Lecture Notes in Computer Science 7134

Commenced Publication in 1973
Founding and Former Series Editors:
Gerhard Goos, Juris Hartmanis, and Jan van Leeuwen

Kristján Jónasson (Ed.)

Applied Parallel and Scientific Computing

10th International Conference, PARA 2010
Reykjavík, Iceland, June 6-9, 2010
Revised Selected Papers, Part II

Springer

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

ISSN 0302-9743 e-ISSN 1611-3349
ISBN 978-3-642-28144-0 e-ISBN 978-3-642-28145-7
DOI 10.1007/978-3-642-28145-7
Springer Heidelberg Dordrecht London New York

Library of Congress Control Number: 2012930011

CR Subject Classification (1998): G.1-4, F.1-2, D.1-3, J.1, C.2

LNCS Sublibrary: SL 1 – Theoretical Computer Science and General Issues

Typesetting: Camera-ready by author, data conversion by Scientific Publishing Services, Chennai, India

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

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 minisymposia 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 valueable 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

Jerzy Waśniewski, Chair, Denmark
Kaj Madsen, Denmark
Anne C. Elster, Norway
Petter Bjørstad, Norway
Hjálmtýr Hafsteinsson, Iceland
Kristján Jónasson, Iceland
Juha Haatja, Finland
Kimmo Koski, Finland
Björn Engquist, Sweden
Bo Kågström, Sweden
Jack Dongarra, Honorary Chair, USA

Local Organizing Committee

Kristján Jónasson, Chair
Sven Þ. Sigurðsson, Vice Chair
Ólafur Rögnvaldsson, Treasurer
Ari Kr. Jónsson
Ebba Þóra Hvannberg
Elínborg Ingunn Ólafsdóttir
Hannes Jónsson
Helmut Neukirchen
Hjálmtýr Hafsteinsson
Jan Valdman
Klaus Marius Hansen
Sigurjón Sindrason
Snorri Agnarsson
Tómas Philip Rúnarsson

Sponsoring Companies

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 *Bartlomiej 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 presentations)
Organized by *Sverker Holmgren*, Uppsala University

Fast PDE Solvers and A Posteriori Error Estimates (8 presentations)
Organized by *Jan Valdman*, 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
Aqrawi, 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
Blaszczyk, 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
Holm, Marcus: Implementing Monte Carlo electrostatics simulations on heterogeneous multicore architectures
Jacobson, Emily R.: A lightweight library for building scalable tools
Jakl, Ondrej: Solution of identification problems in computational mechanics – Parallel processing aspects
Jenz, Domenic: The computational steering framework steereo
Jiang, Steve: GPU-based computational tools for online adaptive cancer radiotherapy
Jónsson, Kristján Valur: Using stackless python for high-performance MMO architecture
Kågström, Bo: Efficient and reliable algorithms for challenging matrix computations targeting multicore architectures and massive parallelism (keynote lecture)
Kamola, Mariusz: Software environment for market balancing mechanisms development, and its application to solving more general problems in parallel way
Karlsson, Lars: Fast reduction to Hessenberg form on multicore architectures
Khan, Malek Olof: Molecular simulations on distributed heterogeneous computing nodes
Kimpe, Dries: Grids and HPC: Not as different as you might think?
Kirschenmann, Wilfried: Multi-target vectorization with MTPS C++ generic library
Kjelgaard Mikkelsen, Carl Christian: Parallel solution of banded and block bidiagonal linear systems
Klüpfel, Peter: Minimization of orbital-density-dependent energy functionals
Knüpfer, Andreas: Rank-specific event tracing for MPI – Extending event tracing to cope with extreme scalability
Kraemer, Walter: High-performance verified computing using C-XSC
Kreutz, Jochen: Black-Scholes and Monte Carlo simulation on accelerator architectures
Krog, Øystein E.: Fast GPU-based fluid simulations using SPH
Kubica, Bartlomiej: Using the second-order information in Pareto-set computations of a multi-criteria problem
Kubica, Bartlomiej: Cache-oblivious matrix formats for computations on interval matrices
Köstler, Harald: Optimized fast wavelet transform utilizing a multicore-aware framework for stencil computations
Lacoursiere, Claude: Direct sparse factorization of blocked saddle point matrices
Langlois, Philippe: Performance evaluation of core numerical algorithms: A tool to measure instruction level parallelism

