High Performance Computing in Science and Engineering ’10

Wolfgang E. Nagel • Dietmar B. Kröner •
Michael M. Resch

Editors

High Performance Computing in Science and Engineering '10

Transactions of the High Performance Computing Center, Stuttgart (HLRS) 2010

Springer

Editors
Wolfgang E. Nagel
Zentrum für Informationsdienste
und Hochleistungsrechnen (ZIH)
Technische Universität Dresden
Zellescher Weg 12-14
01069 Dresden
Germany
wolfgang.nagel@tu-dresden.de

Dietmar B. Kröner
Abteilung für Angewandte Mathematik
Universität Freiburg
Hermann-Herder-Str. 10
79104 Freiburg
Germany
dietmar@mathematik.uni-freiburg.de

Michael M. Resch
Höchstleistungsrechenzentrum
Stuttgart (HLRS)
Universität Stuttgart
Nobelstraße 19
70569 Stuttgart
Germany
resch@hlrs.de

Front cover figure: Temperature isosurface inside a lignite-fired utility boiler with a cross-sectional area of 23 m × 23 m and a height of 150 m. Institut für Feuerungs- und Kraftwerkstechnik, Universität Stuttgart

ISBN 978-3-642-15747-9 e-ISBN 978-3-642-15748-6
DOI 10.1007/978-3-642-15748-6
Springer Heidelberg Dordrecht London New York

Library of Congress Control Number: 2010938287

Mathematics Subject Classification (2010): 65Cxx, 65C99, 68U20

© Springer-Verlag Berlin Heidelberg 2011
This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilm or in any other way, and storage in data banks. Duplication of this publication or parts thereof is permitted only under the provisions of the German Copyright Law of September 9, 1965, in its current version, and permission for use must always be obtained from Springer. Violations are liable to prosecution under the German Copyright Law.
The use of general descriptive names, registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

Cover design: WMXDesign GmbH

Printed on acid-free paper

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

Preface

The Gauss Centre for Supercomputing (GCS) – linking the three national supercomputing centres HLRS (Stuttgart), NIC/JSC (Jülich), and LRZ (Garching) – has established itself as the driving force for high-performance computing (HPC) in Germany, and, even beyond, in Europe. Based on the agreement (Verwaltungsabkommen) between the Federal Ministry of Education and Research (BMBF) and the state ministries for research of Baden-Wuerttemberg, Bavaria, and North Rhine-Westphalia, the overall budget of 400 Million Euros has been allocated – shared equally between federal and state authorities in a five-year time period – to establish the next generation of HPC systems at the GCS. Since the installation of the IBM Blue Gene/P at NIC/JSC in May 2009 – the first phase of the HPC Tier-0 resources – the GCS provides the most powerful high-performance computing infrastructure in Europe today.

It is a pleasure to announce that the next major steps of this agreement will be taken at the HLRS in 2011 and 2013. In 2009/2010, due to the support of the state ministry for research of Baden-Württemberg, the available CPU resources were increased tenfold in an intermediate step, by replacing many of the NEC SX-8 nodes with NEC SX-9/12M192 and installing a remarkably large Intel Nehalem cluster. This has brought a peak performance of 80+ TFLOPs to the users of HLRS. Now, in October 2010 the next round of the GCS infrastructure has been contracted, and the system at the HLRS will be delivered by Cray Inc. in 2011 and 2013. The first delivery phase will be a large Cray XT-6 with a peak speed of roughly 1 PFLOPS. In 2013, in the second delivery phase the final system will be installed, and its peak performance will be roughly 5 PFLOPS, more than twice as fast as the current number-one TOP500-system, and more than 50 times faster than the current systems at the HLRS. After the first upgrade of the HLRS system, the LRZ will upgrade its systems accordingly. The plan is to have a Tier-0 HPC system within the GCS operating at any time within the five year period.

As part of the GCS, HLRS also participates in the European project PRACE (Partnership for Advances Computing in Europe), extending its reach to all European member countries. Within the PRACE project, the GCS will

donate access to high performance computing resources valued at 100 million Euros. These PRACE-activities align well with the activities of the HLRS in the European HPC infrastructure project DEISA (Distributed European Infrastructure for Supercomputing Applications) and in the European HPC support project HPC-Europa2.

While the Gauss Centre for Supercomputing successfully addressed the needs on the high end, it was clear from the beginning that an additional layer of support was required to maintain the longevity of the Centre with a network of competence centers across Germany. This gap is addressed by the Gauß–Allianz, where regional and topical centers team up to create the necessary infrastructure, knowledge and the required methods and tools. The mission of the Allianz is to coordinate the HPC-related activities of its members. By providing versatile computing architectures and by combining the expertise of the participating centers, the ecosystem necessary for computational science is created. Strengthening the research and increasing the visibility to compete at the international level are further goals of the Gauß–Allianz.

