

Michael Griebel
Stephan Knapek
Gerhard Zumbusch

Numerical Simulation in Molecular Dynamics

Numerics, Algorithms,
Parallelization, Applications

With 180 Figures, 43 in Color, and 63 Tables

Table of Contents

1	Computer Simulation – a Key Technology	1
2	From the Schrödinger Equation to Molecular Dynamics	17
2.1	The Schrödinger Equation	17
2.2	A Derivation of Classical Molecular Dynamics	21
2.2.1	TDSCF Approach and Ehrenfest Molecular Dynamics	21
2.2.2	Expansion in the Adiabatic Basis	24
2.2.3	Restriction to the Ground State	26
2.2.4	Approximation of the Potential Energy Hypersurface	26
2.3	An Outlook on Methods of Ab Initio Molecular Dynamics	30
3	The Linked Cell Method for Short-Range Potentials	37
3.1	Time Discretization – the Störmer-Verlet Method	40
3.2	Implementation of the Basic Algorithm	46
3.3	The Cutoff Radius	53
3.4	The Linked Cell Method	56
3.5	Implementation of the Linked Cell Method	58
3.6	First Application Examples and Extensions	64
3.6.1	Collision of Two Bodies I	66
3.6.2	Collision of Two Bodies II	68
3.6.3	Density Gradient	72
3.6.4	Rayleigh-Taylor Instability	73
3.6.5	Rayleigh-Bénard Convection	79
3.6.6	Surface Waves in Granular Materials	82
3.7	Thermostats, Ensembles, and Applications	86
3.7.1	Thermostats and Equilibration	87
3.7.2	Statistical Mechanics and Thermodynamic Quantities	93
3.7.3	Phase Transition of Argon in the NVT Ensemble	96
3.7.4	The Parrinello-Rahman Method	104
3.7.5	Phase Transition of Argon in the NPT Ensemble	107
4	Parallelization	113
4.1	Parallel Computers and Parallelization Strategies	113
4.2	Domain Decomposition for the Linked Cell Method	122
4.3	Implementation	128

4.4	Performance Measurements and Benchmarks	139
4.5	Application Examples	146
4.5.1	Collision of Two Bodies	146
4.5.2	Rayleigh-Taylor Instability	148
5	Extensions to More Complex Potentials and Molecules . .	151
5.1	Many-Body Potentials	151
5.1.1	Cracks in Metals – Finnis-Sinclair Potential	152
5.1.2	Phase Transition in Metals – EAM Potential	160
5.1.3	Fullerenes and Nanotubes – Brenner Potential	167
5.2	Potentials with Fixed Bond Structures	181
5.2.1	Membranes and Minimal Surfaces	181
5.2.2	Systems of Linear Molecules	186
5.2.3	Outlook to More Complex Molecules	202
6	Time Integration Methods	211
6.1	Errors of the Time Integration	212
6.2	Symplectic Methods	221
6.3	Multiple Time Step Methods – the Impulse Method	226
6.4	Constraints – the RATTLE Algorithm	230
7	Mesh-Based Methods for Long-Range Potentials	239
7.1	Solution of the Potential Equation	243
7.1.1	Boundary Conditions	243
7.1.2	Potential Equation and Potential Decomposition	244
7.1.3	Decomposition of the Potential Energy and of the Forces	248
7.2	Short-Range and Long-Range Energy and Force Terms	250
7.2.1	Short-Range Terms – Linked Cell Method	250
7.2.2	Long-Range Terms – Fast Poisson Solvers	252
7.2.3	Some Variants	258
7.3	Smooth Particle-Mesh Ewald Method (SPME)	260
7.3.1	Short-Range Terms	261
7.3.2	Long-Range Terms	263
7.3.3	Implementation of the SPME method	273
7.4	Application Examples and Extensions	281
7.4.1	Rayleigh-Taylor Instability with Coulomb Potential	281
7.4.2	Phase Transition in Ionic Microcrystals	284
7.4.3	Water as a Molecular System	287
7.5	Parallelization	294
7.5.1	Parallelization of the SPME Method	294
7.5.2	Implementation	299
7.5.3	Performance Measurements and Benchmarks	302
7.6	Example Application: Structure of the Universe	306

8	Tree Algorithms for Long-Range Potentials	313
8.1	Series Expansion of the Potential	314
8.2	Tree Structures for the Decomposition of the Far Field	320
8.3	Particle-Cluster Interactions and the Barnes-Hut Method	325
8.3.1	Method	326
8.3.2	Implementation	328
8.3.3	Applications from Astrophysics	339
8.4	Parallel Tree Methods	341
8.4.1	An Implementation with Keys	343
8.4.2	Dynamical Load Balancing	357
8.4.3	Data Distribution with Space-Filling Curves	359
8.4.4	Applications	366
8.5	Methods of Higher Order	370
8.5.1	Implementation	371
8.5.2	Parallelization	376
8.6	Cluster-Cluster Interactions and the Fast Multipole Method	377
8.6.1	Method	377
8.6.2	Implementation	382
8.6.3	Error Estimate	385
8.6.4	Parallelization	386
8.7	Comparisons and Outlook	387
9	Applications from Biochemistry and Biophysics	391
9.1	Bovine Pancreatic Trypsin Inhibitor	392
9.2	Membranes	394
9.3	Peptides and Proteins	398
9.4	Protein-Ligand Complex and Bonding	408
10	Prospects	413
A	Appendix	417
A.1	Newton's, Hamilton's, and Euler-Lagrange's Equations	417
A.2	Suggestions for Coding and Visualization	418
A.3	Parallelization by MPI	421
A.4	Maxwell-Boltzmann Distribution	425
A.5	Parameters	428
	References	431
	Index	467