

| | |
|-------------------------|---|
| 1. Record Nr. | UNISA996483071203316 |
| Autore | Steinhauser M. O (Martin Oliver) |
| Titolo | Computational multiscale modeling of fluids and solids : theory and applications / / Martin Oliver Steinhauser |
| Pubbl/distr/stampa | Cham, Switzerland : , : Springer International Publishing, , [2022] ©2022 |
| ISBN | 9783030989545 9783030989538 |
| Edizione | [3rd ed.] |
| Descrizione fisica | 1 online resource (450 pages) |
| Collana | Graduate Texts in Physics Ser. |
| Disciplina | 532 |
| Soggetti | Fluids - Mathematical models Solids - Mathematical models |
| Lingua di pubblicazione | Inglese |
| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
| Nota di contenuto | <p>Intro -- Preface to the Third Edition -- Preface to the Second Edition -- Preface to the First Edition in 2008 -- Contents -- Acronyms -- List of Algorithms -- List of Boxes -- blackPart I Fundamentals-1pt -- 1</p> <p>Introduction to Multiscale Modeling -- 1.1 Physics on Different Length-and Timescales -- 1.1.1 Electronic/Atomic Scale -- 1.1.2 Atomic/Microscopic Scale -- 1.1.3 Microscopic/Mesoscopic Scale -- 1.1.4 Mesoscopic/Macroscopic Scale -- 1.2 What are Fluids and Solids? -- 1.3 The Objective of Experimental and Theoretical Physics -- 1.4 Computer Simulations-A Review -- 1.4.1 A Brief History of Computer Simulation -- 1.4.2 Computational Materials Science -- 1.5 Suggested Reading -- 2 Multiscale Computational Materials Science -- 2.1 Some Terminology -- 2.2 What is Computational Material Science on Multiscales? -- 2.2.1 Experimental Investigations on Different Length Scales -- 2.3 What is a Model? -- 2.3.1 The Scientific Method -- 2.4 Hierarchical Modeling Concepts Above the Atomic Scale -- 2.4.1 Example: Principle Model Hierarchies in Classical Mechanics -- 2.4.2 Structure-Property Paradigm -- 2.4.3 Physical and Mathematical Modeling -- 2.4.4 Numerical Modeling and Simulation -- 2.5 Unifications and Reductionism in Physical Theories -- 2.5.1 The Four Fundamental Interactions -- 2.5.2 The Standard Model -- 2.5.3 Symmetries, Fields, Particles and the Vacuum -- 2.5.4 Relativistic Wave</p> |

Equations -- 2.5.5 Suggested Reading -- 2.6 Computer Science, Algorithms, Computability and Turing Machines -- 2.6.1 Recursion -- 2.6.2 Divide-and-Conquer -- 2.6.3 Local Search -- 2.6.4 Simulated Annealing and Stochastic Algorithms -- 2.6.5 Computability, Decidability and Turing Machines -- 2.6.6 Efficiency of Algorithms -- 3 Mathematical and Physical Prerequisites -- 3.1 Introduction -- 3.2 Sets and Set Operations -- 3.2.1 Cartesian Product, Product Set. 3.2.2 Functions and Linear Spaces -- 3.3 Topological Spaces -- 3.3.1 Charts -- 3.3.2 Atlas -- 3.3.3 Manifolds -- 3.3.4 Tangent Vectors and Tangent Space -- 3.3.5 Covectors, Cotangent Space and One-Forms -- 3.3.6 Dual Spaces -- 3.3.7 Tensors and Tensor Spaces -- 3.3.8 Affine Connections and Covariant Derivative -- 3.4 Metric Spaces and Metric Connection -- 3.5 Riemannian Manifolds -- 3.5.1 Riemannian Curvature -- 3.6 The Problem of Inertia and Motion: Coordinate Systems in Physics -- 3.6.1 The Special and General Principle of Relativity -- 3.6.2 The Structure of Spacetime -- 3.7 Relativistic Field Equations -- 3.7.1 Relativistic Hydrodynamics -- 3.8 Suggested Reading -- 4 Fundamentals of Numerical Simulation -- 4.1 Basics of Ordinary and Partial Differential Equations in Physics -- 4.1.1 Elliptic Type -- 4.1.2 Parabolic Type -- 4.1.3 Hyperbolic Type -- 4.2 Numerical Solution of Differential Equations -- 4.2.1 Mesh-Based and Mesh-Free Methods -- 4.2.2 Finite Difference Methods -- 4.2.3 Finite Volume Method -- 4.2.4 Finite Element Methods -- 4.3 Elements of Software Design -- 4.3.1 Software Design -- 4.3.2 Writing a Routine -- 4.3.3 Code-Tuning Strategies -- 4.3.4 Suggested Reading -- blackPart II Computational Methods on Multiscales-1pt -- 5 Computational Methods on Electronic/Atomistic Scale -- 5.1 Introduction -- 5.1.1 Scale Separation -- 5.2 Ab-Initio Methods -- 5.3 Physical Foundations of Quantum Theory -- 5.3.1 A Short Description of Quantum Theory -- 5.3.2 A Hamiltonian for a Condensed Matter System -- 5.3.3 The Born-Oppenheimer Approximation -- 5.4 Density Functional Theory -- 5.5 Car-Parrinello Molecular Dynamics -- 5.5.1 Force Calculations: The Hellmann-Feynman Theorem -- 5.5.2 Calculating the Ground State -- 5.6 Solving Schrödinger's Equation for Many-Particle Systems: ... -- 5.6.1 The Hartree-Fock Approximation.

