid and Network", two sessions of "HPC Applied to Security Problems", two sessions of "Clusters and Graphics", one session of "HPC Applied to Cryptology", one session of "ODEs, PDEs and Automatic Differentiation", one session of "Computer Tools", and a special session of "Computer Vendors".

Workshop Proceedings

The proceedings of the PARA 2004 Workshop are divided into two complementary publications, this Springer volume and the following report:

- J. Dongarra, K. Madsen and J. Waśniewski (Eds.)

- Complementary proceedings of the PARA 2004 Workshop on State-of-the-Art in Scientific Computing, Lyngby, Denmark, June, 2004.
- IMM-Technical report-2005-09.
- Informatics and Mathematical Modelling, Technical University of Denmark, DK-2800 Lyngby, Denmark.
- URL: http://www2.imm.dtu.dk/pubdb/views/publication_details.php?id=3927

A list of those papers appearing in the report is given in this volume in Chapter II of the contributed talks.

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The organizers are indebted to the PARA 2004 sponsors, whose support was vital to the success of the workshop. The main sponsor was the Department of Informatics and Mathematical Modelling of the Technical University of Denmark. The other sponsors were:

- HP High Performance Computing USA,
- NAG Numerical Algorithms Group Ltd. UK,
- Comsol A/S Denmark (MATLAB distributor),
- Sun Microsystems Denmark,
- UNI•C Danish Computing Center Denmark,
- Microsoft Denmark, and
- IBM (International Business Machines) Denmark.

The organizers would like to thank Kirsten Probst for her excellent work as PARA 2004 secretary. Dorthe Thøgersen, Henrik Krogh and other staff of the conference also provided very valuable help.

We are very grateful to Prof. Ho Yeol Kwon from the Kangwon National University, Electrical and Computer Engineering Department for taking many photos during the PARA 2004 conference. These are available at the PARA 2004 URL

http://www.imm.dtu.dk/~jw/para04/.

Thanks are also due to Vincent A. Barker for his kind assistance in the preparation of both the workshop and these proceedings.

The PARA 2004 conference ended on June 23, 2004. The evening of June 23, the eve of St. Hans Day, is celebrated in Denmark by the lighting of bonfires. We are indebted to Arriva Denmark A/S for making available two boats for the PARA 2004 participants, from which we could see some of the bonfires and admire beautiful Copenhagen.

Finally, we would like to thank the PARA 2004 referees for their careful evaluation of the workshop papers.

Jack Dongarra
Kaj Madsen
Jerzy Waśniewski

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