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Kristján Jónasson (Ed.)

Applied Parallel and Scientific Computing

10th International Conference, PARA 2010

Reykjavík, Iceland, June 6-9, 2010

Revised Selected Papers, Part I

Volume Editor

Kristján Jónasson
University of Iceland
School of Engineering and Natural Sciences
Department of Computer Science
Hjardarhagi 4, 107 Reykjavík, Iceland
E-mail: jonasson@hi.is

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Preface

The tenth Nordic conference on applied parallel computing, Para 2010: State of the Art in Scientific and Parallel Computing, was held in Reykjavík, Iceland during June 6–9, 2010. The topics of the conference were announced to include software, hardware, algorithms, tools, environments, as well as applications of scientific and high-performance computing. The conference was hosted by the School of Engineering and Natural Sciences of the University of Iceland, and the conference venue was in the School of Education of the University of Iceland. Three companies in Reykjavík supported the conference financially: the video game developer CCP, Microsoft Íslandi, and Opin kerfi (Hewlett Packard distributor for Iceland).

The series of Para meetings began in 1994. The Danish Computing Centre for Research and Education (UNI-C) and the Department of Informatics and Mathematical Modelling of the Technical University of Denmark (IMM/DTU) in Lyngby, Denmark, organized a series of workshops on Applied Parallel Computing, named Para94, Para95 and Para96. Jerzy Waśniewski, senior researcher at DTU, initiated these workshops and Jack Dongarra, professor at the University of Tennessee, became involved during an extended visit to Lyngby. He played a key part in promoting the meetings internationally. Since 1998, the workshops have become a Nordic effort, but both Jerzy and Jack have continued to be an integral part of the meetings. In fact Jerzy has been a keen advocate of holding a Para conference in Iceland. The themes and locations of the Para meetings have been:

PARA94 Parallel Scientific Computing, Lyngby, Denmark

PARA95 Physics, Chemistry and Engineering Science, Lyngby, Denmark

PARA96 Industrial Problems and Optimization, Lyngby, Denmark

PARA 1998 Large Scale Scientific and Industrial Problems, Umeå, Sweden

PARA 2000 New Paradigms for HPC in Industry and Academia, Bergen, Norway

PARA 2002 Advanced Scientific Computing, Helsinki, Finland

PARA 2004 State of the Art in Scientific Computing, Copenhagen, Denmark

PARA 2006 State of the Art in Scientific and Parallel Computing, Umeå, Sweden

PARA 2008 State of the Art in Scientific and Parallel Computing, Trondheim, Norway

PARA 2010 State of the Art in Scientific and Parallel Computing, Reykjavík, Iceland

The Para 2010 conference included five keynote lectures, one tutorial, 11 mini-symposia consisting of a total of 90 presentations, 39 other contributed presentations organized under 10 separate topics, four poster presentations, and eight presentations from industry. Except for the keynote lectures, that were 45 minutes long each, the presentations were organized in five tracks or parallel streams, with 25-minute slots for each presentation, including discussion. The

total number of presentations was thus 147. There were altogether 187 participants from 20 countries:

Denmark 9	Canada 1	Poland 16
Finland 4	Czech Republic 3	Russia 2
Iceland 38	France 12	Spain 7
Norway 13	Germany 32	Switzerland 1
Sweden 17	Italy 1	Turkey 1
Australia 2	Japan 4	USA 20
Austria 2	Netherlands 2	

There were volcanic eruptions in Eyjafjallajökull in southern Iceland from March until June 2010 disrupting international flights, and these may have had an adverse effect on participation.

Extended abstracts (in most cases four pages long) of all the minisymposium and contributed presentations were made available on the conference website, <http://vefir.hi.is/para10>, and in addition a book of short abstracts (also available on the website) was handed out at the conference.

After the conference the presentation authors were invited to submit manuscripts for publication in these peer-reviewed conference proceedings. The reviewing process for the articles appearing here was therefore performed in two stages. In the first stage the extended abstracts were reviewed to select contributions to be presented at the conference, and in the second stage the full papers submitted after the conference were reviewed. As a general rule three referee reports per paper were aimed for, and in most cases these were successfully obtained. However, in cases where it proved difficult to find three willing referees, acquiring only two reports was deemed acceptable.

