

High Performance Computing on Vector Systems 2008

Michael Resch · Sabine Roller · Katharina Benkert ·
Martin Galle · Wolfgang Bez · Hiroaki Kobayashi ·
Toshio Hirayama

Editors

High Performance Computing on Vector Systems 2008

 Springer

Michael Resch
Sabine Roller
Katharina Benkert
Höchstleistungsrechenzentrum
Stuttgart (HLRS)
Universität Stuttgart
Nobelstraße 19
70569 Stuttgart
Germany
resch@hlrs.de
roller@hlrs.de
benkert@hlrs.de

Martin Galle
Wolfgang Bez
NEC Deutschland GmbH
Hansaallee 101
40549 Düsseldorf
Germany
mgalle@hpce.nec.com
wbez@hpce.nec.com

Hiroaki Kobayashi
Cyberscience Center
Tohoku University
6-3 Aramaki-Aza-Aoba
Sendai, 980-8578
Japan
koba@isc.tohoku.ac.jp

Toshio Hirayama
Center for computational science and e-systems
Japan Atomic Energy Agency
Sumitomo fudosan Ueno Bldg. No. 8
6-9-3 Higashi-Ueno Taito-ku
Tokyo, 110-0015
Japan
hirayama.toshio@jaea.go.jp

Front cover figure: Simulation of the UV curing process in automotive coating with multiple ultraviolet lamps. Picture due to IFF, University of Stuttgart, Germany and BMW Group.

ISBN 978-3-540-85868-3

e-ISBN 978-3-540-85869-0

DOI 10.1007/978-3-540-85869-0

Library of Congress Control Number: 2008934396

Mathematics Subject Classification (2000): 68Wxx, 68W10, 68U20, 76-XX, 86A05, 86A10, 70Fxx

© 2009 Springer-Verlag Berlin Heidelberg

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 for 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, Heidelberg

Printed on acid-free paper

987654321

springer.com

Preface

This book covers the results obtained in the Teraflop Workbench project during a four years period from 2004 to 2008. The Teraflop Workbench project is a collaboration between the High Performance Computing Center Stuttgart (HLRS) and NEC Deutschland GmbH (NEC-HPCE) to support users to achieve their research goals using high performance computing.

The Teraflop Workbench supports users of the HLRS systems to enable and facilitate leading edge scientific research. This is achieved by optimizing their codes and improving the process workflow which results from the integration of different modules into a “hybrid vector system”. The assessment and demonstration of industrial relevance is another goal of the cooperation.

The Teraflop Workbench project consists of numerous individual codes, grouped together by application area and developed and maintained by researchers or commercial organizations. Within the project, several of the codes have shown the ability to reach beyond the TFlop/s threshold of sustained performance. This created the possibility for new science and a deeper understanding of the underlying physics. The papers in this book demonstrate the value of the project for different scientific areas.

The work in the Teraflop Workbench project gave us insight into the applications and requirements for current and future HPC systems. We observed the emergence of multi-scale and multi-physics applications, the increase in interdisciplinary work and the growing tendency to use today’s stand-alone application codes as modules in prospective, more complex coupled simulations. At the same time, we noticed the current lack of support for those applications. Our goal is to offer an environment to our users that allows them to concentrate on their area of expertise without spending too much time on computer science itself.

We would like to thank all the contributors of this book and of the Teraflop Workbench project in general.

Stuttgart, July 2008

*Sabine P. Roller
Michael M. Resch*

Contents

I Future Architectures

First Experiences with NEC SX-9	3
Hiroaki Kobayashi, Ryusuke Egawa, Hiroyuki Takizawa, Koki Okabe, Akihiko Musa, Takashi Soga, and Yoichi Shimomura	
1 Introduction	3
2 System Overview	5
3 Performance Evaluation	6
4 Conclusions	9
References	10
Scalable Computing in a Hybrid System Architecture	13
Wilfried Oed	
1 Introduction	13
2 The Need for Scalability	14
3 Processor Trends	15
4 The Cray XT5 _h Hybrid Supercomputer	17
5 The Cray Cascade Program	19
6 Conclusion	20
References	20
Prerequisites for the Productive Usage of Hybrid Systems	23
Danny Sternkopf and Martin Galle	
1 Introduction	23
2 HLRS System Overview	24
3 SW Components for a Hybrid System	25
3.1 Batch System	26
3.2 Global Filesystem	27
3.3 MPI	30
4 Conclusion	31
References	31

