

Table of Contents

Introductory Survey

Molecular Dynamics Simulations: The Limits and Beyond	3
<i>Herman J.C. Berendsen</i>	

I Conformational Dynamics

Steered Molecular Dynamics	39
<i>Sergei Izrailev, Sergey Stepaniants, Barry Isralewitz, Dorina Kosztin, Hui Lu, Ferenc Molnar, Willy Wriggers, Klaus Schulten</i>	
Conformational Transitions of Proteins from Atomistic Simulations	66
<i>Volkhard Helms, J. Andrew McCammon</i>	
Conformational Dynamics Simulations of Proteins	78
<i>Markus Eichinger, Berthold Heymann, Helmut Heller, Helmut Grubmüller, Paul Tavan</i>	
Computation of Essential Molecular Dynamics by Subdivision Techniques	98
<i>Peter Deufloth, Michael Dellnitz, Oliver Junge, Christof Schütte</i>	
Mathematical Model of the Nucleic Acids Conformational Transitions with Hysteresis over Hydration–Dehydration Cycle	116
<i>Michael Ye. Tolstorukov, Konstantin M. Virnik</i>	

II Thermodynamic Modelling

Simulation Studies of Protein-Ligand Interactions	129
<i>Jan Hermans, Geoffrey Mann, Lu Wang, Li Zhang</i>	
Estimating Relative Free Energies from a Single Simulation of the Initial State	149
<i>Alan E. Mark, Heiko Schäfer, Haiyan Liu, Wilfred van Gunsteren</i>	
Exploration of Peptide Free Energy Surfaces	163
<i>Krzysztof Kuczcera</i>	
Prediction of pK_a s of Titratable Residues in Proteins Using a Poisson-Boltzmann Model of the Solute-Solvent System	176

*Jan Antosiewicz, Elżbieta Błachut-Okraśńska, Tomasz Gryczuk,
James M. Briggs, Stanisław T. Włodek, Bogdan Lesyng, J. Andrew
McCammon*

Exploiting Tsallis Statistics	197
<i>John E. Straub, Ioan Andricioaei</i>	

New Techniques for the Construction of Residue Potentials for Protein Folding	212
<i>Arnold Neumaier, Stefan Dallwig, Waltraud Huyer, Hermann Schichl</i>	

III Enhanced Time-Stepping Algorithms

Some Failures and Successes of Long-Timestep Approaches to Biomolecular Simulations	227
<i>Tamar Schlick</i>	

Application of a Stochastic Path Integral Approach to the Computa- tions of an Optimal Path and Ensembles of Trajectories	263
<i>Ron Elber, Benoit Roux, Roberto Olender</i>	

On Some Difficulties in Integrating Highly Oscillatory Hamiltonian Sys- tems	281
<i>Uri M. Ascher, Sebastian Reich</i>	

Molecular Dynamics in Systems with Multiple Time Scales: Reference System Propagator Algorithms	297
<i>Bruce J. Berne</i>	

The Five Femtosecond Time Step Barrier	318
<i>Robert D. Skeel, Jesús A. Izaguirre</i>	

Long Time Step MD Simulations Using Split Integration Symplectic Method	332
<i>Dušanika Janežič, Franci Merzel</i>	

Comparison of Geometric Integrators for Rigid Body Simulation	349
<i>Benedict J. Leimkuhler</i>	

IV Quantum-Classical Simulations

New Methods in Quantum Molecular Dynamics of Large Polyatomic Systems	365
<i>Pavel Jungwirth, R. Benny Gerber</i>	

Approximation Properties and Limits of the Quantum-Classical Molecular Dynamics Model	380
<i>Christof Schütte, Folkmar A. Bornemann</i>	
Numerical Integrators for Quantum-Classical Molecular Dynamics	396
<i>Peter Nettesheim, Christof Schütte</i>	
Symplectic Multiple-Time-Stepping Integrators for Quantum-Classical Molecular Dynamics	412
<i>Peter Nettesheim, Sebastian Reich</i>	
A Bunch of Time Integrators for Quantum/Classical Molecular Dynamics	421
<i>Marlis Hochbruck, Christian Lubich</i>	
Applications of Ab-Initio Molecular Dynamics Simulations in Chemistry and Polymer Science	433
<i>Robert J. Meier</i>	
Polarons of Molecular Crystal Model by Nonlocal Dynamical Coherent Potential Method	442
<i>Sergiy V. Izvekov</i>	

V Parallel Force Field Evaluation

Ewald and Multipole Methods for Periodic N -Body Problems	459
<i>John A. Board, Jr., Christopher W. Humphres, Christophe G. Lambert, William T. Rankin, Abdunour Y. Toukmaji</i>	
Avoiding Algorithmic Obfuscation in a Message-Driven Parallel MD Code	472
<i>James C. Phillips, Robert Brunner, Aritomo Shinozaki, Milind Bhandarkar, Neal Krawetz, Attila Gursoy, Laxmikant Kalé, Robert D. Skeel, Klaus Schulten</i>	
Parallel Molecular Dynamics Using Force Decomposition	483
<i>Daniel Okunbor, Ravi Murty</i>	