Understanding Molecular Simulation Second Edition From Algorithms To Applications Computational Science Series Vol 1

Computer simulation is an indispensable research tool in modeling, understanding and predicting nanoscale phenomena. However, the advanced computer codes used by researchers are too complicated for graduate students wanting to understand computer simulations of physical systems. This book gives students the tools to develop their own codes. Describing advanced algorithms, the book is ideal for students in computational physics, quantum mechanics, atomic and molecular physics, and condensed matter theory. It contains a wide variety of practical examples of varying complexity to help readers at all levels of experience. An algorithm library in Fortran 90, available online at www.cambridge.org/9781107001701, implements the advanced computational approaches described in the text to solve physical problems.

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

Material properties emerge from phenomena on scales ranging from Angstroms to millimeters, and only a multiscale treatment can provide a complete understanding. Materials researchers must therefore understand fundamental concepts and techniques from different fields, and these are presented in a comprehensive and integrated fashion for the first time in this book. Incorporating continuum mechanics, quantum mechanics, statistical mechanics, atomistic simulations and multiscale techniques, the book explains many of the key theoretical ideas behind multiscale modeling. Classical topics are blended with new techniques to demonstrate the connections between different fields and highlight current research trends. Example applications drawn from modern research on the thermo-mechanical properties of crystalline solids are used as a unifying focus throughout the text. Together with its companion book, Continuum Mechanics and Thermodynamics (Cambridge University Press, 2011), this work presents the complete fundamentals of materials modeling for graduate students and researchers in physics, materials science, chemistry and engineering.

For more than four decades, scientists and researchers have relied on the Advances in Chromatography Series for the most up-to-date information on a wide range of developments in chromatographic methods and applications. With contributions from an array of international experts, the latest volume captures new developments in this important field that yields great possibilities in a number of applications. The

authors' clear presentation of topics and vivid illustrations make the material in Volume 48 accessible and engaging to biochemists and analytical, organic, polymer, and pharmaceutical chemists at all levels of technical skill. Topics covered in this new edition include: The retention mechanism in reversed-phase liquid chromatography (RPLC) Thermodynamic modeling of chromatographic separation Ultra-performance liquid chromatography (ULPC) Biointeraction affinity chromatography The characterization of stationary phases in supercritical fluid chromatography with the salvation parameter model Silica-hydride chemistry Multi-dimensional gas chromatography Sample preparation for chromatographic analysis of environmental samples and solid-phase microextraction (SPME) with derivatization Covering the state of the art in separation science, this volume presents timely, cutting-edge reviews on chromatography in the fields of bio-, analytical, organic, polymer, and pharmaceutical chemistry. The information contained in this latest volume will help fuel further research in this burgeoning field across the full spectrum of related disciplines.

This volume focuses on developments in the field of group theory in its broadest sense and is of interest to theoretical and experimental physicists, mathematicians, and scientists in related disciplines who are interested in the latest methods and applications. In an increasingly ultra-specialized world, this volume will demonstrate the interchange of ideas and methods in theoretical and mathematical physics.

Molecular simulation is a widely used tool in biology, chemistry, physics and engineering. This book contains a collection of articles by leading researchers who are developing new methods for molecular modelling and simulation. Topics addressed here include: multiscale formulations for biomolecular modelling, such as quantum-classical methods and advanced solvation techniques; protein folding methods and schemes for sampling complex landscapes; membrane simulations; free energy calculation; and techniques for improving ergodicity. The book is meant to be useful for practitioners in the simulation community and for those new to molecular simulation who require a broad introduction to the state of the art.

