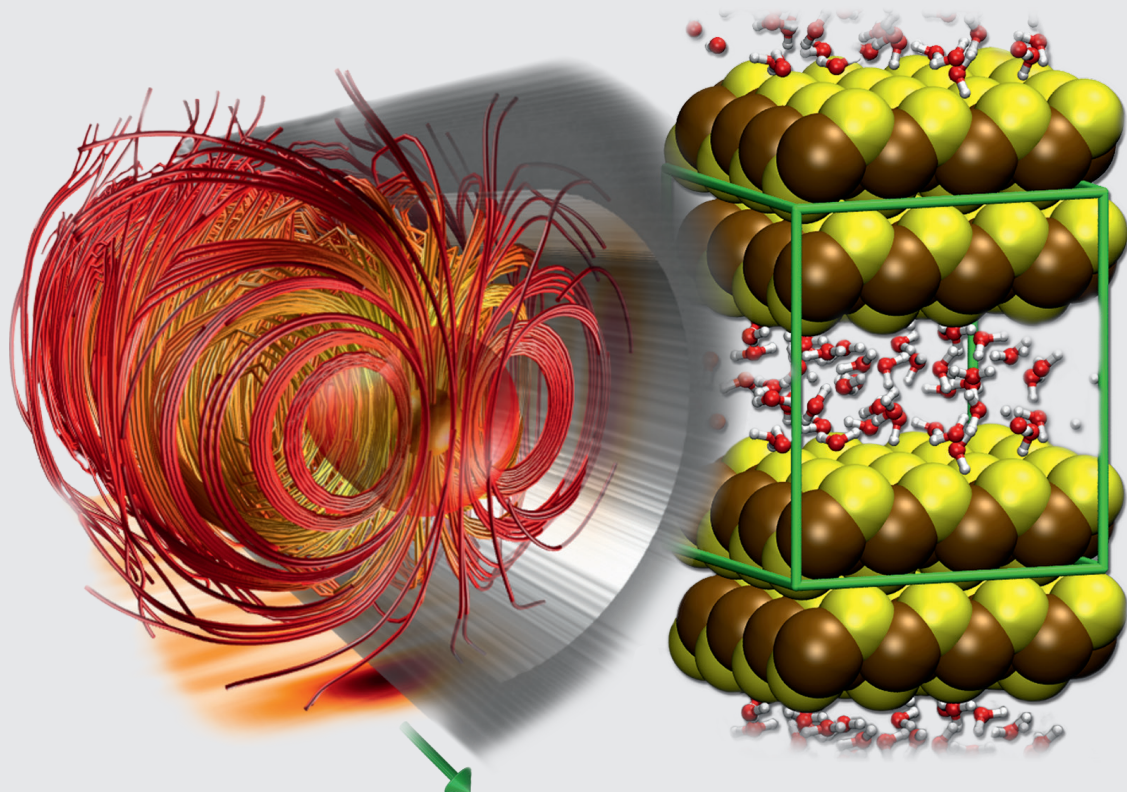


NIC Symposium 2016

11-12 February 2016 | Jülich, Germany

K. Binder, M. Müller, M. Kremer, A. Schnurpfeil (Editors)

Proceedings



Forschungszentrum Jülich GmbH
John von Neumann Institute for Computing (NIC)

NIC Symposium 2016

11-12 February 2016 | Jülich, Germany

K. Binder, M. Müller, M. Kremer, A. Schnurpfeil (Editors)

Proceedings

Publication Series of the John von Neumann Institute for Computing (NIC)

NIC Series

Volume 48

ISBN 978-3-95806-109-5

Contents

Scientific Big Data Analytics by HPC <i>T. Lippert, D. Mallmann, M. Riedel</i>	1
The NIC Research Groups	
Relativistic Quantum Molecular Dynamics Simulations of Multi-Strange Particle Production <i>M. Bleicher, J. Steinheimer, H. Petersen</i>	13
Contact Mechanics and Fluid Leakage Near Percolation <i>W. B. Dapp, M. H. Müser</i>	21
The QCD Phase Transition with Two Quark Flavours <i>C. Czaban, F. Cuteri, O. Philipsen, C. Pinke, A. Sciarra</i>	31
Dynamical Simulations of Lattice QCD <i>K. Jansen, S. Schaefer, H. Simma, R. Sommer</i>	39
Astrophysics	
Introduction <i>P. L. Biermann</i>	49
Formation of Star-Forming Clouds from the Magnetised, Diffuse Interstellar Medium <i>R. Banerjee, B. Körtgen</i>	51
The Formation of Planetesimals: Building Bricks for Planetary Systems <i>H. Klahr, A. Schreiber</i>	61
LOFAR: Calibration and Imaging on JURECA <i>M. Hoeft, A. Horneffer, A. Drabent, S. Fröhlich</i>	69
Turbulence and Its Effect on Protostellar Disk Formation <i>D. Seifried, R. Banerjee, R. S. Klessen</i>	77

