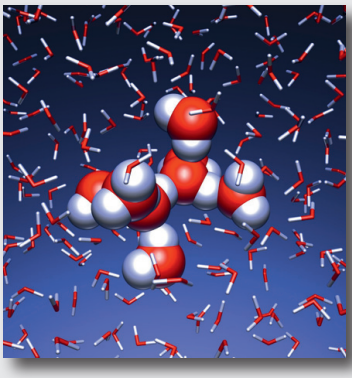

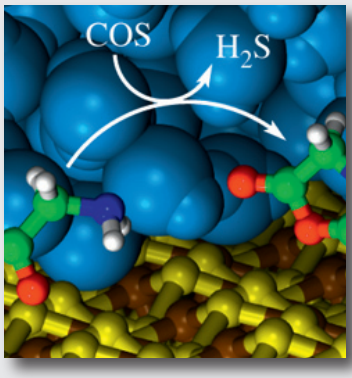

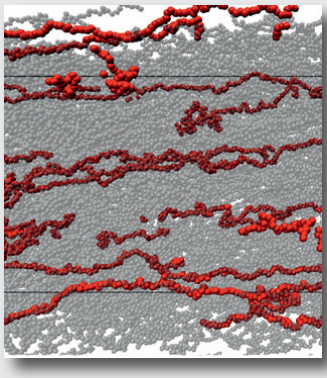

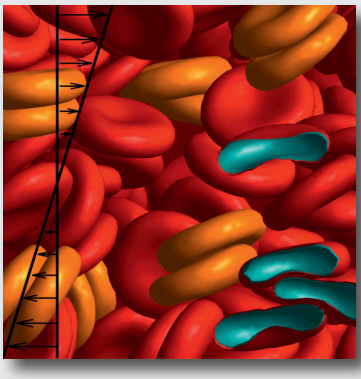

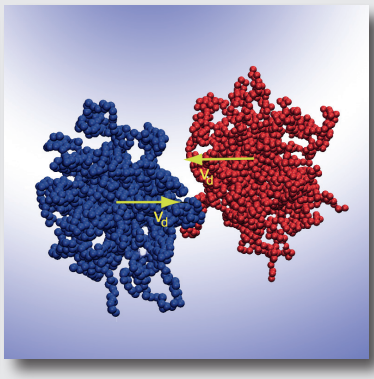

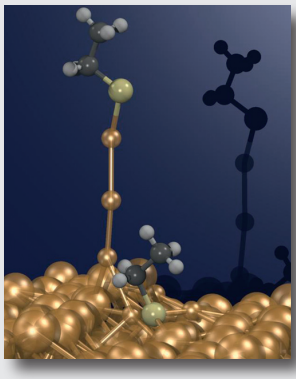

Hierarchical Methods for Dynamics in Complex Molecular Systems Lecture Notes

edited by Johannes Grotendorst, Godehard Sutmann, Gerhard Gompper, Dominik Marx

JÜLICH
FORSCHUNGSZENTRUM

Mitglied der Helmholtz-Gemeinschaft

Forschungszentrum Jülich GmbH
Institute for Advanced Simulation (IAS)
Jülich Supercomputing Centre (JSC)

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IAS Winter School, 5 – 9 March 2012
Forschungszentrum Jülich GmbH
Lecture Notes

Schriften des Forschungszentrums Jülich
IAS Series Volume 10

ISSN 1868-8489 ISBN 978-3-89336-768-9

Contents

Hard and Soft Materials

Simulating Light-Induced Phenomena in Soft Matter
Nikos L. Doltsinis **1**

1 Introduction 1
2 Theoretical Background 4
3 Results and Discussion 22
4 Summary and Outlook 37

Transition Path Sampling of Phase Transitions – Nucleation and Growth in Materials Hard and Soft
Michael Grünwald, Swetlana Jungblut, Christoph Dellago **47**

1 Introduction 47
2 Fundamentals of Transition Path Sampling 50
3 Kinetics 57
4 Identifying the Transition Mechanism 62
5 Applications 66
6 Conclusion and Outlook 75

Neural Network Potentials for Efficient Large-Scale Molecular Dynamics
Jörg Behler **81**

1 Introduction 81
2 Neural Networks 83
3 High-Dimensional Neural Network Potentials 93
4 Discussion 96
5 Conclusions 100

Large-Scale Molecular Dynamics Studies and Scale-Bridging Models for Deformation and Failure of Materials
Alexander Hartmaier **107**