II Multiscale and Multiphysics Simulations

Complex Numerical Simulations in Production Techniques	35
A. Scheibe and E. Westkämper	
1 Problem Statement and Motivation	35
2 Multi-Scale Modeling and Simulation of Manufacturing Systems ..	36
2.1 Vision and Scientific Impact	36
2.2 Challenges, Theoretical Considerations and Definitions ..	37
3 A New Concept Towards a Comprehensive and Holistic Factory	
Simulation Model	38
3.1 Theoretical Aspects	38
3.2 Vectorial Modelling and Simulation Approach Based	
on Business/Organizational Parameters and Technical	
Tolerances	40
4 Complex Example in Automotive Coating Industry	42
5 Conclusions and Future Work	44
References	44

Multi-scale and Multi-physics Applications — User Requirements for Future Applications

Sabine P. Roller	
1 Introduction	45
2 A Glance at Past, Current and Future Simulation Applications	46
3 Future Application Perspective	47
4 Examples	48
4.1 Dynamic Coating Simulation	48
4.2 Ocean Water Plant	48
4.3 Particle-loaden Flows	49
4.4 Multi-scale Aero-acoustics	50
5 Future User Perspective	51
6 Requirements, Architecture and Tools	52
References	52

III Grid Computing & Data Analysis

An Application of the NAREGI Grid Middleware to a Nationwide Joint-Use Environment for Computing

Eisaku Sakane, Manabu Higashida, and Shinji Shimojo	
1 Introduction	55
2 NAREGI Grid Middleware	56
3 Issues	57
3.1 Resource Provisioning	58
3.2 Password / Passphrase Management	58
3.3 Issuance of Grid Certificate	58
3.4 Grid Operations	59
4 Application Method	59

5	Evaluation of Proposed Method	61
6	Cooperative Evaluation	62
7	Summary and future works	63
	References	63

Interoperation between Atomic Energy Grid Infrastructure (AEGIS) and Other Grids 65

Yoshio Suzuki, Noriyuki Kushida, Naoya Teshima, Kohei Nakajima, Akemi Nishida, and Norihiro Nakajima

1	Introduction	65
2	History of Grid Computing Technology at CCSE	66
3	Atomic Energy Grid Infrastructure	68
4	Interoperability Technology based on Atomic Energy Grid Infrastructure	69
5	Collaboration with the High Performance Computing Center Stuttgart (HLRS)	72
6	Collaboration with Grid-TLSE Project Partners	74
7	Collaboration with the U.S. Department of Energy Under the Global Nuclear Energy Partnership	74
8	Summary	75
	References	76

Parallel File Systems in European Grid Projects 79

Peter W. Haas and Michael M. Resch

1	Introduction	79
2	The HLRS Framework	80
	2.1 Target	80
	2.2 Organization	80
	2.3 HLRS Computer Configuration	80
3	Ex@Grid Framework	81
	3.1 Gauss Center for Supercomputing	81
	3.2 Ex@Grid Design	81
4	Consolidation in the Datacenter	82
	4.1 Datacenter Ethernet	82
	4.2 IEEE 802.3ar: Congestion Management	82
5	Multicluster Parallel File Systems	83
	5.1 Multicluster GPFS in DEISA	83
	5.2 Network-centered parallel HSM systems	83
	5.3 Projected mass storage system at HLRS	84
6	The Teraflop Workbench Concept	84
	6.1 Workflow Example	85
	6.2 Fenfloss	85
	6.3 Demonstration in the HLRS Cave	85
	6.4 Virtual Tour of Kiebingen Water Power Plant	86
7	Conclusion	86
	References	87

Development of Cognitive Methodology based Data Analysis System	89
Chiaki Kino, Yoshio Suzuki, Noriyuki Kushida, Akemi Nishida, Sachiko Hayashi, and Norihiro Nakajima	
1	Introduction 89
2	The Basic Idea of CDAS 91
2.1	Data Analysis Process 91
2.2	VV and DD Functions 91
2.3	Synthesis Function 92
2.4	Evaluation and Judgment 92
3	System Configuration 93
3.1	Flow of Data Analysis by CDAS 93
3.2	Implementation on a Grid Computing 94
4	Result and Discussion 94
5	Conclusions and Future Works 96
	References 97

IV Chemical Applications

3D-Flame Modelling in Power Plant Applications	101
Benedetto Riso, Norbert Paßmann, Friedhelm Wessel, Egbert Reinartz	
1	Introduction 101
2	Flame modelling tool and computer hardware 102
3	Neurath A/B boiler model 104
4	Simulation results 105
5	Summary 110
	References 110
Hierarchical Modeling of Combustion Processes	111
Ulrich Maas, Viatcheslav Bykov, Andriy Rybakov, and Rainer Stauch	
1	Introduction 111
2	Dynamics of Reacting Flows 112
3	Detailed Models 114
3.1	Chemical kinetics 115
3.2	Chemistry-Turbulence Coupling 115
3.3	Modeling of Multi-Phase Processes 116
4	Model Reduction 118
4.1	Chemical Kinetics 119
4.2	Chemistry-Turbulence Interaction 121
4.3	Multi-Phase Processes 123
5	Coupling of the Sub-Models 123
6	Summary 125
	References 126