Langou, Julien: Towards an efficient tile matrix inversion of symmetric positive definite matrices on multicore architectures
Langou, Julien: Choosing a reduction tree for communication avoiding QR
Lee, Joo Hong: A hybrid parallel programming model for biological systems simulation
Lieber, Matthias: Highly scalable dynamic load balancing in the atmospheric modeling system COSMO-SPECS+FD4
Luque, Emilio: Scalability and efficiency for SPMD applications on multicore clusters
Luque, Emilio: PAS2P tool, parallel application signature for performance prediction
Lysgaard, Steen: Computational analysis of the interaction of materials for energy storage with water (poster)
Malinen, Mika: The development of fully coupled simulation software by reusing segregated solvers
Mallett, Jacky: Challenges in MMO scaling
Marciniak, Andrzej: An interval version of the Crank-Nicolson method – The first approach
Maronsson, Jón Bergmann: Elastic band of dimers for locating potential energy ridges and second order saddle points
McCulloch, Andrew D.: GPU-accelerated cardiac electrophysiology
Meinel, Michael: The FlowSimulator framework for massively parallel CFD applications
Michalakes, John: Towards petascale for atmospheric simulation (keynote lecture)
Mikkelsen, Kurt V.: Electromagnetic properties of large systems
Missirlis, Nikolaos: The diffusion method using neighbors of path length two in a torus graph
Mitra, Dhrubaditya: Direct numerical simulations of MHD using PENCIL-CODE
Moore, Shirley V.: Scalability study of a quantum simulation code
Morajko, Anna: MATE: Toward scalable automated and dynamic performance tuning environment
Mosegaard, Klaus: Computational limits to nonlinear inversion (keynote lecture)
Mueller, Frank: ScalaTrace: Tracing, analysis and modeling of HPC codes at scale
Mukunoki, Daichi: Implementation and evaluation of quadruple precision BLAS on GPU
Mýrdal, Jón Steinar G.: Computational screening of double cation metal borhydrides for solid Li electrolytes
Nehmeier, Marco: Parallel detection of interval overlapping
Neic, Aurel: Algebraic multigrid solver on clusters of CPUs and GPUs
Neukirchen, Helmut: Testing distributed and parallel systems with TTCN-3
Nguyen, Hong Diep: Efficient implementation for interval matrix multiplication
Nieminen, Risto M.: Algorithmic challenges for electronic-structure calculations (keynote lecture)

Niewiadomska-Szynkiewicz, Ewa: Software environment for parallel optimization of complex systems

Niewiadomska-Szynkiewicz, Ewa: A software tool for federated simulation of wireless sensor networks and mobile ad hoc networks

Pedersen, Andreas: Atomistic dynamics using distributed and grid computing

Pizzagalli, Laurent: Computation of transition states for extended defects in materials science: Issues and challenges from selected exemples

Rahman, Talal: A fast algorithm for a constrained total variation minimization with application to image processing

Remón, Alfredo: Accelerating model reduction of large linear systems with graphics processors

Riedel, Morris: The European middleware initiative: Delivering key technologies to distributed computing infrastructures

Riedel, Morris: Grid infrastructure interoperability in EU FP7th Euforia project

Roman Wyrzykowski: Towards efficient execution of erasure codes on multicore architectures

Ruud, Kenneth: Parallelization and grid adaptation of the Dalton quantum chemistry program

Rögnvaldsson, Ólafur: On-demand high-resolution weather forecast for search-and-rescue (SAR)

Saga, Kazushige: Grid interoperation in the RENKEI grid middleware

Schifano, Sebastiano F.: Monte Carlo simulations of spin systems on multicore processors

