

Contents

Introduction	1
Applications of Dissipative Particle Dynamics	
<i>Robert D. Groot</i>	5
1 Why Mesoscopic Simulation?	5
2 Introduction to DPD	6
2.1 Forces	7
2.2 Simulation Techniques	9
2.3 Parameterisation	10
2.4 Generalisations and Alternatives	12
3 Block Copolymer Mesophase Separation	14
3.1 Polymers in Melt	14
3.2 Expected and Simulated Phase Diagram	16
3.3 Evolution Pathways	20
3.4 Importance of Hydrodynamics	21
4 Polymers and Membranes Interacting with Surfactant Solutions	25
4.1 Polymers and Surfactants in Solution	25
4.2 Biomembrane Morphology	30
4.3 Biomembrane Deformation and Rupture	34
5 Conclusions	36
Simulating the Dynamics of Mesoscopic Systems	
<i>Christopher P. Lowe and Menno W. Dreischor</i>	39
1 Introduction	39
1.1 Renormalizing Static Properties	40
1.2 Time-Scales	41
2 Absolutely Minimal Mesoscopic Dynamics	43
2.1 Modelling the Solvent with an Andersen Thermostat	44
2.2 Langevin Dynamics of a Gaussian Chain	45
2.3 Brownian Dynamics	47
2.4 The Dynamics of a Colloidal Suspension	47
2.5 What Does Minimal Dynamics Teach Us	52
3 More Realistic Solvent Dynamics – Hydrodynamics	52
3.1 The Importance of Hydrodynamics	52
3.2 Putting Back the Hydrodynamics	54

3.3	Dissipative Particle Dynamics and the Lowe–Andersen Thermostat	55
3.4	Parametrically Correct Solvent Modelling	57
3.5	Concluding Remarks	58
4	An Example Problem – A Long Polymer Chain in an External Potential	59
4.1	Renormalizing the Static Properties of the Ideal Chain	59
4.2	Long Polymer Dynamics from Short Model Polymers	61
4.3	Results for the Test Problem	64
4.4	What Do We Learn from This Example	66
5	General Conclusions	66

Statistical Mechanics of Coarse-Graining

<i>Pep Español</i>	69
1 Introduction	69
2 The Theory of Coarse-Graining in a Nutshell	70
3 Example: A Colloidal Suspension	72
3.1 Microscopic Level: Classical Mechanics	72
3.2 Mesoscopic Level 1: Hydrodynamics	74
3.3 Mesoscopic Level 2: Fokker–Planck	76
3.4 Mesoscopic Level 3: Smoluchowski	77
3.5 Mesoscopic Level 4: Fick	78
3.6 Macroscopic Level: Thermodynamics	78
4 The Mathematics of the Theory of Coarse-Graining	79
4.1 The Microscopic Level	80
4.2 Liouville Theorem	80
4.3 Equilibrium at the Microscopic Level	81
4.4 The Mesoscopic Level	82
4.5 Exact Equation for $P(x, t)$	84
4.6 The Fokker–Planck Equation	86
5 Example: Smoluchowski Level	88
6 How to Compute the Objects in the FPE from a MD Simulation?	89
7 GENERIC Structure of the Fokker–Planck Equation	92
7.1 Properties of \mathbf{L} and \mathbf{M}	94
7.2 GENERIC Stochastic Differential Equation	96
7.3 The Size of the Fluctuations and the Deterministic Equations	97
8 Fluid Particle Models for Simulating Complex Fluids	99
8.1 Soft Fluid Particles	102
8.2 Complex Fluids	111
9 Summary	112

Mesoscopic Multi-particle Collision Model for Fluid Flow and Molecular Dynamics

<i>Anatoly Malevanets, Raymond Kapral</i>		116
1	Introduction	116
2	Multi-particle Collision Model for Fluid Flow	117
2.1	Evolution Equation	120
2.2	H-Theorem	121

