Contents

Part I Fluid Dynamics

BESTWIHR: Testing of a Closure Assumption for Fully Developed Turbulent Channel Flow with the Aid of a Lattice Boltzmann Simulation
Peter Lammers, Kamen N. Beronov, Thomas Zeiser, Franz Durst 3

DiSiVGT: Validation of a novel turbulence model using direct numerical simulation
J. Kreuzinger, J. Jovanović, R. Friedrich 19

FlowNoise: Flow Induced Noise Computation on Hitachi SR8000-F1
M. Escobar, I. Ali, M. Kaltenbacher, S. Becker, F. Hülsemann 31

FLUSIB: Fully Three-Dimensional Coupling of Fluid and Thin-Walled Structures
Dominik Scholz, Ernst Rank, Markus Glück, Michael Breuer, Franz Durst 43

ParChem: Efficient Numerical Methods for Chemical Problems related to MOVPE
E. Mesic, M. Mukinovic, L. Kadinski and G. Brenner 51

RexSim: Monte Carlo Simulations of Radiative Heat Transfer in Parallel Computer Architectures
G. Brenner, L. Kadinski, J.G. Marakis, ... 63

SkvG: Cache-Optimal Parallel Solution of PDEs on High Performance Computers Using Space-Trees and Space-Filling Curves
Markus Langlotz, Miriam Mehl, Tobias Weinzierl, Christoph Zenger 71

VISimLab: Optimizing an Interactive CFD Simulation on a Supercomputer for Computational Steering in a Virtual Reality Environment
Petra Wenisch, Oliver Wenisch, Ernst Rank 83

Part II Computer Science and Mathematics

cxHPC: Setting up ByGRID — First Steps Towards an e-Science Infrastructure in Bavaria
Georg Hager, Thomas Zeiser, Helmut Heller 97

FPGA: Exploration of the possibilities for the direct synthesis of concurrent C programs on high-performance computers in FPGAs
Peter Urbanek and Stefan May 103

gridlib: A Parallel, Object-oriented Framework for Hierarchical-hybrid Grid Structures in Technical Simulation and Scientific Visualization
Frank Hülsemann, Stefan Meinlschmidt, Ben Bergen, Günther Greiner, Ulrich Rüde 117

LRZ: The Suitability of Contemporary Processors for Quantum Chemical Computations
Ludger Palm 129

MethWerk: Scalable Mesh-based Simulation on Clusters of SMPs
Amitava Gupta, Peter Luksch, Andreas C. Schmidt 141

OPTILAS: Numerical Optimization as a Key Tool for the Improvement of Advanced Multi-Beam Laser Welding Techniques
Verena Petzet, Christof Büskens, Hans Josef Pesch, Victor Karkhin, Maksym Makhutin, Andrey Prikhodovsky, Vasily Ploshikhin 153

ParEXPDE: Expression Templates and Advanced PDE Software Design on the Hitachi SR8000
Christoph Freundl, Ben Bergen, Frank Hülsemann, Ulrich Rüde 167

ParRichy: Parallel Simulation of Bioreactive Multicomponent Transport Processes in Porous Media
S. Kräutle, M. Bause, A. Prechtel, F. Radu, P. Knabner 181

Peridot: Towards Automated Runtime Detection of Performance Bottlenecks
Karl Fürlinger, Michael Gerndt 193

Part III Natural Sciences

CUHE: Electron-Spin Interaction in High-T_c Superconductors
Zhongbing Huang, Werner Hanke, and Enrico Arrigoni 205

ENZYMECH: Computer Simulations of Enzyme Reaction Mechanisms: Application of a Hybrid Genetic Algorithm for the Superimposition of Three-Dimensional Chemical Structures
Alexander von Homeyer, Johann Gasteiger 213

FreeWIHR: Lattice Boltzmann Methods with Free Surfaces and their Application in Material Technology
Carolin Körner, Thomas Pohl, Ulrich Rüde, Nils Thürey, Torsten Hofmann . . 225

HQS@HPC: Comparative numerical study of Anderson localisation in disordered electron systems
Gerald Schubert, Alexander Weiße, Gerhard Wellein, Holger Fehske 237

NBW: Computational Seismology: Narrowing the Gap Between Theory and Observations
Bernhard Schuberth, Michael Ewald, Heiner Igel, Markus Treml, Haijiang Wang, Gilbert Brietzke 251

OOPCV: Phasediagram and Scaling Properties of the Projected SO(5) Model in Three Dimensions
Martin Jöstingmeier, Ansgar Dorneich, Enrico Arrigoni, Werner Hanke, S.C. Zhang 263

ParBaum: A Fast Program for Phylogenetic Tree Inference with Maximum Likelihood
Alexandros P. Stamatakis, Thomas Ludwig and Harald Meier 275

ParaGauss: The Density Functional Program ParaGauss for Complex Systems in Chemistry
Notker Rösch, Sven Krüger, Vladimir A. Nasluzov', Alexei V. Matveev 285

Appendix Color figures

Color figures 297