Schmelling, Michael: Boosting data analysis for the LHC experiments

Schnupp, Michael: Experimental performance of I/O-optimal sparse matrix dense vector multiplication algorithms within main memory

Schwanke, Christoph: Parallel particle-in-cell Monte Carlo algorithm for simulation of gas discharges under PVM and MPI (poster)

Shende, Sameer Suresh: Improving the scalability of performance evaluation tools

Signell, Artur: An efficient approximative method for generating spatially correlated multivariate random normals in parallel

Skovhede, Kenneth: CSP channels for CELL-BE

Skúlason, Egill: Simulations of atomic scale transitions at charged interfaces

Strey, Alfred: Implementation of clustering algorithms on manycore architectures

Strzelczyk, Jacek: Parallel kriging algorithm for unevenly spaced data

Stussak, Christian: Parallel computation of bivariate polynomial resultants on graphics processing units

Tillenius, Martin: An efficient task-based approach for solving the n-body problem on multicore architectures

Tudruj, Marek: Distributed Java programs initial mapping based on extremal optimization

Tudruj, Marek: Scheduling parallel programs with architecturally supported regions

Tudruj, Marek: Streaming model computation of the FDTD problem (poster)

Ujaldón, Manuel: The GPU on the 2D wavelet transform survey and contributions

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

Unat, Didem: Optimizing Aliev-Panfilov model of cardiac excitation on heterogeneous systems

Urbah, Etienne: EDGI brings desktop grids to distributed computing interoperability

Valdman, Jan: Fast MATLAB assembly of FEM stiffness- and mass matrices in 2D and 3D: Nodal elements

Vazquez-Poletti, Jose Luis: A model for efficient onboard actualization of an instrumental cyclogram for the Mars MetNet mission on a public cloud infrastructure

Vialle, Stéphane: InterCell: A software suite for rapid prototyping and parallel execution of fine-grained applications

Waśniewski, Jerzy: New algorithms and data structures for matrices in the multi/manycore era, part 3 (tutorial)

Widener, Patrick: High-performance computing tools for data-intensive research patterns

Wikfeldt, Kjartan Thor: Thermodynamical and x-ray spectroscopic insights on the structure of liquid water from large-scale molecular dynamics simulations

Wolf, Felix: Further improving the scalability of the Scalasca toolset

Wylie, Brian J.N.: Performance engineering of GemsFDTD computational electromagnetics solver

Wyrzykowski, Roman: Towards efficient execution of erasure codes on multicore architectures

Table of Contents – Part II

Part II – Minisymposium Papers

Simulations of Atomic Scale Systems

Free Energy Monte Carlo Simulations on a Distributed Network 1
Luke Czapla, Alexey Siretskiy, John Grime, and Malek O. Khan

Numerical Investigation of the Cumulant Expansion for Fourier Path Integrals 13
Nuria Plattner, Sharif Kunikeev, David L. Freeman, and Jimmie D. Doll

Optimization of Functionals of Orthonormal Functions in the Absence of Unitary Invariance 23
Peter Klüpfel, Simon Klüpfel, Kiril Tsemekhman, and Hannes Jónsson

Simulated Annealing with Coarse Graining and Distributed Computing 34
Andreas Pedersen, Jean-Claude Berthet, and Hannes Jónsson

Path Optimization with Application to Tunneling 45
Dóróthea M. Einarsdóttir, Andri Arnaldsson, Finnbogi Óskarsson, and Hannes Jónsson

Tools and Environments for Accelerator Based Computational Biomedicine

Shallow Water Simulations on Multiple GPUs 56
Martin Lilleeng Sætra and André Rigland Brodtkorb

High Performance Computing Techniques for Scaling Image Analysis Workflows 67
Patrick M. Widener, Tahsin Kurc, Wenjin Chen, Fusheng Wang, Lin Yang, Jun Hu, Vijay Kumar, Vicky Chu, Lee Cooper, Jun Kong, Ashish Sharma, Tony Pan, Joel H. Saltz, and David J. Foran