Computational Biology and Biophysics

Introduction <i>W. Wenzel</i>	85
Structural Predictions of Intrinsically Disordered Proteins with Computational Methods <i>E. Abad, G. Rossetti</i>	89
Towards Restoring Catalytic Activity of Glutamine Synthetase With a Clinically Relevant Mutation <i>B. Frieg, D. Häussinger, H. Gohlke</i>	97
Using Molecular Dynamics to Model the Stacking Behaviour of Perylene Bisimide Derivatives in Aromatic Solvent <i>M. Hollfelder, S. Gekle</i>	105

Computational Chemistry

Introduction <i>C. Peter</i>	115
<i>Ab Initio</i> Molecular Dynamics Simulations of Ionic Liquids <i>M. Thomas, I. Sancho Sanz, O. Hollóczki, B. Kirchner</i>	117
Prebiotic Chemistry in Nanoconfinement <i>D. Muñoz-Santiburcio, D. Marx</i>	125
Simulation of Electron Transfer and Electron Transport in Molecular Systems at Surfaces <i>P. B. Coto, C. Hofmeister, V. Prucker, D. Weckbecker, M. Thoss</i>	133

Elementary Particle Physics

Introduction <i>G. Münster</i>	143
The Mass Difference Between Protons and Neutrons and the Fine Tuning of Physical Constants <i>Sz. Borsanyi, S. Dürr, Z. Fodor, C. Hölbling, S. D. Katz, S. Krieg, L. Lellouch, T. Lippert, A. Portelli, K. K. Szabó, B. C. Tóth</i>	145

The Pseudocritical Line in the QCD Phase Diagram	
<i>H.-T. Ding, P. Hegde, O. Kaczmarek, F. Karsch, E. Laermann, S. Mukherjee, P. Petreczky, H. Sandmeyer, C. Schmidt, P. Steinbrecher, W. Söldner</i>	153
Pushing the Boundaries of Nuclear Physics with Lattice Simulations	
<i>U.-G. Meißner, T. A. Lähde, T. Luu</i>	161
Hadron Structure from Lattice QCD	
<i>A. Schäfer</i>	169
The Strong Interaction at Neutron-Rich Extremes	
<i>A. Gezerlis, K. Hebeler, J. D. Holt, J. Menéndez, A. Schwenk, J. Simonis, I. Tews</i>	179

Materials Science

Introduction	
<i>R. O. Jones</i>	189
Nanostructured Metallic Glasses: Tailoring the Mechanical Properties of Amorphous Metals	
<i>T. Brink, O. Adjaoud, K. Albe</i>	191
Understanding Tribology and Machining Processes through Computationally Intensive Large Scale MD	
<i>P. A. Romero, M. Moseler</i>	199
Memory Effect in Crystallisation of Amorphous Ge₂Sb₂Te₅	
<i>R. O. Jones, J. Kalikka, J. Akola</i>	209
Anisotropic Magneto-Thermopower in $M/Co/M$ ($M = \text{Cu, Pd, Pt}$) Trilayer Systems	
<i>V. Popescu, P. Kratzer</i>	217

Condensed Matter

Introduction	
<i>K. Binder</i>	227
Structures and Phases in (Nano-)Systems in Confined Geometry	
<i>M. Beck, A. Haller, D. Kawatzki, M. Matt, M. Pütz, M. Ring, R. Schmid, K. Scholz, U. Siems, P. Nielaba</i>	229

Quantum Monte Carlo Simulations of Strongly Correlated Electron Systems: The Dimensional Crossover	
<i>M. Raczkowski, M. Bercx, M. Weber, S. Beyl, J. Hofmann, F. Parisen Toldin, M. Hohenadler, F. F. Assaad</i>	241

Optical Spectra of Carbon-Based Nanostructures	
<i>M. Rohlfing</i>	249

Computational Soft Matter Science

Introduction	
<i>K. Kremer</i>	259

Hierarchical Modelling of High-Molecular Weight Polymer Melts: From Soft Blobs to Microscopic Description	
<i>G. Zhang, T. Stuehn, K. Ch. Daoulas, K. Kremer</i>	261