Fred G. Gustavson, emeritus scientist at IBM Research, New York, and professor at Umeå University, and Jerzy Waśniewski gave a tutorial on matrix algorithms in the new many core era. Fred celebrated his 75th birthday on May 29, 2010, and the Linear Algebra Minisymposium was held in his honor. The material of the tutorial is covered in Fred Gustavson's article in these proceedings.

A conference of this size requires considerable organization and many helping hands. The role of the minisymposium organizers was very important. They reviewed and/or organized reviewing of contributions to their respective minisymposia, both the original extended abstracts and the articles for these proceedings, and in addition they managed the minisymposium sessions at the conference. Several members of the local Organizing Committee helped with the reviewing of other contributed extended abstracts: Elínborg I. Ólafsdóttir, Hjálmtýr Hafsteinsson, Klaus Marius Hansen, Ólafur Rögnvaldsson, Snorri Agnarsson and Sven Þ. Sigurðsson. Other colleagues who helped with this task were Halldór Björnsson, Kristín Vogfjörð and Viðar Guðmundsson.

The editor of these proceedings organized the reviewing of manuscripts falling outside minisymposia, as well as manuscripts authored by the minisymposium organizers themselves. There were 56 such submissions. The following people played a key role in helping him with this task: Sven Þ. Sigurðsson, Julien

Langou, Bo Kågström, Sverker Holmgren, Michael Bader, Jerzy Waśniewski, Klaus Marius Hansen, Kimmo Koski and Halldór Björnsson. Many thanks are also due to all the anonymous referees, whose extremely valuable work must not be forgotten.

The conference bureau Your Host in Iceland managed by Inga Sólnes did an excellent job of organizing and helping with many tasks, including conference registration, hotel bookings, social program, financial management, and maintaining the conference website. Apart from Inga, Kristjana Magnúsdóttir of Your Host was a key person and Einar Samúelsson oversaw the website design. Ólafía Lárusdóttir took photographs for the conference website. The baroque group Custos and the Tibia Trio, both led by recorder player Helga A. Jónsdóttir, and Helgi Kristjánsson (piano) provided music for the social program. Ólafur Rögnvaldsson helped to secure financial support from industry. Jón Blöndal and Stefán Ingi Valdimarsson provided valuable TeX help for the editing of the proceedings.

Finally, I wish to devote a separate paragraph to acknowledge the help of my colleague Sven Þ. Sigurðsson, who played a key role in helping with the conference organization and editing of the proceedings through all stages.

October 2011

Kristján Jónasson

Organization

PARA 2010 was organized by the School of Engineering and Natural Sciences of the University of Iceland.

Steering Committee

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CCP, Reykjavík – video game developer
Microsoft Íslandi, Reykjavík
Opin kerfi, Reykjavík – Hewlett Packard in Iceland

PARA 2010 Scientific Program

Keynote Presentations

Impact of Architecture and Technology for Extreme Scale on Software and Algorithm Design

Jack Dongarra, University of Tennessee and Oak Ridge National Laboratory

Towards Petascale for Atmospheric Simulation

John Michalakes, National Center for Atmospheric Research (NCAR), Boulder, Colorado

Algorithmic Challenges for Electronic-Structure Calculations

Risto M. Nieminen, Aalto University School of Science and Technology, Helsinki

Computational Limits to Nonlinear Inversion

Klaus Mosegaard, Technical University of Denmark

Efficient and Reliable Algorithms for Challenging Matrix Computations Targeting Multicore Architectures and Massive Parallelism

Bo Kågström, Umeå University

Tutorial

New Algorithms and Data Structures for Matrices in the Multi/Many Core Era

Fred G. Gustavson, Umeå University and Emeritus Scientist at IBM Research, New York, and *Jerzy Waśniewski*, Danish Technical University

General Topics

Cloud Computing (1 presentation)

HPC Algorithms (7 presentations and 1 poster)

HPC Programming Tools (4 presentations)

HPC in Meteorology (3 presentations)

