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Numerical Simulation in Molecular Dynamics
Introduction to Practice of Molecular Simulation
Proceeding of the 2nd International Symposium on Algorithms for Macromolecular Modelling, Berlin, May 21–24, 1997
Modeling and Simulation of Functionalized Materials for Additive Manufacturing and 3D Printing: Continuous and Discrete Media
Fundamentals and Applications
From Classical to Quantum Methods
Computational Chemistry
Molecular Modeling at the Atomic Scale
Proceedings of the International Conference on Computational Methods in Continuum Mechanics (CMCM 2021), Volume 2
Simulation Methods for Polymers
Computer Aided Drug Design (CADD): From Ligand-Based Methods to Structure-Based Approaches

HARRISON CLINTON

Molecular Modeling and Simulation World Scientific
Makes Numerical Programming More Accessible to a Wider Audience Bearing in mind the evolution of modern programming, most specifically emergent programming languages that reflect modern practice, Numerical Programming: A Practical Guide for Scientists and Engineers Using Python and C/C++ utilizes the author’s many years of practical research and teaching experience to offer a systematic approach to relevant programming concepts. Adopting a practical, broad appeal, this user-friendly book offers guidance to anyone interested in using numerical programming to solve science and engineering problems. Emphasizing methods generally used in physics and engineering—from elementary methods to complex algorithms—it gradually incorporates algorithmic elements with increasing complexity. Develop a Combination of Theoretical Knowledge, Efficient Analysis Skills, and Code Design Know-How The book encourages algorithmic thinking, which is essential to numerical analysis. Establishing the fundamental numerical methods, application numerical behavior and graphical output needed to foster algorithmic reasoning, coding dexterity, and a scientific programming style, it enables readers to successfully navigate relevant algorithms, understand coding design, and develop efficient programming skills. The book incorporates real code, and includes examples and problem sets to assist in hands-on learning. Begins with an overview on approximate numbers and programming in Python and C/C++, followed by discussion of basic sorting and indexing methods, as well as portable graphic functionality Contains methods for function evaluation, solving algebraic and transcendental equations, systems of linear algebraic equations, ordinary differential equations, and eigenvalue problems Addresses approximation of tabulated functions, regression, integration of one- and multi-dimensional functions by classical and Gaussian quadratures, Monte Carlo integration techniques, generation of random variables, discretization methods for ordinary and partial differential equations, and stability analysis This text introduces platform-independent numerical

programming using Python and C/C++, and appeals to advanced undergraduate and graduate students in natural sciences and engineering, researchers involved in scientific computing, and engineers carrying out applicative calculations.
Molecular Modelling for Beginners CRC Press
Within the last decade, several industrialized countries have stressed the importance of advanced manufacturing to their economies. Many of these plans have highlighted the development of additive manufacturing techniques, such as 3D printing which, as of 2018, are still in their infancy. The objective is to develop superior products, produced at lower overall operational costs. For these goals to be realized, a deep understanding of the essential ingredients comprising the materials involved in additive manufacturing is needed. The combination of rigorous material modeling theories, coupled with the dramatic increase of computational power can potentially play a significant role in the analysis, control, and design of many emerging additive manufacturing processes. Specialized materials and the precise design of their properties are key factors in the processes. Specifically, particle-functionalized materials play a central role in this field, in three main regimes: (1) to enhance overall filament-based material properties, by embedding particles within a binder, which is then passed through a heating element and the deposited onto a surface, (2) to “functionalize” inks by adding particles to freely flowing solvents forming a mixture, which is then deposited onto a surface and (3) to directly deposit particles, as dry powders, onto surfaces and then to heat them with a laser, e-beam or other external source, in order to fuse them into place. The goal of these processes is primarily to build surface structures which are extremely difficult to construct using classical manufacturing methods. The objective of this monograph is introduce the readers to basic techniques which can allow them to rapidly develop and analyze particulate-based materials needed in such additive manufacturing processes. This monograph is broken into two main parts: “Continuum Method” (CM) approaches and “Discrete Element Method” (DEM) approaches. The materials associated with methods (1) and (2) are closely related types of continua (particles embedded in a continuous binder) and are treated using continuum approaches. The materials in method (3), which are of a discrete particulate character, are analyzed using discrete element methods.