At the moment, the entire HPC community in Germany is awaiting the funding decisions of the second BMBF HPC-call of May 2010. This call is directed towards proposals to enable and support petascale applications on more than 100,000 processors. While the projects of the first funding round started in early 2009, the follow-up call has been delayed by more than 18 months. Nevertheless, all experts and administration authorities continue to see the strong need for such a program, given that the main issue seen in nearly all applications is one of scalability. The strategic plan involves spending another 20 Million Euros each year over the next three years for projects to develop scalable algorithms, methods, and tools to support massively parallel systems. This may seem like a very large investment. Nevertheless, in relation to the investment in hardware in Germany over this five years period, it is still comparatively small. And furthermore, it will produce brains – brains we will need in order to use the newly developed innovative methods and tools to accomplish technological breakthroughs in scientific as well as industrial fields of application. Even more, the target will not be the Petascale only but also Exascale systems. As we all know, we do not only need competitive hardware but also excellent software and methods to address – and solve – the most demanding problems in science and engineering. The success of this approach is of significant importance for our community and will also greatly influence the development of new technologies and industrial products; beyond that, this will finally determine whether Germany will be an accepted partner alongside the leading technology and research nations.

Since 1996, the HLRS has supported the scientific community as part of its official mission. Just as in the past years, the major results of the last 12 months were presented at the 14th annual Results and Review Workshop on High Performance Computing in Science and Engineering, which was held on October 4–5, 2010 at the Stuttgart University. The workshop proceedings contain the written versions of the research work presented. The papers were

selected from all projects running at the HLRS and the SSC Karlsruhe during the one-year period beginning October 2009. Overall, 44 papers were chosen from Physics, Solid State Physics, Reactive Flow, Computational Fluid Dynamics (CFD), Transport and Climate, and numerous other fields. The largest number of contributions – as in many previous years – came from CFD with 16 papers. Even though such a small collection cannot entirely represent such a vast area, the selected papers demonstrate the state-of-the-art in high performance computing in Germany. The authors were encouraged to emphasize computational techniques used in solving the problems examined. This often forgotten aspect was the major focus of these proceedings. Nevertheless, the importance of the newly computed scientific results for the specific disciplines should not be disregarded.

We gratefully acknowledge the continuing support of the federal state of Baden-Württemberg in promoting and supporting high performance computing. Grateful acknowledgement is also due to the German Research Foundation (Deutsche Forschungsgemeinschaft (DFG)), as many projects pursued on the HLRS and SSC computing machines could not have been carried out without its support. Also, we thank Springer Verlag for publishing this volume and, thus, helping to position the local activities in an international framework. We hope that this series of publications contributes to the global promotion of high performance scientific computing.

Stuttgart, October 2010

Wolfgang E. Nagel
Dietmar Kröner
Michael Resch

Contents

Physics
P. Nielaba 1

Spin-Liquid Phase in the Hubbard Model on the Honeycomb Lattice
Z.Y. Meng, T.C. Lang, S. Wessel, F.F. Assaad, and A. Muramatsu 5

Massive and Massless Four-Loop Integrals
J.H. Kühn, P. Marquard, M. Steinhauser, and M. Tentyukov 19

Ligand Protected Gold Alloy Clusters as Superatoms
M. Walter 29

The Chiral Critical Surface of QCD
Ph. de Forcrand and O. Philipsen 43

Mesoscopic Simulations of Polyelectrolyte Electrophoresis in Nanochannels
J. Smiatek and F. Schmid 53

The SuperN-Project: An Update on Core-Collapse Supernova Simulations
B. Müller, L. Hüdepohl, A. Marek, F. Hanke, and H.-Th. Janka 69

Higgs Boson Mass Bounds from a Chirally Invariant Lattice Higgs-Yukawa Model
P. Gerhold, K. Jansen, and J. Kallarackal 85

Dust, Chemistry & Radiation Transport in MRI-Turbulent Protoplanetary Discs
M. Flaig, W. Kley, R. Kissman, and P. Ruoff 103

Solid State Physics
W. Hanke 117

Organic-Metal Interface: Adsorption of Cysteine on Au(110) from First Principles
B. Höffling, F. Ortmann, K. Hannewald, and F. Bechstedt 119

Ab-initio Characterization of Electronic Properties of PbTe Quantum Dots Embedded in a CdTe Matrix
R. Leitsmann and F. Bechstedt 135

Si(111)-In Nanowire Optical Response from Large-scale Ab Initio Calculations
W.G. Schmidt, S. Wippermann, E. Rauls, U. Gerstmann, S. Sanna, C. Thierfelder, M. Landmann, and L.S. dos Santos 149

Laser Ablation of Metals
J. Roth, C. Trichet, H.-R. Trebin, and S. Sonntag 159

Conductance and Noise Correlations of Correlated Nanostructures
A. Branschädel and P. Schmitteckert 169

Cu Substitutionals and Defect Complexes in the Lead-Free Ferroelectric KNN
S. Körbel and C. Elsässer 181