Parallel Numerical Algorithms (8 presentations and 1 poster)

Parallel Computing in Physics (2 presentations and 1 poster)

Scientific Computing Tools (10 presentations)

HPC Software Engineering (2 presentations and 1 poster)

Hardware (1 presentation)

Presentations from Industry (8 presentations)

Minisymposia

Simulations of Atomic Scale Systems (15 presentations)

Organized by *Hannes Jónsson*, University of Iceland

Tools and Environments for Accelerator-Based Computational Biomedicine
(6 presentations)

Organized by *Scott B. Baden*, University of California, San Diego

GPU Computing (9 presentations)

Organized by *Anne C. Elster*, NTNU, Trondheim

High-Performance Computing Interval Methods (6 presentations)

Organized by *Bartłomiej Kubica*, Warsaw University of Technology

Real-Time Access and Processing of Large Data Sets (6 presentations)

Organized by *Helmut Neukirchen*, University of Iceland and *Michael Schmelling*, Max Planck Institute for Nuclear Physics, Heidelberg

Linear Algebra Algorithms and Software for Multicore and Hybrid Architectures,
in honor of Fred Gustavson on his 75th birthday (10 presentations)

Organized by *Jack Dongarra*, University of Tennessee and *Bo Kågström*,
Umeå University

Memory and Multicore Issues in Scientific Computing – Theory and Practice
(6 presentations)

Organized by *Michael Bader*, Universität Stuttgart and *Riko Jacob*,
Technische Universität München

Multicore Algorithms and Implementations for Application Problems (9 presen-
tations)

Organized by *Sverker Holmgren*, Uppsala University

Fast PDE Solvers and A Posteriori Error Estimates (8 presentations)

Organized by *Jan Valdmán*, University of Iceland and *Talal Rahman*,
University College Bergen

Scalable Tools for High-Performance Computing (12 presentations)

Organized by *Luiz DeRose*, Cray Inc. and *Felix Wolf*, German Research
School for Simulation Sciences

Distributed Computing Infrastructure Interoperability (4 presentations)

Organized by *Morris Riedel*, Forschungszentrum Jülich

Speakers and Presentations

For a full list of authors and extended abstracts, see <http://vefir.hi.is/para10>.

- Abrahamowicz, Michal: Alternating conditional estimation of complex constrained models for survival analysis
- Abramson, David: Scalable parallel debugging: Challenges and solutions
- Agnarsson, Snorri: Parallel programming in Morpho
- Agullo, Emmanuel: Towards a complexity analysis of sparse hybrid linear solvers
- Aliaga, José I.: Parallelization of multilevel ILU preconditioners on distributed-memory multiprocessors
- Anzt, Hartwig: Mixed precision error correction methods for linear systems – Convergence analysis based on Krylov subspace methods
- Aqrabi, Ahmed Adnan: Accelerating disk access using compression for large seismic datasets on modern GPU and CPU
- Arbenz, Peter: A fast parallel poisson solver on irregular domains
- Bader, Michael: Memory-efficient Sierpinski-order traversals on dynamically adaptive, recursively structured triangular grids
- Bartels, Soeren: A posteriori error estimation for phase field models
- Belsø, Rene: Structural changes within the high-performance computing (HPC) landscape
- Bientinesi, Paolo: The algorithm of multiple relatively robust representations for multicore processors
- Bjarnason, Jón: Fighting real time – The challenge of simulating large-scale space battles within the Eve architecture
- Błaszczak, Jacek Piotr: Aggregated pumping station operation planning problem (APSOP) for large-scale water transmission system
- Bohlender, Gerd: Fast and exact accumulation of products
- Borkowski, Janusz: Global asynchronous parallel program control for multicore processors
- Bozejko, Wojciech: Parallelization of the tabu search algorithm for the hybrid flow shop problem
- Breitbart, Jens: Semiautomatic cache optimizations using OpenMP
- Brian J. N. Wylie: Performance engineering of GemsFDTD computational electromagnetics solver
- Britsch, Markward: The computing framework for physics analysis at LHCb
- Brodtkorb, André R.: State of the art in heterogeneous computing
- Buttari, Alfredo: Fine granularity sparse QR factorization for multicore-based systems
- Cai, Xiao-Chuan: A parallel domain decomposition algorithm for an inverse problem in elastic materials
- Cai, Xing: Detailed numerical analyses of the Aliev-Panfilov model on GPGPU
- Cambruzzi, Sandro: The new features of Windows HPC Server 2008 V3 and Microsoft's HPC strategy
- Cankur, Reydan: Parallel experiments on PostgreSQL (poster)
- Casas, Marc: Multiplexing hardware counters by spectral analysis