3	Hydrodynamic Equations and Transport Properties	126
3.1	Evolution Equations for Mean Dynamical Variables	126
3.2	Kinetic Equations for Conserved Variables	128
3.3	General Form of the Kinetic Equation	132
3.4	Hydrodynamic Equations	133
4	Simulations of Fluid Flow	135
5	Mesoscopic Model for Solute Molecular Dynamics	136
6	Simulations of Hybrid Dynamics	138
6.1	Brownian Motion	138
6.2	Cluster Dynamics	142
6.3	Polymer Dynamics	144
6.4	Complex Fluids	146
7	Conclusion and Perspectives	147

Molecular Dynamics of Complex Systems: Non-Hamiltonian, Constrained, Quantum-Classical

	<i>Giovanni Ciccotti and Galina Kalibaeva</i>	150
1	Introduction	150
2	Non-Hamiltonian Molecular Dynamics	150
2.1	Nosé–Hoover “Demonstration”	150
2.2	Invariant Measure for Non-Hamiltonian Dynamical Systems	152
2.3	Liouville Equation and Its Stationary Solutions	154
2.4	The Correct Rules to Construct the Equilibrium Ensemble of Extended Variables Dynamical Systems	156
2.5	The True Statistics of the Nosé–Hoover Ensemble	157
2.6	New Atomic “iso”-stats (NVT, NPT)	159
2.7	Molecular NPT with Constraints	162
3	Implementations	167
3.1	Reversible Integrators	167
3.2	Constraints (SHAKE)	172
3.3	Concluding Remarks for Non-Hamiltonian Molecular Dynamics	177
4	Dynamics and (Some) Statistical Mechanics of Quantum-Classical Systems	177
4.1	Quantum-Classical Non-adiabatic Dynamics	177
4.2	Quantum-Classical Statistical Mechanics	184
4.3	Concluding Remarks for Quantum-Classical Systems	188

Hybrid Models: Bridging Particle and Continuum Scales in Hydrodynamic Flow Simulations

	<i>Eirik G. Flekkøy, Sean McNamara, Knut Jørgen Måløy, Jens Feder, Geri Wagner</i>	190
1	Introduction	190
2	A Hybrid Model for Diffusion	191
2.1	Simulations and Results	193
2.2	Transport Properties and Continuity of the Discrete-Continuous Interface	194
2.3	Equilibrium Fluctuations	196

X Contents

3	A Hybrid Model for the Navier–Stokes Equation	201
4	A Hybrid Model for the Coupling of Gas and Grains	205
4.1	Gas Dynamics	206
4.2	Particle Dynamics	208
4.3	Implementation	210
4.4	Sedimentation	211
4.5	Fluidized Beds	213
4.6	Experimental Verification	214
5	Conclusions	215

**On the Reduction of Molecular Degrees of Freedom
in Computer Simulations**

<i>Alexander P. Lyubartsev and Aatto Laaksonen</i>		219
1	Introduction	219
1.1	Atomistic Force Fields	220
1.2	Parameterization of Force Fields	224
2	Reduction of Molecular Degrees of Freedom	225
2.1	Eliminating Fast Fluctuations	226
2.2	Simplifying Molecular Models	227
2.3	Elimination of Explicit Solvent Molecules	227
3	Effective Potentials and the Inverse Monte Carlo Method	228
3.1	Inverse Problem in Statistical Mechanics	228
3.2	The Method	229
3.3	How to Implement the Method for More General Systems	231
4	Some Examples and Discussion	232
4.1	<i>Ab-Initio</i> Effective Potentials	232
4.2	Effective Solvent-Mediated Potentials	236
4.3	Effective Potentials for Macromolecules	241
5	Summary	242

