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Applied Parallel Computing

State of the Art
in Scientific Computing

8th International Workshop, PARA 2006
Umeå, Sweden, June 18-21, 2006
Revised Selected Papers

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Preface

The Eighth International Workshop on Applied Parallel Computing (PARA 2006) was held in Umeå, Sweden, June 18–21, 2006. The workshop was organized by the High Performance Computing Center North (HPC2N) and the Department of Computing Science at Umeå University. The general theme for PARA 2006 was “State of the Art in Scientific and Parallel Computing.” Topics covered at PARA 2006 included basic algorithms and software for scientific, parallel and grid computing, tools and environments for developing high-performance computing applications, as well as a broad spectrum of applications from science and engineering.

The workshop included 7 plenary keynote presentations, 15 invited minisymposia organized in 30 sessions, and 16 sessions of contributed talks. The minisymposia and the contributed talks were held in five to six parallel sessions. The main workshop program was preceded by two half-day tutorials. In total, 205 presentations were held at PARA 2006, by speakers representing 28 countries. Extended abstracts for all presentations were made available at the PARA 2006 Web site (www.hpc2n.umu.se/para06).

The reviewing process was performed in two stages for evaluation of originality, appropriateness, and significance. In the first stage, extended abstracts were reviewed for selection of contributions to be presented at the workshop. In the second stage the full papers submitted after the workshop were reviewed. In total, 120 papers were selected for publication in this peer-reviewed post-conference proceedings.

A number of people contributed in different regards to the organization and the accomplishment of PARA 2006. First of all the Local Organization Committee did a greatly appreciated and enthusiastic job. We also acknowledge the following people for the assistance and support during the workshop days: Yvonne Löwstedt and Anne-Lie Persson; Niklas Edmundsson, Roger Oscarsson, and Mattias Wadenstein. A special thanks goes to the PARA 2006 secretary, Lena Hellman, to Anders Backman and Björn Torkelsson for designing and managing the PARA 2006 Web site including the electronic paper submission system, powered by Commence, and to Mats Nylén and Mikael Rännar for their professional assistance in compiling and editing the PARA 2006 program, the booklet of extended abstracts, and the final proceedings. PARA 2006 would not have been possible without the personal involvement of all these fine people. We also greatly acknowledge all minisymposia organizers, the review coordinators and all the referees for their evaluations in the second review stage, which included several rounds and resulted in these professionally peer-reviewed post-workshop proceedings. Finally, we would also like to thank the sponsoring institutions for their generous financial support.

Since 1996 the international PARA conferences have become biennial and are organized by one of the Nordic countries. The three first workshops including PARA 1996 and the last PARA 2004 were held in Lyngby, Denmark. The other three, besides this one, were held in Umeå, Sweden (PARA 1998), in Bergen, Norway (PARA 2000), and in Espoo, Finland (PARA 2002). The PARA 2008 workshop will take place in Trondheim, Norway, May 13–16, 2008.

March 2007

Bo Kågström
Erik Elmroth
Jack Dongarra
Jerzy Wasniewski

In Memoriam and Dedication

Every day we are reminded of the perishables of life and that our individual lives are only a gift for a finite time. Unfortunately, at PARA 2006 this was no exception. Our colleague Amelia De Vivo, Università degli Studi della Basilicata, Italy, passed away during the conference on June 21, 2006 in Umeå, Sweden. Another of our colleagues, Olav Beckmann, Imperial College London, UK died on November 9, 2006; this workshop was the last professional engagement of his career. As a token of our friendship and admiration of Amelia De Vivo and Olav Beckmann, we dedicate the PARA 2006 conference proceedings to them, from all PARA 2006 participants and with our regards to their families.

Organization

PARA 2006 was organized by the High Performance Computing Center North (HPC2N) and the Department of Computing Science at Umeå University.