Process-Directed Self-Assembly of Copolymer Materials	
<i>M. Müller</i>	271

Calculation of the Work of Adhesion of Solid-Liquid Interfaces by Molecular Dynamics Simulations	
<i>F. Leroy, F. Müller-Plathe</i>	279

Earth and Environment

Introduction	
<i>U. Hansen</i>	289

Very High Resolution Simulations of African Climate with the Regional Climate Model REMO	
<i>A. Hänsler, N. Koldunov, D. Sein, W. Sauf, D. Jacob</i>	291

Forward and Inverse Modelling of Lithospheric Deformation on Geological Timescales	
<i>B. J. P. Kaus, A. A. Popov, T. S. Baumann, A. E. Püsök, A. Bauville, N. Fernandez, M. Collignon</i>	299

Computational Aspects of High-Resolution Global Gravity Field Determination – Numbering Schemes and Reordering	
<i>J. M. Brockmann, W.-D. Schuh</i>	309

Towards a Better Understanding of Rotating Turbulent Convection in Geo- and Astrophysical Systems	
<i>S. Stellmach, J. Verhoeven, M. Lischper, U. Hansen</i>	319

Computer Science and Numerical Mathematics

Introduction	
<i>D. Kröner</i>	331
Massively Parallel Large Scale Stokes Flow Simulation	
<i>B. Gmeiner, M. Huber, L. John, U. Rüde, C. Waluga, B. Wohlmuth</i>	333
Analysing the Scalability of Climate Codes Using New Features of Scalasca	
<i>M. Harlacher, A. Calotoiu, J. Dennis, F. Wolf</i>	343

Fluid Mechanics

Introduction	
<i>N. A. Adams</i>	353
Numerical Analysis of the FDA Centrifugal Blood Pump	
<i>V. Marinova, I. Kerroumi, A. Lintermann, J. H. Göbbert, C. Moulinec, S. Rible, Y. Fournier, M. Behbahani</i>	355
Direct Numerical Simulations of Impeller Driven Turbulence and Dynamo Action	
<i>S. Kreuzahler, R. Grauer, H. Homann, Y. Ponty</i>	365
Highly-Resolved Numerical Simulation of the Turbulent Combustion Process in Experimental Burners	
<i>F. Proch, M. Rieth, A. Rittler, A. Kempf</i>	373
Supercomputing Studies in Turbulent Rayleigh-Bénard Convection: Challenges and Perspectives	
<i>M. S. Emran, P. Götzfried, A. Kolchinskaya, J. D. Scheel, J. Schumacher</i>	381
On the Parametrisation of Lattice Boltzmann Method in Pore-Scale Flow Simulations	
<i>S. Khirevich, U. Tallarek</i>	389

Computational Plasma Physics

Introduction

K.-H. Spatschek

399

Towards Plasma-Driven Free-Electron Lasers

*I. Dornmair, L. T. Campbell, J. T. Henderson, S. Jalas, O. Karger, M. Kirchen,
A. Knetsch, G. G. Manhan, G. Wittig, B. Hidding, B. W. J. McNeil, A. R. Maier*

401

Collisionless Shocks and Mediating Instabilities

A. Stockem Novo, P. Alves, K. Schoeffler, L. O. Silva, R. Schlickeiser

409

The John von Neumann Institute for Computing (NIC) was established in 1998 by Forschungszentrum Jülich and Deutsches Elektronen-Synchrotron DESY to support the supercomputer-oriented simulation sciences. In 2006, GSI Helmholtzzentrum für Schwerionenforschung joined NIC as a contract partner.

The core task of NIC is the peer-reviewed allocation of supercomputing resources to computational science projects in Germany and Europe. The NIC partners also support supercomputer-aided research in science and engineering through a three-way strategy:

- Provision of supercomputing resources for projects in science, research, and industry.
- Supercomputer-oriented research and development by research groups in selected fields of physics and natural sciences.
- Education and training in all areas of supercomputing by symposia, workshops, summer schools, seminars, courses, and guest programmes for scientists and students.

The NIC Symposium is held biennially to give an overview on activities and results obtained by the NIC projects in the last two years. The contributions for this 8th NIC Symposium are from projects that have been supported by the supercomputers JUROPA, JURECA, and JUQUEEN in Jülich. They cover selected topics in the fields of Astrophysics, Biology and Biophysics, Chemistry, Elementary Particle Physics, Materials Science, Condensed Matter, Soft Matter Science, Earth and Environment, Computer Science and Numerical Mathematics, Fluid Mechanics, and Plasma Physics.



Deutsches
Elektronen-Synchrotron