Understanding Molecular Recognition and Self-Assembly from Large-Scale Numerical Simulations	129
Stephan Blankenburg and Wolf Gero Schmidt	
1 Introduction	129
2 Computational Method	131
3 Results and Discussion	131
4 Conclusions	136
References	137
Large Scale Particle-in-cell Plasma Simulation	139
Seiji Ishiguro	
1 Introduction	139
2 Parallelization of 3D Particle-in-cell Code using High Performance Fortran	140
3 PIC Simulation of Blob Transport	141
4 Conclusion	143
References	144
Multi-scale Modeling of Crack Propagation	145
Mitsuhiro Itakura, Hideo Kaburaki, Masatake Yamaguchi, and Ken-ichi Ebihara	
1 Introduction	145
2 Multi-scale Model of SCC	146
2.1 Oxygen Embrittlement Mechanism	146
2.2 Mechanics Modeling of Crack Growth	147
2.3 Oxygen Diffusion Modeling	149
3 Simulation Details and Results	149
4 Conclusions	151
References	152
V Climate Modeling, Hydro- and Aerodynamics	
The Climate Model ECHAM5 on NEC SX-8	155
Stefan Borowski	
1 Introduction	155
2 Runtime Analysis	156
3 Optimizations	157
3.1 Single CPU Optimizations	157
3.2 Scalability Optimizations	158
4 Performance Results	158
4.1 Single CPU Performance	158
4.2 Scalability	159
5 Conclusions	161
References	162

A Large Spectrum of Free Oceanic Oscillations	163	
Malte Müller		
1	Introduction	163
2	State of Knowledge	164
3	Free Oceanic Oscillation Model with Consideration of LSA	165
3.1	Theory	166
3.2	The Implicitly Restarted Arnoldi Method	167
3.3	The Parallelization with MPI	169
3.4	The Performance of the Model	169
4	Results	170
4.1	Gravitational Modes	171
4.2	Vorticity Modes	171
5	Conclusion	174
	References	174
Direct Numerical Simulation of Controlled Shear Flows	177	
Markus J. Kloker, Tillmann A. Friederich, Jens Linn		
1	Laminar-Flow-Control Case	177
1.1	Introduction	177
1.2	Numerical Model	179
1.3	Secondary Instability and Control Setup	180
1.4	Control Results and Conclusions	181
2	Effusion Cooling Case at <Mach 6.8> Flight Conditions	184
2.1	Introduction	184
2.2	Numerical Model	184
2.3	Blowing Through Slits	185
2.4	Blowing Through Holes	188
3	Computational Aspects and Outlook	191
	References	193
Fluid-Structure Interaction in Turbine Simulation	195	
Felix Lippold and Albert Ruprecht		
1	Introduction	195
2	Basic Equations	196
3	Fluid-Structure Coupling	200
4	Efficient Moving Mesh Scheme	201
5	Coupled Codes and Architecture	202
5.1	FENFLOSS — CFD on Vector Systems	202
5.2	FSI Coupling with FENFLOSS on SX-8	203
6	von Karman Vortex Street	204
7	FSI Benchmark Application	206
8	Tidal Turbine Runner	209
8.1	Computational Model and Performance	210
8.2	Fluid-Structure Interaction Results	210
9	Summary	212
	References	213

Heterogeneous Parallel Aero-Acoustics Using PACX-MPI 215
 Harald Klimach and Sabine Roller and Claus-Dieter Munz

- 1 The Aero-Acoustic Application 215
 - 1.1 Structure of the Application 216
 - 1.2 Coupling Scheme 216
 - 1.3 Parallelization 217
- 2 PACX-MPI 218
 - 2.1 Communication Layout 218
 - 2.2 Heterogeneous Environment 219
 - 2.3 Starting an Application Using PACX-MPI 219
- 3 Heterogeneous Computations 219
- 4 Conclusion 221
- References 222

Meandering of Wing-Tip Vortices Interacting with a Cold Jet in the Extended Wake 223
 Frank T. Zurheide, Matthias Meinke, and Wolfgang Schröder

- 1 Introduction 223
- 2 Governing Equations 225
- 3 Boundary Conditions 226
 - 3.1 Experimental set-up 226
 - 3.2 Inflow boundary conditions 227
- 4 Results 228
- 5 Computational Resources 238
- 6 Conclusions 239
- References 240