Adsorption and Diffusion CRC Press
Nanostructured materials with multiple components and complex structures are the current focus of research and are expected to develop further for material designs in many applications in electrochemical, colloidal, medical, pharmaceutical, and several other fields. This book discusses complex nanostructured systems exemplified by nanoporous silicates, spontaneously formed gels from silica-nanocolloidal solutions, and related systems, and examines them using molecular dynamics simulations. Nanoporous materials, nanocolloidal systems, and gels are useful in many applications and can be used in electric devices and storage, and for gas, ion, and drug delivery. The book gives an overview of the history, current status, and frontiers of the field. It also discusses the fundamental aspects related to the common behaviors of some of these systems and common analytical methods to treat them.
Molecular Dynamics, Monte Carlo, Brownian Dynamics, Lattice Boltzmann and Dissipative Particle Dynamics Elsevier
The idea of the book is to provide a comprehensive overview of computational physics methods and techniques, that are used for materials modeling on different length and time scales. Each chapter first provides an overview of the basic physical principles which are the basis for the numerical and mathematical modeling on the respective length-scale. The book includes the micro-scale, the meso-scale and the macro-scale, and the chapters follow this classification. The book explains in detail many tricks of the trade of some of the most important methods and techniques that are used to simulate materials on the perspective levels of spatial and temporal resolution. Case studies are included to further illustrate some methods or theoretical considerations. Example applications for all techniques are provided, some of which are from the author’s own contributions to some of the research areas. The second edition has been expanded by new sections in computational models on meso/macroscopic scales for ocean and atmosphere dynamics. Numerous applications in environmental physics and geophysics had been added.
Classical and Quantum Dynamics in Condensed Phase Simulations Elsevier
"In the opening chapter of An Introduction to Molecular Dynamics, the method of statistical geometry, based on the construction of a Voronoi polyhedral, is applied to the pattern recognition of atomic environments and to the investigation of the local order in molecular dynamics-simulated materials. Next, the authors discuss the methodology of bimolecular simulations and their advancements, as well as their applications in the field of nanoparticle-biomolecular interactions. The theory of molecular dynamics simulation and some of the recent molecular dynamics methods such as steered molecular dynamics, umbrella sampling, and coarse-grained simulation are also discussed. The use of auxiliary programs in the cases of modified cyclodextrins is discussed. Additionally, results from molecular dynamics studies on cases of inclusion compounds of molecules of different sizes and shapes encapsulated in the same host cyclodextrin have been examined and compared. In closing, the authors discuss the methodology of molecular dynamics simulation with a non-constant force field. In the context of molecular simulations, the term "force field" refers to a set of equations and parameters for the calculation of forces acting on the particles of the system and its potential energy"--
Dynamics of Engineered Artificial Membranes and Biosensors CRC Press
Molecular Dynamics is a two-volume compendium of the ever-growing applications of molecular dynamics simulations to solve a wider range of scientific and engineering challenges. The contents illustrate the rapid progress on molecular dynamics simulations in many fields of science and technology, such as nanotechnology, energy research, and biology, due to the advances of new dynamics theories and the extraordinary power of today's computers. This second book begins with an introduction of molecular dynamics simulations to macromolecules and then illustrates the computer experiments using molecular dynamics simulations in the studies of synthetic and biological macromolecules, plasmas, and nanomachines. Coverage of this book includes: Complex formation and dynamics of polymers Dynamics of lipid bilayers, peptides, DNA, RNA, and proteins Complex liquids and plasmas Dynamics of molecules on surfaces Nanofluidics and nanomachines
Computational Approaches for Chemistry Under Extreme Conditions Elsevier
"Provides a lot of reading pleasure and many new insights." -Journal of Molecular Structure "This is the most entertaining, stimulating and useful book which can be thoroughly recommended to anyone with an interest in computer simulation." - Contemporary Physics "A very useful introduction . . . more interesting to read than the often dry equation-based texts." -

Journal of the American Chemical Society Written especially for the novice, Molecular Dynamics Simulation demonstrates how molecular dynamics simulations work and how to perform them, focusing on how to devise a model for specific molecules and then how to simulate their movements using a computer. This book provides a collection of methods that until now have been scattered through the literature of the last 25 years. It reviews elements of sampling theory and discusses how modern notions of chaos and nonlinear dynamics explain the workings of molecular dynamics. Stresses easy-to-use molecules * Provides sample calculations and figures * Includes four complete FORTRAN codes