1 Introduction 107
2 Large-Scale Molecular Dynamics Simulations 108
3 Scale-Bridging Models 110
4 Concluding Remarks 112

Biomolecular Systems

Exploration of Multi-Dimensional Free Energy Landscapes in Molecular Dynamics
Mark E. Tuckerman **115**
1 Introduction 115
2 Adiabatic Free Energy Molecular Dynamics and Temperature-Accelerated Molecular Dynamics 117
3 Long Time-Step Molecular Dynamics 126

Methods on TDDFT-Based Nonadiabatic Dynamics with Applications
Ivano Tavernelli **139**
1 Introduction 139
2 Mixed Quantum-Classical Nonadiabatic Molecular Dynamics: A TDDFT-Based Prospective 140
3 TDDFT Quantities for Nonadiabatic Dynamics 152

Hybrid Car-Parrinello Molecular Dynamics / Molecular Mechanics Simulations: A Powerful Tool for the Investigation of Biological Systems
Emiliano Ippoliti, Jens Dreyer, Paolo Carloni, Ursula Röthlisberger **163**
1 Introduction 163
2 Methods 164
3 Applications to Biological Systems 173
4 Concluding Remarks 175

Simulation Techniques for Studying the Impact of Force on (Bio)chemical Processes
Frauke Graeter, Wenjin Li **183**
1 Introduction: How Force Affects Chemical Bonds 183
2 Methods 184
3 Application: Disulphide Bond Reduction 189
4 Outlook 192

Coarse Grained Models for Multiscale Simulations of Biomolecular Systems
Christine Peter **195**
1 Introduction 195
2 Deriving CG Interaction Potentials 196
3 Systematic Coarse Graining: Challenges 207

Particle-Based Dynamics Simulations of Multi-Protein Systems and Cellular Compartments
Volkhard Helms, Po-Hsien Lee, Tihamér Geyer **219**
1 Introduction 219
2 Coarse-Grained Simulations of Proteins 220
3 Applications 224
4 Summary and Outlook 231

Advanced Methods

Algorithmic Rethinking and Code Reengineering for Truly Massively Parallel *ab initio* Molecular Dynamics Simulations
Costas Bekas, Alessandro Curioni **235**

1 Introduction 235
2 Task Groups Strategy for 3D Parallel FFTs 236
3 Large Scale Wavefunction Orthogonalization 241
4 Initialization from Atomic Orbitals 259
5 Discussion 267

Non-Equilibrium Molecular Dynamics for Biomolecular Systems Using Fluctuation Theorems
Gerhard Hummer **269**

1 Introduction 269
2 Equilibrium Thermodynamics from Non-Equilibrium Simulations and Experiments 270
3 Concluding Remarks 276

Multigrid QM/MM Approaches in *ab initio* Molecular Dynamics
Teodoro Laino **279**

1 Introduction 279
2 Renormalization of the QM/MM Hamiltonian 281
3 Wave-Function Optimization 286
4 QM/MM Coupling for Isolated Systems 290
5 Extension to Periodic Boundary Conditions 293
6 Tests and Applications 300
7 QM/MM Study on Silica: Motivation 303
8 Conclusion 312

Accelerated Molecular Dynamics Methods
Danny Perez, Blas. P. Uberuaga, Arthur F. Voter **329**

1 Background 330
2 Parallel-Replica Dynamics 334
3 Hyperdynamics 336
4 Temperature Accelerated Dynamics 338
5 Choosing the Right AMD Method 342
6 Conclusion 343

Tracking the Dynamics of Systems Evolving through Infrequent Transitions in a Network of Discrete States
Doros N. Theodorou **347**
1 Introduction 347
2 Identifying States 349
3 Calculating Rate Constants 351
4 Kinetic Monte Carlo Simulation 361
5 Analytical Solution of the Master Equation 362
6 Example: Diffusion of Xenon in Silicalite 365
7 Example: Diffusion of CO_2 in Poly(amide imide) 371
8 Dynamic Integration of a Markovian Web and its Application to Structural Relaxation in Glasses 376
9 Lumping 382
10 Summary 384

