Wolfgang E. Nagel · Willi Jäger · Michael Resch
Editors

High Performance Computing in Science and Engineering '06

Transactions of the High Performance Computing Center
Stuttgart (HLRS) 2006

With 312 Figures, 101 in Colour, and 46 Tables

Contents

Physics

H. Ruder and R. Speith 1

Gravitational Wave Signals from Simulations of Black Hole Dynamics

*B. Brügmann, J. Gonzalez, M. Hannam, S. Husa, P. Marronetti,
U. Sperhake, and W. Tichy* 3

The SuperN-Project: Understanding Core Collapse Supernovae

A. Marek, K. Kifonidis, H.-Th. Janka, and B. Müller 19

MHD Code Optimizations and Jets in Dense Gaseous Halos

V. Gaibler, M. Vigelius, M. Krause, and M. Camenzind 35

Anomalous Water Optical Absorption:

Large-Scale *First-Principles* Simulations

*W.G. Schmidt, S. Blankenburg, S. Wippermann, A. Hermann,
P.H. Hahn, M. Preuss, K. Seino, and F. Bechstedt* 49

The Electronic Structures of Nanosystems:

Calculating the Ground States of Sodium Nanoclusters

and the Actuation of Carbon Nanotubes

B. Huber, L. Pastewka, P. Koskinen, M. Moseler 59

Object-Oriented SPH-Simulations with Surface Tension

S. Ganzenmüller, A. Nagel, S. Holtwick, W. Rosenstiel, and H. Ruder .. 69

Simulations of Particle Suspensions at the Institute

for Computational Physics

J. Harting, M. Hecht, and H. Herrmann 83

Solid State Physics

<i>W. Hanke</i>	93
-----------------------	----

Nano-Systems in External Fields and Reduced Geometry:

Numerical Investigations

<i>P. Henseler, C. Schieback, K. Franzrahe, F. Bürzle, M. Dreher, J. Neder, W. Quester, M. Kläui, U. Rüdiger, and P. Nielaba</i>	97
--	----

Signal Transport and Finite Bias Conductance

in and Through Correlated Nanostructures

<i>P. Schmitteckert and G. Schneider</i>	113
--	-----

Atomistic Simulations of Dislocation – Crack Interaction

<i>E. Bitzek and P. Gumbsch</i>	127
---------------------------------------	-----

Monte Carlo Simulations of Strongly Correlated

and Frustrated Quantum Systems

<i>C. Lavalie, S.R. Manmana, S. Wessel, and A. Muramatsu</i>	137
--	-----

Chemistry

<i>C. van Wüllen</i>	153
----------------------------	-----

Characterization of Catalyst Surfaces by STM Image Calculations

<i>R. Kovacik, B. Meyer, and D. Marx</i>	155
--	-----

Theoretical Investigation of the Self-Diffusion on Au(100)

<i>K. Pötting, T. Jacob, and W. Schmickler</i>	171
--	-----

TrpAQP: Computer Simulations to Determine

the Selectivity of Aquaporins

<i>M. Dynowski and U. Ludewig</i>	187
---	-----

Computational Fluid Dynamics

<i>S. Wagner</i>	199
------------------------	-----

Direct Numerical Simulation and Analysis of the Flow Field

Around a Swept Laminar Separation Bubble

<i>T. Hetsch and U. Rist</i>	205
------------------------------------	-----

Direct Numerical Simulation of Primary Breakup Phenomena

in Liquid Sheets

<i>W. Sander and B. Weigand</i>	223
---------------------------------------	-----

Direct Numerical Simulation of Mixing and Chemical Reactions

in a Round Jet into a Crossflow – a Benchmark

<i>J.A. Denev, J. Fröhlich, and H. Bockhorn</i>	237
---	-----

Numerical Simulation of the Bursting

<i>O. Marxen and D. Henningson</i>	253
--	-----

Parallel Large Eddy Simulation with UG <i>A. Hauser and G. Wittum</i>	269
LES and DNS of Melt Flow and Heat Transfer in Czochralski Crystal Growth <i>A. Raufeisen, M. Breuer, V. Kumar, T. Botsch, and F. Durst</i>	279
Efficient Implementation of Nonlinear Deconvolution Methods for Implicit Large-Eddy Simulation <i>S. Hickel and N.A. Adams</i>	293
Large-Eddy Simulation of Tundish Flow <i>N. Alkishriwi, M. Meinke, and W. Schröder</i>	307
Large Eddy Simulation of Open-Channel Flow Over Spheres <i>T. Stoesser and W. Rodi</i>	321
Prediction of the Resonance Characteristics of Combustion Chambers on the Basis of Large-Eddy Simulation <i>F. Magagnato, B. Pritz, H. Büchner, and M. Gabi</i>	331
Investigations of Flow and Species Transport in Packed Beds by Lattice Boltzmann Simulations <i>T. Zeiser</i>	343
Rheological Properties of Binary and Ternary Amphiphilic Fluid Mixtures <i>J. Harting and G. Giupponi</i>	355
The Effects of Vortex Generator Arrays on Heat Transfer and Flow Field <i>C.F. Dietz, M. Henze, S.O. Neumann, J. von Wolfersdorf, and B. Weigand</i>	365
Investigation of the Influence of the Inlet Geometry on the Flow in a Swirl Burner <i>M. García-Villalba, J. Fröhlich, and W. Rodi</i>	381
Numerical Investigation and Simulation of Transition Effects in Hypersonic Intake Flows <i>M. Krause, B. Reinartz, and J. Ballmann</i>	391
Aeroelastic Simulations of Isolated Rotors Using Weak Fluid-Structure Coupling <i>M. Dietz, M. Kessler, and E. Krämer</i>	407
Computational Study of the Aeroelastic Equilibrium Configuration of a Swept Wind Tunnel Wing Model in Subsonic Flow <i>L. Reimer, C. Braun, and J. Ballmann</i>	421

Structural Mechanics

P. Wriggers 435

Numerical Prediction of the Residual Stress State after Shot Peening

M. Klemenž, M. Zimmermann, V. Schulze, and D. Löhe 437

Computer-Aided Destruction of Complex Structures by Blasting

S. Mattern, G. Blankenhorn, and K. Schweizerhof 449

Wave Propagation in Automotive Structures Induced by Impact Events

S. Mattern and K. Schweizerhof 459

Miscellaneous Topics

W. Schröder 471

Continental Growth and Thermal Convection in the Earth's Mantle

U. Walzer, R. Hendel, and J. Baumgardner 473

Efficient Satellite Based Geopotential Recovery

O. Baur, G. Austen, and W. Keller 499

Molecular Modeling of Hydrogen Bonding Fluids: Monomethylamine,
Dimethylamine, and Water Revised

T. Schnabel, J. Vrabec, and H. Hasse 515

The Application of a Black-Box Solver with Error Estimate
to Different Systems of PDEs

T. Adolph and W. Schönauer 527

Scalable Parallel Suffix Array Construction

F. Kulla and P. Sanders 543