This volume consists of a selection of research-type articles on dynamical systems, evolution equations, analytic number theory and closely related topics. A strong emphasis is on a fair balance between theoretical and more applied work, thus spanning the chasm between abstract insight and actual application. Several of the articles are expected to be in the intersection of dynamical systems theory and number theory. One article will likely relate the topics presented to the academic achievements and interests of Prof. Leutbecher and shed light on common threads among all the contributions. Contents:PrefaceBiographical Note on Armin Leutbecher (S Walcher)Das Jahr 1934 ... (J Fischer)Explicit Expressions for Equivariant Minimal Lagrangian Surfaces (J F Dorfmeister & H Ma)Rational Parameter Rays of the Multibrot Sets (D Eberlein, S Mukherjee & D Schleicher)The Matovich-Pearson Equations Revisited (T Hagen)Diffeomorphisms with Stable Manifolds as Basin Boundaries (S Hayes & Ch Wolf)A New Type of Functional Equations of Euler Products (B Heim)The Hexagonal Lattice and the Epstein Zeta Function (A Henn)On Putative q-Analogues of the Fano Plane (Th Honold & M Kiermaier)Integral Orthogonal Groups (A Krieg)The Role of Fourier Analysis in X-Ray Crystallography (F Rupp & J Scheurle)An Elementary Proof for Joint Continuity of Semiflows (S Schmitz)A Convergent String Method (H Schwetlick & J Zimmer)Variational Symmetries and Pluri-Lagrangian Systems (Y B Suris) Readership: Researchers in algebra and number theory, dynamical systems and analysis and differential equations. Key Features:This versatile book covers state-of-the art work in dynamical systems, analytic number theory and applied analysisIt appeals to a wide audience due to its broad range of topics, highlighting both the breadth and the depth of modern analytical work without losing sight of a common coreKeywords:Dynamical Systems;Evolution Equations;Number Theory;Differential Geometry

The scope of this book is to identify and emphasize the successful link between computational materials modeling as a simulation and design

tool and its synergistic application to experimental research and alloy development. The book provides a more balanced perspective of the role that computational modeling can play in every day research and development efforts. Each chapter describes one or more particular computational tool and how they are best used.

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

Applications of numerical mathematics and scientific computing to chemical engineering.

Gathering leading specialists in the field of structure prediction, this book provides a unique view of this complex and rapidly developing field, reflecting the numerous viewpoints of the different authors. A summary of the major achievements over the last few years and of the challenges still remaining makes this monograph very timely.

This paper introduces time-continuous numerical schemes to simulate stochastic differential equations (SDEs) arising in mathematical finance, population dynamics, chemical kinetics, epidemiology, biophysics, and polymeric fluids. These schemes are obtained by spatially discretizing the Kolmogorov equation associated with the SDE in such a way that the resulting semi-discrete equation generates a Markov jump process that can be realized exactly using a Monte Carlo method. In this construction the jump size of the approximation can be bounded uniformly in space, which often guarantees that the schemes are numerically stable for both finite and long time simulation of SDEs.

Kjelstrup, Bedeaux, Johannessen, and Gross describe what non-equilibrium thermodynamics is in a simple and practical way and how it can add to engineering design. They explain how to describe proper equations of transport that are more precise than those used so far, and how to use them to understand the waste of energy resources in central process units in the industry. The authors introduce the entropy balance as an additional equation to use in engineering; to create consistent thermodynamic models, and to systematically minimize energy losses that are connected with the transport of heat, mass, charge and momentum.Non-equilibrium Thermodynamics for Engineers teaches the essence of non-equilibrium thermodynamics and its applications at a level comprehensible to engineering students, practitioner engineers, and scientists working on industrial problems. The book may be used as a textbook in basic engineering curricula or graduate courses.

This book highlights the most recent advances in nano science from leading researchers in Ukraine, Europe and beyond. It features contributions from participants of the 3rd International Summer School “Nanotechnology: From Fundamental Research to Innovations,” held in Yaremche, Ukraine on August 23-26, 2014 and of the 2nd International NANO-2014 Conference, held in Lviv, Ukraine on August 27-30, 2014. These events took place within the framework of the European Commission FP7 project Nano twinning and were organized jointly by the Institute of Physics of the National Academy of Sciences of Ukraine, University of Tartu (Estonia), University of Turin (Italy) and Pierre and Marie Curie University (France). Internationally recognized experts from a

wide range of universities and research institutions share their knowledge and key results in the areas of nanocomposites and nanomaterials, nanostructured surfaces, microscopy of nano-objects, nano-optics and nano photonics, nano plasmonics, nano chemistry, nano biotechnology and surface enhanced spectroscopy. Covers nanocomposites, nano structured surfaces and nano biotechnology Presents state-of-the-art advances in nano plasmonics, nanomaterials characterization and surface enhanced spectroscopy Represents essential reading for advanced undergraduate and graduate students through practicing university and industry researchers