Organization and Program Committee

Bo Kågström	Umeå University and HPC2N, Sweden <i>PARA 2006 Chairman</i>
Erik Elmroth	Umeå University and HPC2N, Sweden <i>PARA 2006 Coordinator</i>
Jack Dongarra	University of Tennessee and Oak Ridge National Laboratory, USA
Jerzy Wasniewski	Technical University of Denmark

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Christoph Kessler	Hans Stockinger
David Kincaid	Jerzy Wasniewski
Sinisa Krajnovic	Jan Westerholm
Daniel Kressner	Felix Wolf
	Anders Ynnerman

Sponsoring Institutions

The Swedish Research Council (VR) via the Swedish National Infrastructure for Computing (SNIC).

Umeå University via the Vice-Chancellor, the High Performance Computing Center North (HPC2N), and the Department of Computing Science.

PARA 2006 Tutorials

Python in High-Performance Computing

Organizers and Lecturers: *Xing Cai*, *Hans Petter Langtangen*, and *Kent-Andre Mardal*, Simula Research Laboratory and Oslo University, Norway

Introduction to Object-Oriented Modeling and Simulation with Modelica

Organizers and Lecturers: *Peter Fritzson* and *Anders Sandahl*, Linköping University, Sweden

PARA 2006 Keynote Presentations

Implementing Advanced Force Fields for Simulation of Physical and Biological Processes

Tom Darden, National Institute of Environmental Health Science, North Carolina, USA

The Future of LAPACK and ScaLAPACK

James Demmel, University of California, Berkeley, USA

Supercomputers and Clusters and Grids, Oh My!

Jack Dongarra, University of Tennessee, Knoxville and Oak Ridge National Laboratory, USA

Large-Scale Ill-Posed Problems and Applications

Per Christian Hansen, Technical University of Denmark, Lyngby, Denmark

Mixed-Language Programming for HPC Applications

Hans Petter Langtangen, Simula Research Laboratory and Oslo University, Norway

Parallel MATLAB

Cleve Moler, The MathWorks Inc., USA

Recent Advances in Rendering and Interaction for Volumetric Data in Medical Applications

Anders Ynnerman, Linköping University, Sweden

PARA 2006 Minisymposia

Stretching Time and Length Scales in Biomolecular Modelling (18 presentations)

Organizer: *Aatto Laaksonen*, Stockholm University, Sweden

Recent Advances in Dense Linear Algebra (11 presentations)

Organizers: *Daniel Kressner*, University of Zagreb, Croatia and Umeå University, Sweden; *Julien Langou*, The University of Tennessee, Knoxville, USA

CFD Applications for High-Performance Computing (6 presentations)

Organizer: *Sinisa Krajinovic*, Chalmers, Sweden

HPC Environments: Visualization and Parallelization Tools (12 presentations)

Organizers: *Anne C. Elster*, Norwegian University of Science and Technology, Norway; *Otto Anshus*, University of Tromsø, Norway

Tools, Frameworks and Applications for High-Performance Computing (17 presentations)

Organizer: *Osní Marques*, Lawrence Berkeley National Laboratory, Berkeley, USA

Grid Data Management (5 presentations)

Organizers: *Siegfried Benkner*, University of Vienna, Austria; *Heinz Stockinger*, Swiss Institute of Bioinformatics, Lausanne, Switzerland

Simulations in Geophysics and Space Physics (9 presentations)

Organizers: *Mats Holmström*, Swedish Institute of Space Physics, Kiruna, Sweden; *Kjell Rönnmark*, Umeå University, Sweden

Tools for Parallel Performance Analysis (12 presentations)

Organizer: *Felix Wolf*, Forschungszentrum Jülich GmbH, Germany

Grids for Scientific Computing (9 presentations)

Organizer: *Oxana Smirnova*, Lund University, Sweden

Simulations of Materials (12 presentations)

Organizer: *Lars Nordström*, Uppsala University, Sweden

Novel Data Formats and Algorithms for Dense Linear Algebra Computations (13 presentations)

Organizers: *Fred Gustavson*, IBM T.J. Watson Research Center, New York, USA and Umeå University; *Jerzy Wasniewski*, Technical University of Denmark, Lyngby, Denmark

Bioinformatics and Computational Biology (5 presentations)