5.7 What Holds a Solid Together? -- 5.7.1 Homonuclear Diatomic Molecules -- 5.8 Semi-empirical Methods -- 5.8.1 Tight-Binding Method -- 5.9 Bridging Scales: Quantum Mechanics (QM) - Molecular Mechanics (MM) -- 5.10 Concluding Remarks -- 6 Computational Methods on Atomistic/Microscopic Scale -- 6.1 Introduction -- 6.1.1 Thermodynamics and Statistical Ensembles -- 6.2 Fundamentals of Statistical Physics and Thermodynamics -- 6.2.1 Probabilities -- 6.2.2 Measurements and the Ergodic Hypotheses -- 6.2.3 Statistics in Phase Space and Statistical Ensembles -- 6.2.4 Virtual Ensembles -- 6.2.5 Entropy and Temperature -- 6.3 Classical Interatomic and Intermolecular Potentials -- 6.3.1 Charged Systems -- 6.3.2 Ewald Summation -- 6.3.3 The P3M Algorithm -- 6.3.4 Van der Waals Potential -- 6.3.5 Covalent Bonds -- 6.3.6 Embedded Atom Potentials -- 6.3.7 Pair Potentials -- 6.4 Classical Molecular Dynamics Simulations -- 6.4.1 Numerical Ingredients of MD Simulations -- 6.4.2 Integrating the Equations of Motion -- 6.4.3 Periodic Boundary Conditions -- 6.4.4 The Minimum Image Convention -- 6.4.5 Efficient Search Strategies for Interacting Particles -- 6.4.6 Making Measurements -- 6.5 Liquids, Soft Matter and Polymers -- 6.5.1 Bonded Interactions -- 6.5.2 Scaling and Universality of Polymers -- 6.6 Monte Carlo Simulations -- 7 Computational Methods on Mesoscopic/Macroscopic Scale -- 7.1 Example: Meso- and Macroscale Shock-Wave Experiments -- 7.2 Statistical Methods: Voronoi

Tesselations and Power Diagrams for Modeling ... -- 7.2.1 Reverse Monte Carlo Optimization -- 7.3 Dissipative Particle Dynamics -- 7.4 Ginzburg-Landau/Cahn-Hilliard Field Theoretic Mesoscale Simulation Method -- 7.5 Bridging Scales: Soft Particle Discrete Elements for Shock Wave Applications -- 7.6 Bridging Scales: Energetic Links Between MD and FEM -- 7.6.1 Bridging Scales: Work-Hardening.
7.7 Physical Theories for Macroscopic Phenomena: The Continuum Approach -- 7.7.1 The Description of Fluid Motion -- 7.8 Continuum Theory -- 7.8.1 The Continuum Hypothesis -- 7.9 Theory of Elasticity -- 7.9.1 Kinematic Equations -- 7.9.2 The Stress Tensor -- 7.9.3 Equations of Motion of the Theory of Elasticity -- 7.9.4 Constitutive Equations -- 7.10 Bridging Scale Application: Crack Propagation -- 8 Perspectives in Multiscale Materials Modeling -- A Further Reading -- A.1 Foundations of Physics -- A.2 Programming Techniques -- A.3 Journals and Conferences on Multiscale Materials Modeling and Simulation -- B Mathematical Definitions -- C Sample Code for the Main Routine in a MD Program -- D A Sample Makefile -- E Tables of Physical Constants -- E.1 International System of Units (SI or mksA System) -- E.2 Conversion Factors of Energy -- References -- Index.