Computer Simulations of the Electric Double Layer

<i>André G. Moreira and Roland R. Netz</i>		245
1	Introduction	245
2	Numerics of the Coulomb Interaction	246
2.1	Electrostatic Energy for Periodic Systems	248
2.2	Precision of the Lekner Summation	252
3	Counterions Close to a Single Charged Wall	253
3.1	Counterion Density Profile	257
3.2	Two-Dimensional Liquid and Crystal	259
3.3	Finite-Size Effects	262
3.4	Other Boundary Conditions	263
4	Charge-Modulated Substrate	265
5	Interacting Double Layers	270
6	Concluding Remarks	275

Lattice Boltzmann Modeling of Complex Fluids: Colloidal Suspensions and Fluid Mixtures

<i>Ignacio Pagonabarraga</i>	279
1 Introduction	279
2 Lattice Boltzmann: The Model	280
2.1 Elementary Variables	282
2.2 Time Evolution	282
2.3 The Equilibrium Distribution	283
2.4 Macroscopic Dynamics	284
3 Colloidal Suspensions	286
3.1 Modeling Solid Particles	286
3.2 Colloidal Hydrodynamics	289
3.3 Colloids at High Confinement	290
4 Non-ideal Fluids: A Binary Mixture	298
4.1 The Model	299
4.2 Spinodal Decomposition	301
5 Conclusions	306

Reverse Non-equilibrium Molecular Dynamics

<i>Florian Müller-Plathe, Patrice Bordat</i>	310
1 Introduction	310
2 Introduction: Transport Coefficients	310
3 Illustration of the RNEMD Method: Calculating Shear Viscosity	312
4 Modification of the RNEMD Method: Thermal Conductivity	317
5 Digression: Features of the RNEMD Method	319
6 The RNEMD and Higher-Order Transport Coefficients: The Ludwig–Soret Effect as an Example	320
7 Molecular Fluids and the RNEMD Method	321
8 A Bibliography of Applications of the RNEMD Method	323
8.1 Shear Flow, Viscosity	323
8.2 Thermal Conductivity	323
8.3 Thermal Diffusion, Soret Coefficient	324
9 Status and Future Potential of the RNEMD Method	324

Coarse-Graining in Polymer Simulations

<i>Séverine Girard and Florian Müller-Plathe</i>	327
1 Introduction	327
2 From Quantum Chemistry to Atomistic Simulation	329
2.1 The Bonded-Potential	330
2.2 The Non-bonded Potential	331
2.3 Force Field Optimisation	332
3 Coarse-Graining from Atomistic to Mesoscopic Models	335
3.1 The Super-Atoms	336
3.2 Definition and Optimisation of the Potential	339
4 Reverse Mapping	347
5 Relation to Other Coarse-Graining Procedures	349
5.1 Lattice Models	349

5.2	Coarse-Graining Further: From Super-Atoms to Blobs	354
6	Conclusions	354
Phase-Field Modeling of Dynamical Interface Phenomena in Fluids		
	<i>Tapio Ala-Nissila, Sami Majaniemi, Ken Elder</i>	357
1	Introduction to Coarse-Graining	357
2	Phase-Field Modeling	359
2.1	Construction of Free Energy	360
2.2	The Phase-Field	361
3	Sharp Interface Limit	364
3.1	Droplets	364
3.2	Dynamics of Gently Curved Fronts	366
3.3	Kinetic Roughening	368
3.4	Universality	370
4	Advantages of the Phase-Field Approach	371
5	Alphabet Soup of Models	372
6	Application: Kinetic Roughening in Imbibition	374
6.1	Background	374
6.2	Phase-Field Model of Imbibition	375
6.3	Evaporation and Gravity	379
6.4	Capillaries	381
7	Phase-Field Models and Hydrodynamics	382
8	Summary and Conclusions	384
	Index	389

Novel Methods in Soft Matter Simulations

Karttunen, M.; Vattulainen, I.; Lukkarinen, A. (Eds.)

2004, XIV, 393 p. 61 illus., Hardcover

ISBN: 978-3-540-20916-4