Adaptive Resolution Molecular Dynamics: Extension to Quantum Problems
Luigi Delle Site **391**
1 Introduction 391
2 The AdResS Method 392
3 Quantum-Classical Adaptive Resolution: The Conceptual Problem 394
4 Path Integral Molecular Dynamics 395
5 Quantum-Classical Adaptive Resolution Simulation via PIMD 398
6 Conclusions and Perspectives 400

Flow Simulation and Transport

Coupling Molecular Dynamics and Lattice Boltzmann to Simulate Brownian Motion with Hydrodynamic Interactions
Burkhard Dünweg **403**
1 Introduction 403
2 Coupling Scheme 405
3 Low Mach Number Physics 407
4 Lattice Boltzmann 1: Statistical Mechanics 407
5 Lattice Boltzmann 2: Stochastic Collisions 410
6 Lattice Boltzmann 3: Chapman–Enskog Expansion 410
7 A Polymer Chain in Solvent 412

Flow Simulations with Multiparticle Collision Dynamics
Roland G. Winkler **417**
1 Introduction 417
2 Multiparticle Collision Dynamics 418
3 Embedded Objects and Boundary Conditions 420
4 Cell-Level Canonical Thermostat 421
5 Transport Coefficients 423
6 MPC without Hydrodynamics 431
7 External Fields 431
8 Hydrodynamic Simulations of Polymers in Flow Fields 436
9 Conclusions 440

Dissipative Particle Dynamics
Pep Español **445**
1 Introduction 445
2 The Meaning of a Dissipative Particle 446
3 DPD for Unbounded Atoms: The Simulation of Simple Fluids 447
4 Two Technical Points: Integrators and Boundary Conditions 456
5 Microscopic Foundation of DPD 457
6 Conclusion 462

Large-Scale Simulations of Blood Flows with Coarse-Grained Cells
Simone Melchionna **469**
1 Introduction 469
2 Solvent Representation 470
3 Diffused Particle Model (DPM) 472
4 Solid Particle Model (SPM) 480
5 Excluded Volume Interactions 484
6 Conclusions 486

Simulations of Blood Flow on the Cell Scale
Dmitry A. Fedosov **489**
1 Introduction 489
2 Red Blood Cells 490
3 Methods and Models 491
4 Simulation Results and Discussion 499
5 Summary 506

Parallel Computing and Numerical Methods

Introduction to Parallel Computing
Bernd Mohr **511**
1 Introduction 511
2 Programming Models 514
3 MPI 516
4 OpenMP 519
5 Parallel Debugging 520
6 Parallel Performance Analysis 520
7 Summary 522

Scalability of $\mu\varphi$ and the Parallel Algebraic Multigrid Solver of DUNE-ISTL
Olaf Ippisch, Markus Blatt **527**
1 Introduction 527
2 Algebraic Multigrid as Parallel Linear Solver 527
3 Test Cases 528
4 Results 529

Highly Parallel Geometric Multigrid Algorithm for Hierarchical Hybrid Grids
Björn Gmeiner, Tobias Gradl, Harald Köstler, Ulrich Rüde **533**
1 Introduction 533
2 Grid Partitioning and the Coarsest Grids 535
3 Scaling on JUGENE 536
4 Conclusions and Future Work 539

The focus of this Winter School was on hierarchical methods for dynamical problems having primarily in mind systems described in terms of many atoms or molecules. One end of relevant time scales certainly is nonadiabatic quantum dynamics methods, which operate on the subfemtosecond time scale but influence dynamical events that are orders of magnitude slower. Examples for such phenomena might be photoinduced switching of individual molecules, which results into large-amplitude relaxation in liquids or photodriven phase transitions of liquid crystals. On the other end of the relevant time scales methods are important to investigate and understand the non-equilibrium dynamics of complex fluids, with typical time scales in the range from microseconds to seconds. Examples are the flow of polymer solutions, or the flow of blood through microvessels.

The Lecture Notes contain state-of-the-art information on methodological foundations and methods coming from materials science, soft matter, life science and fluid dynamics. In addition to introducing discipline-specific methods, modern numerical algorithms and parallel programming techniques are presented in detail.

This publication was edited at the Jülich Supercomputing Centre (JSC) which is an integral part of the Institute for Advanced Simulation (IAS). The IAS combines the Jülich simulation sciences and the supercomputer facility in one organizational unit. It includes those parts of the scientific institutes at Forschungszentrum Jülich which use simulation on supercomputers as their main research methodology.

IAS Series
Volume 10
ISBN 978-3-89336-768-9

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