
Contents

Part I Fundamentals

1	Introduction	3
1.1	Physics on Different Length- and Timescales	4
1.1.1	Electronic/Atomistic Scale	5
1.1.2	Atomistic/Microscopic Scale	7
1.1.3	Microscopic/Mesoscopic Scale	8
1.1.4	Mesoscopic/Macroscopic Scale	9
1.2	What are Fluids and Solids?	9
1.3	The Objective of Experimental and Theoretical Physics	12
1.4	Computer Simulations – A Review	13
1.4.1	A Brief History of Computer Simulation	15
1.4.2	Computational Materials Science	23
1.5	Suggested Reading	25
2	Multiscale Computational Materials Science	27
2.1	Some Terminology	30
2.2	What is Computational Material Science on Multiscales?	31
2.2.1	Experimental Investigations on Different Length Scales	32
2.3	What is a Model?	35
2.3.1	The Scientific Method	36
2.4	Hierarchical Modeling Concepts above the Atomic Scale	44
2.4.1	Example: Principle Model Hierarchies in Classical Mechanics	45
2.4.2	Structure-Property Paradigm	47
2.4.3	Physical and Mathematical Modeling	47
2.4.4	Numerical Modeling and Simulation	55
2.5	Unification and Reductionism in Physical Theories	55
2.5.1	The Four Fundamental Interactions	58
2.5.2	The Standard Model	59
2.5.3	Symmetries, Fields, Particles and the Vacuum	61

2.5.4	Relativistic Wave Equations	69
2.5.5	Suggested Reading	77
2.6	Computer Science, Algorithms, Computability and Turing Machines	77
2.6.1	Recursion	80
2.6.2	Divide-and-Conquer	81
2.6.3	Local Search	85
2.6.4	Simulated Annealing and Stochastic Algorithms	87
2.6.5	Computability, Decidability and Turing Machines	88
2.6.6	Efficiency of Algorithms	99
2.6.7	Suggested Reading	105
	Problems	106
3	Mathematical and Physical Prerequisites	109
3.1	Introduction	109
3.2	Sets and Set Operations	113
3.2.1	Cartesian Product, Product Set	116
3.2.2	Functions and Linear Spaces	117
3.3	Topological Spaces	127
3.3.1	Charts	134
3.3.2	Atlas	135
3.3.3	Manifolds	137
3.3.4	Tangent Vectors and Tangent Space	140
3.3.5	Covectors, Cotangent Space and One-Forms	143
3.3.6	Dual Spaces	148
3.3.7	Tensors and Tensor Spaces	150
3.3.8	Affine Connections and Covariant Derivative	155
3.4	Metric Spaces and Metric Connection	159
3.5	Riemannian Manifolds	162
3.5.1	Riemannian Curvature	163
3.6	The Problem of Inertia and Motion: Coordinate Systems in Physics	165
3.6.1	The Special and General Principle of Relativity	166
3.6.2	The Structure of Spacetime	170
3.7	Relativistic Field Equations	171
3.7.1	Relativistic Hydrodynamics	172
3.8	Suggested Reading	175
	Problems	175
4	Fundamentals of Numerical Simulation	179
4.1	Basics of Ordinary and Partial Differential Equations in Physics	179
4.1.1	Elliptic Type	184
4.1.2	Parabolic Type	185
4.1.3	Hyperbolic Type	187
4.2	Numerical Solution of Differential Equations	189

4.2.1	Mesh-based and Mesh-free Methods	190
4.2.2	Finite Difference Methods	196
4.2.3	Finite Volume Method	198
4.2.4	Finite Element Methods	202
4.3	Elements of Software Design	205
4.3.1	Software Design	207
4.3.2	Writing a Routine	210
4.3.3	Code-Tuning Strategies	214
4.3.4	Suggested Reading	217
	Problems	217

