

# 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 Furlinger, Michael Gerndt* ..... 193

---

**Part III Natural Sciences**

---

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

---

<b>ENZYMECH: Computer Simulations of Enzyme Reaction Mechanisms: Application of a Hybrid Genetic Algorithm for the Superimposition of Three-Dimensional Chemical Structures</b> <i>Alexander von Homeyer, Johann Gasteiger</i> .....	213
<b>FreeWIHR: Lattice Boltzmann Methods with Free Surfaces and their Application in Material Technology</b> <i>Carolin Körner, Thomas Pohl, Ulrich Rüde, Nils Thürey, Torsten Hofmann</i> ..	225
<b>HQS@HPC: Comparative numerical study of Anderson localisation in disordered electron systems</b> <i>Gerald Schubert, Alexander Weiße, Gerhard Wellein, Holger Fehske</i> .....	237
<b>NBW: Computational Seismology: Narrowing the Gap Between Theory and Observations</b> <i>Bernhard Schuberth, Michael Ewald, Heiner Igel, Markus Trembl, Haijiang Wang, Gilbert Brietzke</i> .....	251
<b>OOPCV: Phasediagram and Scaling Properties of the Projected SO(5) Model in Three Dimensions</b> <i>Martin Jöstingmeier, Ansgar Dorneich, Enrico Arrigoni, Werner Hanke, S.C. Zhang</i> .....	263
<b>ParBaum: A Fast Program for Phylogenetic Tree Inference with Maximum Likelihood</b> <i>Alexandros P. Stamatakis, Thomas Ludwig and Harald Meier</i> .....	275
<b>ParaGauss: The Density Functional Program ParaGauss for Complex Systems in Chemistry</b> <i>Notker Rösch, Sven Krüger, Vladimir A. Nasluzov, Alexei V. Matveev</i> .....	285
<hr/>	
<b>Appendix Color figures</b>	
<b>Color figures</b> .....	297

---

High Performance Computing in Science and  
Engineering, Garching 2004

Transaction of the KONWIHR Result Workshop, October  
14-15, 2004, Technical University of Munich, Garching,  
Germany

Bode, A.; Durst, F. (Eds.)

2005, XI, 301 p., Hardcover

ISBN: 978-3-540-26145-2