Organizers: *Ann-Charlotte Berglund Sonnhammer* and *Sverker Holmgren*, Uppsala University, Sweden

Scientific Visualization and HPC Applications (4 presentations)

Organizers: *Matt Cooper* and *Anders Ynnerman*, Linköping University, Sweden

Software Tools for Parallel CFD Applications (7 presentations)

Organizers: *Xing Cai* and *Hans Petter Langtangen*, Simula Research Laboratory and Oslo University, Norway

Multi-scale Physics (6 presentations)

Organizer: *Mats G. Larson*, Umeå University, Sweden

PARA 2006 Speakers

The keynote, minisymposia and contributed papers that are published in the proceedings were presented by the speakers listed below (the names are in the same order as the papers appear in the Table of Contents). We refer to the PARA 2006 program for a complete listing of all presentations and speakers.

Keynote Papers

Jack Dongarra
James W. Demmel

Per Christian Hansen
Hans Petter Langtangen

Minisymposia Papers

Peter G. Kusalik
Peter Ahlström
Christophe Labbez
Mikael Lund
Mikael Peräkylä
Paweł Sałek
Yaoquan Tu
David van der Spoel
Björn Adlerborn
Robert Granat
Craig Lucas
Jakub Kurzak
Enrique S. Quintana-Ortí
Håkan Nilsson
John Markus Bjørndalen
Espen Skjelnes Johnsen
Jan C. Meyer
Thorvald Natvig
Ingar Saltvik
Daniel Stødle
Peter Arbenz
L. Anthony Drummond
Viral B. Shah
Lutz Gross
Zsolt I. Lázár
Sameer Shende

Siegfried Benkner
Brian Coghlan
Carmela Comito
Francisco Almeida
Werner Bengler
Pablo López
Madelene Jeanette Parviainen
Jörgen Vedin
Genaro Costa
Karl Furlinger
Felix Wolf
Josep Jorba
Edmond Kereku
Andreas Knüpfer
Sameer Shende
Hung-Hsun Su
Brian J. N. Wylie
Oxana Smirnova
Sigve Haug
Roman Wyrzykowski
Pooja M. Panchmatia
Levente Vitos
Michael Bader
Isak Jonsson
Fred G. Gustavson
Lars Karlsson

Tadeusz Swirszcz
 Jerzy Waśniewski
 José R. Herrero
 Przemysław Stpczyński
 Jennifer A. Scott
 Enrique S. Quintana-Ortí
 Tetsuya Sakurai
 Mahen Jayawardena
 Paul Sjöberg
 Jeanette Tångrot

Paul R. Woodward
 Markus Blatt
 Bruno Carpentieri
 Xing Cai
 Hiroshi Okuda
 Kent-Andre Mardal
 Christophe Prud'homme
 Eugene V. Shilnikov
 Fredrik Bengzon

Contributed Papers

Juan A. Acebrón
 Torsten Adolph
 Nikolaos M. Missirlis
 Scott B. Baden
 Michael Spevak
 Jorge Andrade
 Amy Krause
 Krzysztof Benedyczak
 Jan Kwiatkowski
 Gabriele Pierantoni
 Olaf Schneider
 Marilton S. de Aguiar
 Tamito Kajiyama
 Dries Kimpe
 Carmen B. Navarrete
 Gerhard Zumbusch
 Jan Westerholm
 Cevdet Aykanat
 Kamen Yotov
 Pascal Hénon
 Takahiro Katagiri
 Mariana Kolberg
 Claude Lacoursière

Marzio Sala
 Marzio Sala
 Teruo Tanaka
 René Heinzl
 Christoph Kessler
 Margreet Nool
 Constantine Bekas
 Nils Smeds
 Vladimir A. Tcheverda
 Bartłomiej Jacek Kubica
 Tomas Lindén
 Paul R. Woodward
 Juan-Pedro Martínez-Gallar
 Stéphane Vialle
 Yurong Chen
 Raimondas Čiegis
 Jacek Dąbrowski
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 Thomas Fischer
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 Myungho Lee
 Daisuke Takahashi

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