Understanding Molecular Simulation: From Algorithms to Applications explains the physics behind the "recipes" of molecular simulation for materials science. Computer simulators are continuously confronted with questions concerning the choice of a particular technique for a given application. A wide variety of tools exist, so the choice of technique requires a good understanding of the basic principles. More importantly, such understanding may greatly improve the efficiency of a simulation program. The implementation of simulation methods is illustrated in pseudocodes and their practical use in the case studies used in the text. Since the first edition only five years ago, the simulation world has changed significantly -- current techniques have matured and new ones have appeared. This new edition deals with these new developments; in particular, there are sections on: · Transition path sampling and diffusive barrier crossing to simulaterare events · Dissipative particle dynamic as a course-grained simulation technique · Novel schemes to compute the long-ranged forces · Hamiltonian and non-Hamiltonian dynamics in the context constant-temperature and constant-pressure molecular dynamics simulations · Multiple-time step algorithms as an alternative for constraints · Defects in solids · The pruned-enriched Rosenbluth sampling, recoil-growth, and concerted rotations for complex molecules · Parallel tempering for glassy Hamiltonians Examples are included that highlight current applications and the codes of case studies are available on the World Wide Web. Several new examples have been added since the first edition to illustrate recent applications. Questions are included in this new edition. No prior knowledge of computer simulation is assumed.

Understanding Molecular SimulationFrom Algorithms to ApplicationsElsevier

Recently, there has been a surge of activity to elucidate the behavior of highly charged soft matter and Coulomb fluids in general. Such systems are ubiquitous, especially in biological matter where the length scale and the strength of the interaction between highly charged biomolecules are governed by strong electrostatic effects. Several interesting limits have been discovered in the parameter space of highly charged many-particle Coulomb matter where analytical progress is possible and completely novel and unexpected results have been obtained. One of the challenges in highly charged matter is to correctly describe systems with finite coupling strength in the transition regime between weak and strong couplings. After studying the fluctuations of both, several theories have been developed that describe this experimentally highly relevant regime. At the same time, computer simulation algorithms and computing power have advanced to the level where all-ion simulations, including many-body and polarization effects, are possible; the new theories thus can be

subjected to numerical confirmation. Another important question is the effect of the structural disorder on electrostatic interactions. It has recently been demonstrated, both theoretically and experimentally, that charge disorder can impose long-range interaction between charged or even uncharged surfaces. These interactions might become very significant in biological processes. Filling a void in the literature, this volume cross-pollinates different theoretical and simulation approaches with new experiments and ties together the low temperature, high coupling constant, and disorder parameters in a unified description of the electrostatic interactions, which largely determine the stability and conformations of most important biological macromolecules. With striking graphical illustrations, the book presents a unified view of the current advances in the field of Coulomb (bio)colloidal systems, building on previous literature that summarized the field over 20 years ago. Leading scientists in the field offer a detailed introduction to different modern methods in statistical physics of Coulomb systems. They detail various approaches to elucidate the behavior of strongly charged soft matter. They also provide experimental and theoretical descriptions of disorder effects in Coulomb systems, which have not been discussed in any other book.

Amber is the collective name for a suite of programs that allow users to carry out molecular dynamics simulations, particularly on biomolecules. None of the individual programs carries this name, but the various parts work reasonably well together, and provide a powerful framework for many common calculations. The term Amber is also used to refer to the empirical force fields that are implemented here. It should be recognized, however, that the code and force field are separate: several other computer packages have implemented the Amber force fields, and other force fields can be implemented with the Amber programs. Further, the force fields are in the public domain, whereas the codes are distributed under a license agreement. The Amber software suite is divided into two parts: AmberTools21, a collection of freely available programs mostly under the GPL license, and Amber20, which is centered around the pmemd simulation program, and which continues to be licensed as before, under a more restrictive license. Amber20 represents a significant change from the most recent previous version, Amber18. (We have moved to numbering Amber releases by the last two digits of the calendar year, so there are no odd-numbered versions.) Please see https://ambermd.org for an overview of the most important changes. AmberTools is a set of programs for biomolecular simulation and analysis. They are designed to work well with each other, and with the “regular” Amber suite of programs. You can perform many simulation tasks with AmberTools, and you can do more extensive simulations with the combination of AmberTools and Amber itself. Most components of AmberTools are released under the GNU General Public License (GPL). A few components are in the public domain or have other open-source licenses. See the README file for more information.

A self-contained account of energy landscape theory aimed at graduate students and researchers.