Theoretical Developments and Applications in Nanotechnology and Energy Springer Science & Business Media Although molecular modeling has been around for a while, the groundbreaking advancement of massively parallel supercomputers and novel algorithms for parallelization is shaping this field into an exciting new area. Developments in molecular modeling from experimental and computational techniques have enabled a wide range of biological applications. Responding to this renaissance, Molecular Modeling at the Atomic Scale: Methods and Applications in Quantitative Biology includes discussions of advanced techniques of molecular modeling and the latest research advancements in biomolecular applications from leading experts. The book begins with a brief introduction of major methods and applications, then covers the development of cutting-edge methods/algorithms, new polarizable force fields, and massively parallel computing techniques, followed by descriptions of how these novel techniques can be applied in various research areas in molecular biology. It also examines the self-assembly of biomacromolecules, including protein folding, RNA folding, amyloid peptide aggregation, and membrane lipid bilayer formation. Additional topics highlight biomolecular interactions, including protein interactions with DNA/RNA, membrane, ligands, and nanoparticles. Discussion of emerging topics in biomolecular modeling such as DNA sequencing with solid-state nanopores and biological water under nanoconfinement round out the coverage. This timely summary contains the perspectives of leading experts on this transformation in molecular biology and includes state-of-the-art examples of how molecular modeling approaches are being applied to critical questions in modern quantitative biology. It pulls together the latest research and applications of molecular modeling and real-world expertise that can boost your research and development of applications in this rapidly changing field.

Introduction to Computational Materials Science BoD – Books on Demand First time paperback of successful physics monograph. Copyright © Libri GmbH. All rights reserved.

Elementary Methods Springer On May 21-24, 1997 the Second International Symposium on Algorithms for Macromolecular Modelling was held at the Konrad Zuse Zentrum in Berlin. The event brought together computational scientists in fields like biochemistry, biophysics, physical chemistry, or statistical physics and numerical analysts as well as computer scientists working on the advancement of algorithms, for a total of over 120 participants from 19 countries. In the course of the symposium, the speakers agreed to produce a representative volume that combines survey articles and original papers (all refereed) to give an impression of the present state of the art of Molecular Dynamics. The 29 articles of the book reflect the main topics of the Berlin meeting which were i) Conformational Dynamics, ii) Thermodynamic Modelling, iii) Advanced Time-Stepping Algorithms, iv) Quantum-Classical Simulations and Fast Force Field and v) Fast Force Field Evaluation.

Reviews of Current Trends Springer Science & Business Media Emphasising essential methods and universal principles, this textbook provides everything students need to understand the basics of simulating materials behavior. All the key topics are covered from electronic structure methods to microstructural evolution, appendices provide crucial background material, and a wealth of practical resources are available online to complete the teaching package. Modeling is examined at a broad range of scales, from the atomic to the mesoscale, providing students with a solid foundation for future study and research. Detailed, accessible explanations of the fundamental equations underpinning materials modelling are presented, including a full chapter summarising essential mathematical background. Extensive appendices, including essential background on classical and quantum mechanics, electrostatics, statistical thermodynamics and linear elasticity, provide the background necessary to fully engage with the fundamentals of computational modelling. Exercises, worked examples, computer codes and discussions of practical implementations methods are all provided online giving students the hands-on experience they need.

Computational Chemistry: Reviews of Current Trends CRC Press This book is devoted to a description of the modeling of nanosystems and a detailed exposition of the application of molecular dynamics methods to problems from various fields of technology: material science, the formation of composite molecular complexes, and transport of nanosystems. The research results of the modeling of various nanosystems are presented: soft supramolecular nanostructures, nanosized beams of single-crystal Cu, metallic nanosized crystals, drug delivery systems, and systems stabilized by hydrogen bonds. The information from this book will be useful for engineers, technologists, researchers, and postgraduate students interested in the study of the whole complex of computer simulation based on the concept of molecular dynamics methods for the task of designing and producing nanomaterials with controlled properties.

Advanced Computational Methods for Knowledge Engineering Elsevier Molecular Dynamics is a two-volume compendium of the ever-growing applications of molecular dynamics simulations to solve a wider range of scientific and engineering challenges. The contents illustrate the rapid progress on molecular dynamics simulations in many fields of science and technology, such as nanotechnology, energy research, and biology, due to the advances of new dynamics theories and the extraordinary power of today's computers. This first book begins with a general description of underlying theories of molecular dynamics simulations and provides extensive coverage of molecular dynamics simulations in nanotechnology and energy. Coverage of this book includes: Recent advances of molecular dynamics theory Formation and evolution of nanoparticles of up to 106 atoms Diffusion and dissociation of gas and liquid molecules on silicon, metal, or metal organic frameworks Conductivity of ionic species in solid oxides Ion solvation in liquid mixtures Nuclear structures

Ab Initio Molecular Dynamics World Scientific Publishing Company Incorporated The book consists of 29 extended chapters which have been selected and invited from the submissions to the 1st International Conference on Computer Science, Applied

Mathematics and Applications (ICCSAMA 2013) held on 9-10 May, 2013 in Warsaw, Poland. The book is organized into five parts, which are: Advanced Optimization Methods and Their Applications, Queuing Theory and Applications, Computational Methods for Knowledge Engineering, Knowledge Engineering with Cloud and Grid Computing, and Logic Based Methods for Decision Making and Data Mining, respectively. All chapters in the book discuss theoretical and practical issues connected with computational methods and optimization methods for knowledge engineering.