GPU Computing

Parallel Computation of Bivariate Polynomial Resultants on Graphics Processing Units 78
Christian Stussak and Peter Schenzel

Accelerating Model Reduction of Large Linear Systems with Graphics Processors 88
Peter Benner, Pablo Ezzatti, Daniel Kressner, Enrique S. Quintana-Ortí, and Alfredo Remón

Fast GPU-Based Fluid Simulations Using SPH 98
Øystein E. Krog and Anne C. Elster

Toward Techniques for Auto-tuning GPU Algorithms 110
Andrew Davidson and John Owens

High Performance Computing Interval Methods

An Interval Version of the Crank-Nicolson Method – The First Approach 120
Andrzej Marciniak

Parallel Detection of Interval Overlapping 127
Marco Nehmeier, Stefan Siegel, and Jürgen Wolff von Gudenberg

Using the Second-Order Information in Pareto-set Computations of a Multi-criteria Problem 137
Bartłomiej Jacek Kubica and Adam Woźniak

Comments on Fast and Exact Accumulation of Products 148
Gerd Bohlender and Ulrich Kulisch

An Interval Finite Difference Method of Crank-Nicolson Type for Solving the One-Dimensional Heat Conduction Equation with Mixed Boundary Conditions 157
Malgorzata A. Jankowska

Using C-XSC for High Performance Verified Computing 168
Walter Krämer, Michael Zimmer, and Werner Hofschuster

Efficient Implementation of Interval Matrix Multiplication 179
Hong Diep Nguyen

Real-Time Access and Processing of Large Data Sets

The Computing Framework for Physics Analysis at LHCb 189
Markward Britsch

Taming the Raven – Testing the Random Access, Visualization and Exploration Network RAVEN 196
Helmut Neukirchen

RAVEN – Boosting Data Analysis for the LHC Experiments 206
Michael Schmelling, Markward Britsch, Nikolai Gagunashvili, Hans Kristjan Gudmundsson, Helmut Neukirchen, and Nicola Whitehead

Bridging HPC and Grid File I/O with IOFSL 215
Jason Cope, Kamil Iskra, Dries Kimpe, and Robert Ross

Linear Algebra Algorithms and Software for Multicore and Hybrid Architectures in Honor of Fred Gustavson on His 75th Birthday

Fine Granularity Sparse *QR* Factorization for Multicore Based Systems 226
Alfredo Buttari

Mixed Precision Iterative Refinement Methods for Linear Systems: Convergence Analysis Based on Krylov Subspace Methods 237
Hartwig Anzt, Vincent Heuveline, and Björn Rocker

An Implementation of the Tile QR Factorization for a GPU and Multiple CPUs 248
Jakub Kurzak, Rajib Nath, Peng Du, and Jack Dongarra

Efficient Reduction from Block Hessenberg Form to Hessenberg Form Using Shared Memory 258
Lars Karlsson and Bo Kågström

Cache-Oblivious Algorithms and Matrix Formats for Computations on Interval Matrices 269
Rafał Dabrowski and Bartłomiej Jacek Kubica

Parallel Solution of Narrow Banded Diagonally Dominant Linear Systems 280
Carl Christian Kjelgaard Mikkelsen and Bo Kågström

Memory and Multicore Issues in Scientific Computing - Theory and Practice

An Approach for Semiautomatic Locality Optimizations Using OpenMP 291
Jens Breitbart

Memory-Efficient Sierpinski-Order Traversals on Dynamically Adaptive, Recursively Structured Triangular Grids 302
Michael Bader, Kaveh Rahnema, and Csaba Vigh

Fast Wavelet Transform Utilizing a Multicore-Aware Framework 313
Markus Stürmer, Harald Köstler, and Ulrich Rüde

Multicore Algorithms and Implementations for Application Problems

Direct Sparse Factorization of Blocked Saddle Point Matrices 324
Claude Lacoursière, Mattias Linde, and Olof Sabelström