Lipid science and technology has grown exponentially since the turn of the millennium. The replacement of unhealthy fats in the foods we eat, and of petroleum-based ingredients in the cosmetics we use, is a top priority for consumers, government, and industry alike. Particularly for the food industry, removing trans fats and reducing saturated fat in foods has produced a major challenge: How do we create structure with a minimum amount of structuring material? A comprehensive omnibus, Structure and Properties of Fat Crystal Networks, Second Edition clarifies the complex relationship between triglyceride composition of vegetable oils and fats, the physicochemical properties of triglycerides in simple and complex model systems, their crystallization, and melting behavior. Furthermore, it dives into the implications of these materials on the functional properties in food systems. Replacing ingredients, optimizing functionality, and improving health necessitate the ability to relate the structural organization present in a material to macroscopic properties. Revisiting concepts and approaches used in the study of fat crystal networks, the second edition includes new developments, particularly intermolecular interactions, and thoroughly updated analytical methods. Succinct, clear, and complete, this book is designed to help students and early-career researchers make the study of fats a more focused, less frustrating, and less expensive endeavor.

FROM REVIEWS OF THE SERIES "Reviews in Computational Chemistry remains the most valuable reference to methods and techniques in computational chemistry." -JOURNAL OF MOLECULAR GRAPHICS AND MODELLING "One cannot generally do better than to try to find an appropriate article in the highly successful Reviews in Computational Chemistry. The basic philosophy of the editors seems to be to help the authors produce chapters that are complete, accurate, clear, and accessible to experimentalists (in particular) and other nonspecialists (in general)." -JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

Free energy constitutes the most important thermodynamic quantity to understand how chemical species recognize each other, associate or react. Examples of problems in which knowledge of the underlying free energy behaviour is required, include conformational equilibria and molecular association, partitioning between immiscible liquids, receptor-drug interaction, protein-protein and protein-DNA association, and protein stability. This volume sets out to present a coherent and comprehensive account of the concepts that underlie different approaches devised for the determination of free energies. The reader will gain the necessary insight into the theoretical and computational foundations of the subject and will be presented with relevant applications from molecular-level modelling and simulations of chemical and biological systems. Both formally accurate and approximate methods are covered using both classical and quantum mechanical descriptions. A central theme of the book is that the wide variety of free energy calculation techniques available today can be understood as different implementations of a few basic principles. The book is aimed at a broad readership of

graduate students and researchers having a background in chemistry, physics, engineering and physical biology.
This book provides a unique and comprehensive overview of the latest advances, challenges and accomplishments in the rapidly growing field of theoretical and computational materials science. Today, an increasing number of industrial communities rely more and more on advanced atomic-scale methods to obtain reliable predictions of materials properties, complement qualitative experimental analyses and circumvent experimental difficulties. The book examines some of the latest and most advanced simulation techniques currently available, as well as up-to-date theoretical approaches adopted by a selected panel of twelve international research teams. It covers a wide range of novel and advanced materials, exploring their structural, elastic, optical, mass and electronic transport properties. The cutting-edge techniques presented appeal to physicists, applied mathematicians and engineers interested in advanced simulation methods in materials science. The book can also be used as additional literature for undergraduate and postgraduate students with majors in physics, chemistry, applied mathematics and engineering.
Annual Reports in Computational Chemistry is a new periodical providing timely and critical reviews of important topics in computational chemistry as applied to all chemical disciplines. Topics covered include quantum chemistry, molecular mechanics, force fields, chemical education, and applications in academic and industrial settings. Each volume is organized into (thematic) sections with contributions written by experts. Focusing on the most recent literature and advances in the field, each article covers a specific topic of importance to computational chemists. Annual Reports in Computational Chemistry is a 'must' for researchers and students wishing to stay up-to-date on current developments in computational chemistry. * Broad coverage of computational chemistry and up-to-date information * The topics covered include quantum chemistry, molecular mechanics, force fields, chemical education, and applications in academic and industrial settings * Each chapter reviews the most recent literature on a specific topic of interest to computational chemists
Biomateriomics is the holistic study of biological material systems. While such systems are undoubtedly complex, we frequently encounter similar components -- universal building blocks and hierarchical structure motifs -- which result in a diverse set of functionalities. Similar to the way music or language arises from a limited set of music notes and words, we exploit the relationships between form and function in a meaningful way by recognizing the similarities between Beethoven and bone, or Shakespeare and silk. Through the investigation of material properties, examining fundamental links between processes, structures, and properties at multiple scales and their interactions, materiomics explains system functionality from the level of building blocks. Biomateriomics specifically focuses the analysis of the role of materials in the context of biological processes, the transfer of biological material principles towards biomimetic and bioinspired applications, and the study of interfaces between living