Understanding Molecular Simulation World Scientific

This book shows how nanofabrication techniques and nanomaterials can be used to customize packaging for nano devices with applications to electronics, photonics, biological and biomedical research and products. It covers topics such as bio sensing electronics, bio device packaging, MEMS for bio devices and much more, including: Offers a comprehensive overview of nano and bio packaging and their materials based on their chemical and physical sciences and mechanical, electrical and material engineering perspectives; Discusses nano materials as power energy sources, computational analyses of nano materials including molecular dynamic (MD) simulations and DFT calculations; Analyzes nanotubes, superhydrophobic self-clean Lotus surfaces; Covers nano chemistry for bio sensor/bio material device packaging. This second edition includes new chapters on soft materials-enabled packaging for stretchable and wearable electronics, state of the art miniaturization for active implantable medical devices, recent LED packaging and progress, nanomaterials for recent energy storage devices such as lithium ion batteries and supercapacitors and their packaging. Nano- Bio- Electronic, Photonic and MEMS Packaging is the ideal book for all biomedical engineers, industrial electronics packaging engineers, and those engaged in bio nanotechnology applications research.

Computational Molecular Dynamics: Challenges, Methods, Ideas Wiley-Interscience

The field of quantum and molecular simulations has experienced strong growth since the time of the early software packages. A recent study, showed a large increase in the number of people publishing papers based on ab initio methods from about 3,000 in 1991 to roughly 20,000 in 2009, with particularly strong growth in East Asia. Looking to the future, the question remains as to how these methods can be further integrated into the R&D value chain, bridging the gap from engineering to manufacturing. Using successful case studies as a framework, Industrial Applications of Molecular Simulations demonstrates the capability of molecular modeling to tackle problems of industrial relevance. This book presents a wide range of various modeling techniques, including methods based on quantum or classical mechanics, molecular dynamics, Monte Carlo simulations, etc. It also explores a wide range of materials, from soft materials such as polymeric blends widely used in the chemical industry to hard or inorganic materials such as glasses and alumina. Features Demonstrates how modeling can solve everyday problems for scientists in industry Provides a broad overview of theoretical approaches Presents a wide range of applications in areas such as materials research, catalysis, pharmaceutical development and electronics Emphasizes the relationship between theory and experiments

A Practical Guide for Scientists and Engineers Using Python and C/C++ Springer

The latest developments in quantum and classical molecular dynamics, related techniques, and their applications to several fields of science and engineering. Molecular simulations include a broad range of methodologies such as Monte Carlo, Brownian dynamics, lattice dynamics, and molecular dynamics (MD). Features of this book: • Presents advances in methodologies, introduces quantum methods and lists new techniques for classical MD • Deals with complex systems: biomolecules, aqueous solutions, ice and clathrates, liquid crystals, polymers • Provides chemical reactions, interfaces, catalysis, surface phenomena and solids Although the book is not formally divided into methods and applications, the chapters are arranged starting with those that discuss new algorithms, methods and techniques, followed by several important applications.

Methods and Applications in Quantitative Biology CRC Press

"Vast progress in the area of computational chemistry has been achieved in the last decade. Theoretical methods such as quantum mechanics, molecular dynamics and statistical mechanics have been successfully used to characterize chemical systems and to design new materials, drugs and chemicals. The reviews presented in this volume discuss the current advances in computational methodologies and their applications. The areas covered include materials science, nanotechnology, inorganic and biological systems. The major thrust of the book is to bring timely overviews of new findings and methods applied in the rapidly changing field of computational chemistry."--BOOK JACKET.

Molecular Simulation of Fluids Springer Nature

Until the late 20th century, computational studies of biomolecules and nanomaterials had considered the two subjects separately. A thorough presentation of state-of-the-art simulations for studying the nanoscale behavior of materials, Simulations in Nanobiotechnology discusses computational simulations of biomolecules and nanomaterials together. Th

Basic Theory and Advanced Methods Cambridge University Press

Very broad overview of the field intended for an interdisciplinary audience; Lively discussion of current challenges written in a colloquial style; Author is a rising star in this discipline; Suitably accessible for beginners and suitably rigorous for experts; Features extensive four-color illustrations; Appendices featuring homework assignments and reading lists complement the material in the main text

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