Multi-Target Vectorization with MTPS C++ Generic Library 336
Wilfried Kirschenmann, Laurent Plagne, and Stéphane Vialle

Analysis of Gravitational Wave Signals on Heterogeneous Architectures 347
Maciej Cytowski

Towards Efficient Execution of Erasure Codes on Multicore Architectures 357
Roman Wyrzykowski, Lukasz Kuczynski, and Marcin Wozniak

Communication-Efficient Algorithms for Numerical Quantum Dynamics 368
Magnus Gustafsson, Katharina Kormann, and Sverker Holmgren

Efficiently Implementing Monte Carlo Electrostatics Simulations on Multicore Accelerators 379
Marcus Holm and Sverker Holmgren

Fast PDE Solvers and a Posteriori Error Estimates

Algebraic Multigrid Solver on Clusters of CPUs and GPUs 389
Aurel Neic, Manfred Liebmann, Gundolf Haase, and Gernot Plank

Solution of Identification Problems in Computational Mechanics – Parallel Processing Aspects 399
Radim Blaheta, Roman Kohut, and Ondřej Jakl

Scalable Tools for High Performance Computing

ScalaTrace: Tracing, Analysis and Modeling of HPC Codes at Scale 410
Frank Mueller, Xing Wu, Martin Schulz, Bronis R. de Supinski, and Todd Gamblin

A Lightweight Library for Building Scalable Tools 419
Emily R. Jacobson, Michael J. Brim, and Barton P. Miller

MATE: Toward Scalable Automated and Dynamic Performance Tuning Environment 430
Anna Morajko, Andrea Martínez, Eduardo César, Tomàs Margalef, and Joan Sorribes

Improving the Scalability of Performance Evaluation Tools 441
Sameer Suresh Shende, Allen D. Malony, and Alan Morris

Automatic Performance Analysis of OpenMP Codes on a Scalable Shared Memory System Using Periscope 452
Shajulin Benedict and Michael Gerndt

Further Improving the Scalability of the Scalasca Toolset 463
Markus Geimer, Pavel Saviankou, Alexandre Strube, Zoltán Szebenyi, Felix Wolf, and Brian J.N. Wylie

Author Index 475

Table of Contents – Part I

Part I – Keynote Papers and General Topics

Keynote Papers

On Aggressive Early Deflation in Parallel Variants of the QR Algorithm 1
Bo Kågström, Daniel Kressner, and Meiyue Shao

Limits to Nonlinear Inversion 11
Klaus Mosegaard

Cache Blocking 22
Fred G. Gustavson

General Topics

Cloud Computing

A Model for Efficient Onboard Actualization of an Instrumental Cyclogram for the Mars MetNet Mission on a Public Cloud Infrastructure 33
Jose Luis Vázquez-Poletti, Gonzalo Barderas, Ignacio M. Llorente, and Pilar Romero

HPC Algorithms

Impact of Asynchronism on GPU Accelerated Parallel Iterative Computations 43
Sylvain Contassot-Vivier, Thomas Jost, and Stéphane Vialle

Simulation of Seismic Waves Propagation in Multiscale Media: Impact of Cavernous/Fractured Reservoirs 54
Victor Kostin, Vadim Lisitsa, Galina Reshetova, and Vladimir Tcheverda

Improvements of a Fast Parallel Poisson Solver on Irregular Domains . . . 65
Andreas Adelmann, Peter Arbenz, and Yves Ineichen

Distributed Java Programs Initial Mapping Based on Extremal Optimization 75
Eryk Laskowski, Marek Tudruj, Ivanoe De Falco, Umberto Scafuri, Ernesto Tarantino, and Richard Olejnik

HPC Programming Tools

Software Environment for Parallel Optimization of Complex Systems ... 86
Ewa Niewiadomska-Szynkiewicz and Michal Marks