- Cheverda, Vladimir A.: Simulation of seismic waves propagation in multiscale media: Impact of cavernous/fractured reservoirs
- Cheverda, Vladimir A.: Parallel algorithm for finite difference simulation of acoustic logging
- Contassot-Vivier, Sylvain: Impact of asynchronism on GPU accelerated parallel iterative computations
- Cytowski, Maciej: Analysis of gravitational wave signals on heterogeneous architecture
- Danek, Tomasz: GPU accelerated wave form inversion through Monte Carlo sampling
- Davidson, Andrew: Toward techniques for auto-tuning GPU algorithms
- DeRose, Luiz: Automatic detection of load imbalance
- Doll, Jimmie D.: Recent developments in rare-event Monte Carlo methods
- Dongarra, Jack: Impact of architecture and technology for extreme scale on software and algorithm design (keynote lecture)
- Dongarra, Jack: LINPACK on future manycore and GPU-based systems
- Dubcova, Lenka: Automatic hp-adaptivity for inductively heated incompressible flow of liquid metal
- Einarsdóttir, Dóróthea M.: Calculation of tunneling paths and rates in systems with many degrees of freedom
- Ekström, Ulf Egil: Automatic differentiation in quantum chemistry
- Elster, Anne C.: Current and future trends in GPU computing
- Elster, Anne C.: Visualization and large data processing – State of the art and challenges
- Fjukstad, Bård: Interactive weather simulation and visualization on a display wall with manycore compute nodes
- Fujino, Seiji: Performance evaluation of IDR(s)-based Jacobi method
- Gagunashvili, Nikolai: Intellectual data processing for rare event selection using a RAVEN network
- Gepner, Pawel: Performance evaluation of Intel® Xeon® 7500 family processors for HPC
- Gerndt, Michael: Performance analysis tool complexity
- Gjermundsen, Aleksander: LBM vs. SOR solvers on GPU for real-time fluid simulations
- Goerling, Andreas: Novel density-functional methods for ground and excited states of molecules and first steps towards their efficient implementation
- Greiner, Gero: Evaluating non-square sparse bilinear forms on multiple vector pairs in the I/O-model
- Gross, Lutz: Algebraic upwinding with flux correction in 3D numerical simulations in geosciences
- Guðjónsson, Halldór Fannar: HPC and the Eve cluster game architecture
- Gustafsson, Magnus: Communication-efficient Krylov methods for exponential integration in quantum dynamics
- Gustavson, Fred G.: New Algorithms and data structures for matrices in the multi/manycore era, parts 1, 2, 4 (tutorial)

- Gustavson, Fred G.: Enduring linear algebra
- Henkelman, Graeme: Accelerating molecular dynamics with parallel computing resources
- Hess, Berk: Molecular simulation on multicore clusters and GPUs
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- Jenz, Domenic: The computational steering framework stereo
- Jiang, Steve: GPU-based computational tools for online adaptive cancer radiotherapy
- Jónsson, Kristján Valur: Using stackless python for high-performance MMO architecture
- Kåggström, Bo: Efficient and reliable algorithms for challenging matrix computations targeting multicore architectures and massive parallelism (keynote lecture)
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- Langou, Julien: Choosing a reduction tree for communication avoiding QR
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- Michalakes, John: Towards petascale for atmospheric simulation (keynote lecture)
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- Tudruj, Marek: Scheduling parallel programs with architecturally supported regions
- Tudruj, Marek: Streaming model computation of the FDTD problem (poster)

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- Ujaldón, Manuel: CUDA 2D stencil computations for the Jacobi method
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