Part II Computational Methods on Multiscales

	Summary of Part I	221
5	Computational Methods on Electronic/Atomistic Scale	225
5.1	Introduction	225
5.2	Ab-initio Methods	226
5.3	Physical Foundations of Quantum Theory	230
5.3.1	A Short Historical Account of Quantum Theory	231
5.3.2	A Hamiltonian for a Condensed Matter System	234
5.3.3	The Born-Oppenheimer Approximation	234
5.4	Density Functional Theory	237
5.5	Car-Parinello Molecular Dynamics	239
5.5.1	Force Calculations: The Hellmann-Feynman Theorem	240
5.5.2	Calculating the Ground State	242
5.6	Solving Schrödinger's Equation for Many-Particle Systems: Quantum Mechanics of Identical Particles	243
5.6.1	The Hartree-Fock Approximation	245
5.7	What Holds a Solid Together?	256
5.7.1	Homonuclear Diatomic Molecules	256
5.8	Semi-empirical Methods	259
5.8.1	Tight-Binding Method	260
5.9	Bridging Scales: Quantum Mechanics (QM) – Molecular Mechanics (MM)	265
5.10	Concluding Remarks	266
6	Computational Methods on Atomistic/Microscopic Scale	269
6.1	Introduction	269
6.1.1	Thermodynamics and Statistical Ensembles	273
6.2	Fundamentals of Statistical Physics and Thermodynamics	275
6.2.1	Probabilities	275
6.2.2	Measurements and the Ergodic Hypotheses	276
6.2.3	Statistics in Phase Space and Statistical Ensembles	278

XVI Contents

6.2.4	Virtual Ensembles	282
6.2.5	Entropy and Temperature	284
6.3	Classical Interatomic and Intermolecular Potentials	284
6.3.1	Charged Systems	285
6.3.2	Ewald Summation	287
6.3.3	The P^3M Algorithm	288
6.3.4	Van der Waals Potential	288
6.3.5	Covalent Bonds	289
6.3.6	Embedded Atom Potentials	290
6.3.7	Pair Potentials	292
6.4	Classical Molecular Dynamics Simulations	294
6.4.1	Numerical Ingredients of MD Simulations	295
6.4.2	Integrating the Equations of Motion	299
6.4.3	Periodic Boundary Conditions	303
6.4.4	The Minimum Image Convention	305
6.4.5	Efficient Search Strategies for Interacting Particles	306
6.4.6	Making Measurements	309
6.5	Liquids, Soft Matter and Polymers	313
6.5.1	Scaling and Universality of Polymers	317
6.6	Monte Carlo Method	323
	Problems	327
7	Computational Methods on Mesoscopic/Macroscopic Scale	329
7.1	Example: Meso- and Macroscale Shock-Wave Experiments with Ceramics	332
7.2	Statistical Methods: Voronoi Tesselations and Power Diagrams for Modeling Microstructures of Ceramics	334
7.2.1	Reverse Monte Carlo Optimization	336
7.3	Dissipative Particle Dynamics	340
7.4	Theoretic Mesoscale Simulation Method	342
7.5	Bridging Scales: Soft Particle Discrete Elements	344
7.6	Bridging Scales: Energetic Links between MD and FEM	354
7.6.1	Bridging Scales: Work-Hardening	356
7.7	Physical Theories for Macroscopic Phenomena:	357
7.7.1	The Description of Fluid Motion	358
7.8	Continuum Theory	360
7.8.1	The Continuum Hypothesis	360
7.9	Theory of Elasticity	363
7.9.1	Kinematic Equations	365
7.9.2	The Stress Tensor	371
7.9.3	Equations of Motion of the Theory of Elasticity	373
7.9.4	Constitutive Equations	373
7.10	Bridging Scale Application: Crack Propagation in a Brittle Specimen	375

8 Perspectives in Multiscale Materials Modeling	377
A Further Reading	381
B Mathematical Definitions	383
C Sample Code for the Main Routine of a MD Simulation	385
D A Sample Makefile	387
E Tables of Physical Constants	389
E.1 International System of Units (SI or mksA System)	389
E.2 Conversion Factors of Energy	390
List of Algorithms	391
List of Boxes	393
Solutions	395
References	401
Index	423