Parallel Programming in Morpho ... 97
Snorri Agnarsson

Extending Distributed Shared Memory for the Cell Broadband Engine to a Channel Model ... 108
Kenneth Skovhede, Morten N. Larsen, and Brian Vinter

Global Asynchronous Parallel Program Control for Multicore Processors ... 119
Janusz Borkowski, Marek Tudruj, Adam Smyk, and Damian Kopanski

HPC in Meteorology

Highly Scalable Dynamic Load Balancing in the Atmospheric Modeling System COSMO-SPECS+FD4 ... 131
Matthias Lieber, Verena Grützun, Ralf Wolke, Matthias S. Müller, and Wolfgang E. Nagel

Interactive Weather Simulation and Visualization on a Display Wall with Many-Core Compute Nodes ... 142
Bård Fjukstad, Tor-Magne Stien Hagen, Daniel Stødle, Phuong Hoai Ha, John Markus Bjørndalen, and Otto Anshus

Parallel Numerical Algorithms

The Algorithm of Multiple Relatively Robust Representations for Multi-core Processors ... 152
Matthias Petschow and Paolo Bientinesi

Parallelization of Multilevel ILU Preconditioners on Distributed-Memory Multiprocessors ... 162
José I. Aliaga, Matthias Bollhöfer, Alberto F. Martín, and Enrique S. Quintana-Ortí

CUDA 2D Stencil Computations for the Jacobi Method ... 173
José María Cecilia, José Manuel García, and Manuel Ujaldón

Streaming Model Computation of the FDTD Problem ... 184
Adam Smyk and Marek Tudruj

Numerical Aspects of Spectral Segmentation on Polygonal Grids ... 193
Anna Matsekh, Alexei Skurikhin, Lakshman Prasad, and Edward Rosten

Parallel Kriging Algorithm for Unevenly Spaced Data 204
Jacek Strzelczyk and Stanislawa Porzycka

Parallel Computing in Physics

Parallel Particle-in-Cell Monte-Carlo Algorithm for Simulation of Gas Discharges under PVM and MPI 213
Christoph Schwanke, Andreas Pflug, Michael Siemers, and Bernd Szyszka

Monte Carlo Simulations of Spin Systems on Multi-core Processors 220
Marco Guidetti, Andrea Maiorano, Filippo Mantovani, Marcello Pivanti, Sebastiano F. Schifano, and Raffaele Tripiccione

Software Environment for Market Balancing Mechanisms Development, and Its Application to Solving More General Problems in Parallel Way 231
Mariusz Kamola

The Development of Fully Coupled Simulation Software by Reusing Segregated Solvers 242
Mika Malinen

Implementation and Evaluation of Quadruple Precision BLAS Functions on GPUs 249
Daichi Mukunoki and Daisuke Takahashi

Aggregated Pumping Station Operation Planning Problem (APSOP) for Large Scale Water Transmission System 260
Jacek Błaszczyk, Krzysztof Malinowski, and Alnoor Allidina

PerPI: A Tool to Measure Instruction Level Parallelism 270
Bernard Goossens, Philippe Langlois, David Parello, and Eric Petit

InterCell: A Software Suite for Rapid Prototyping and Parallel Execution of Fine Grained Applications 282
Jens Gustedt, Stéphane Vialle, Hervé Frezza-Buet, D'havh Boumba Sitou, Nicolas Fressengeas, and Jeremy Fix

PAS2P Tool, Parallel Application Signature for Performance Prediction 293
Alvaro Wong, Dolores Rexachs, and Emilio Luque

A Software Tool for Federated Simulation of Wireless Sensor Networks and Mobile Ad Hoc Networks 303
Ewa Niewiadomska-Szynkiewicz and Andrzej Sikora

HPC Software Engineering

Performance Engineering of GemsFDTD Computational Electromagnetics Solver 314
Ulf Andersson and Brian J.N. Wylie

Scheduling Architecture–Supported Regions in Parallel Programs 325
Marek Tudruj and Łukasz Maśko

Author Index 337