Reacting Flows
D. Kröner 189

Scalar Mixing in Droplet Arrays in Stagnant and Convective Environments
A. Kronenburg, M.R.G. Zoby, S. Navarro-Martinez, and A.J. Marquis . . 191

Euler-Lagrange Simulation of a LOX/H2 Model Combustor with Single Shear Coaxial Injector
M. Lempke, P. Gerlinger, M. Rachner, and M. Aigner 203

Simulation of Triflux Heat Exchangers in Utility Boilers
A. Matschke, M. Müller, U. Schnell, and G. Scheffknecht 217

Computational Fluid Dynamics
S. Wagner 229

Direct Numerical Simulation of Swept-Wing Laminar Flow Control Using Pinpoint Suction
T.A. Friederich and M.J. Kloker 231

A Numerical Study of Turbulent Stably-Stratified Plane Couette Flow
M. García-Villalba, E. Azagra, and M. Uhlmann 251

DNS of Unsteady Heat Transfer Increase on a Curved Surface Due to Wake-Induced Turbulence
D. von Terzi, L. Venema, H.-J. Bauer, and W. Rodi 263

Application of a Novel Turbulence Generator to Multiphase Flow Computations
C. Huber, H. Gomaa, and B. Weigand 273

Numerical Investigation on the Deformation of Droplets in High-Pressure Homogenizers
K. Kissling, S. Schütz, and M. Piesche 287

Direct Numerical Simulation of Sediment Transport in Turbulent Open Channel Flow
C. Chan-Braun, M. García-Villalba, and M. Uhlmann 295

Grid Sensitivity of LES Heat Transfer Results of a Turbulent Round Impinging Jet
S.O. Neumann, N. Uddin, and B. Weigand 307

Large Eddy Simulations of a Jet in Crossflow
F.C.C. Galeazzo, P. Habisreuther, and N. Zarzalis 327

The Impact of Secondary Mean Vortices on Turbulent Separation in 3D Diffusers
D. von Terzi, H. Schneider, and H.-J. Bauer 339

Time-Dependent Three-Dimensional Simulation of the Turbulent Flow and Heat Transfer in Czochralski Crystal Growth Including the Three-Phase Boundary Movement
A. Raufeisen, M. Breuer, T. Botsch, and A. Delgado 353

Numerical Investigation of Shock Wave Boundary-Layer Interaction Using a Zonal RANS-LES Ansatz
B. Roidl, M. Meinke, and W. Schröder 369

Large Eddy Simulation of the Cyclic Variations in an Internal Combustion Engine
F. Magagnato, A. Walcker, and M. Gabi 385

CFD-CSD-Coupled Simulations of Helicopter Rotors Using an Unstructured Flow Solver
F. Bensing, M. Keßler, and E. Krämer 393

Wake Signature of Finite-Span Flapping Rigid Wings
J.E. Guerrero 407

Computational Design Study of a 3D Hypersonic Intake for Scramjet Demonstrator Testing
B. Reinartz and M. Behr 429

Characterization of Mixing in Food Extrusion and Emulsification Processes by Using CFD
M.A. Emin, K. Köhler, M. Schlender, and H.P. Schuchmann 443

Transport and Climate
C. Kottmeier 463

Modelling Regional Climate Change in Germany
P. Berg, H.-J. Panitz, G. Schädler, H. Feldmann, and C. Kottmeier 467

Modelling the Extratropical Transition of Tropical Cyclones and Its Downstream Impact
C.M. Grams and S.C. Jones 479

Global Long-Term MIPAS Data Processing: Some Aspects of the Dynamics of the Atmosphere from Lower Stratosphere to Lower Thermosphere
M. Kiefer, B. Funke, U. Grabowski, and A. Linden 501

Miscellaneous Topics
W. Schröder 515

Computer Simulation for Building Implosion Using LS-DYNA
G. Michaloudis, S. Mattern, and K. Schweizerhof 519

Quaero Speech-to-Text and Text Translation Evaluation Systems
S. Stüker, K. Kilgour, and J. Niehues 529

Molecular Modeling of Hydrogen Bonding Fluids: Transport Properties and Vapor-Liquid Coexistence
J. Vrabec, G. Guevara-Carrion, T. Merker, and H. Hasse 543

Software Framework UG: Parallel Simulation of a Three-Dimensional Benchmark Problem for Thermohaline-Driven Flow
M. Lampe, A. Grillo, and G. Wittum 553

Tailored Usage of the NEC SX-8 and SX-9 Systems in Satellite Geodesy
M. Roth, O. Baur, and W. Keller 561

A Geodynamic Model of the Evolution of the Earth's Chemical Mantle Reservoirs
U. Walzer and R. Hendel 573

Three-Dimensional Simulation of Rarefied Plasma Flows Using a High Order Particle in Cell Method
J. Neudorfer, T. Stindl, A. Stock, R. Schneider, D. Petkow, S. Roller, C.-D. Munz, and M. Auweter-Kurtz 593