and non-living systems. The challenges of biological materials are vast, but the convergence of biology, mathematics and engineering as well as computational and experimental techniques have resulted in the toolset necessary to describe complex material systems, from nano to macro. Applying biomateriomics can unlock Nature's secret to high performance materials such as spider silk, bone, and nacre, and elucidate the progression and diagnosis or the treatment of diseases. Similarly, it contributes to develop a de novo understanding of biological material processes and to the potential of exploiting novel concepts in innovation, material synthesis and design.

This book presents a collection of papers presented at the 3rd World Congress on Integrated Computational Materials Engineering (ICME), a specialty conference organized by The Minerals, Metals & Materials Society (TMS). This meeting convened ICME stakeholders to examine topics relevant to the global advancement of ICME as an engineering discipline. The papers presented in these proceedings are divided into six sections: (1) ICME Applications; (2) ICME Building Blocks; (3) ICME Success Stories and Applications (4) Integration of ICME Building Blocks: Multi-scale Modeling; (5) Modeling, Data and Infrastructure Tools, and (6) Process Optimization. . These papers are intended to further the global implementation of ICME, broaden the variety of applications to which ICME is applied, and ultimately help industry design and produce new materials more efficiently and effectively.

A systematic discussion of the fundamental principles, written by a leading contributor to the field.

Computer simulations provide an essential set of tools for understanding the macroscopic properties of liquid crystals and of their phase transitions in terms of molecular models. While simulations of liquid crystals are based on the same general Monte Carlo and molecular dynamics techniques as are used for other fluids, they present a number of specific problems and peculiarities connected to the intrinsic properties of these mesophases. The field of computer simulations of anisotropic fluids is interdisciplinary and is evolving very rapidly. The present volume covers a variety of techniques and model systems, from lattices to hard particle and Gay-Berne to atomistic, for thermotropics, lyotropics, and some biologically interesting liquid crystals. Contributions are written by an excellent panel of international lecturers and provides a timely account of the techniques and problems in the field.

Molecular simulation allows researchers unique insight into the structures and interactions at play in fluids. Since publication of the first edition of Molecular Simulation of Fluids, novel developments in theory, algorithms and computer hardware have generated enormous growth in simulation capabilities. This 2nd edition has been fully updated and expanded to highlight this recent progress, encompassing both Monte Carlo and molecular dynamic techniques, and providing details of theory, algorithms and implementation. Beginning with a clear introduction and review of theoretical foundations, the book goes on to explore intermolecular potentials before discussing the calculation of molecular interactions in more detail. Monte Carlo simulation and integrators for molecular dynamics are then discussed further, followed by non-equilibrium molecular dynamics and molecular simulation of ensembles and phase equilibria. Finally, practical parallel algorithms, and molecular simulation and object-orientation

are reviewed. Drawing on the extensive experience of its expert author, Molecular Simulation of Fluids, 2nd Edition is a practical, accessible guide to this complex topic for all those currently using, or interested in using, molecular simulation to study fluids
A modern approach to mathematical modeling, featuring unique applications from the field of mechanics An Introduction to Mathematical Modeling: A Course in Mechanics is designed to survey the mathematical models that form the foundations of modern science and incorporates examples that illustrate how the most successful models arise from basic principles in modern and classical mathematical physics. Written by a world authority on mathematical theory and computational mechanics, the book presents an account of continuum mechanics, electromagnetic field theory, quantum mechanics, and statistical mechanics for readers with varied backgrounds in engineering, computer science, mathematics, and physics. The author streamlines a comprehensive understanding of the topic in three clearly organized sections: Nonlinear Continuum Mechanics introduces kinematics as well as force and stress in deformable bodies; mass and momentum; balance of linear and angular momentum; conservation of energy; and constitutive equations Electromagnetic Field Theory and Quantum Mechanics contains a brief account of electromagnetic wave theory and Maxwell's equations as well as an introductory account of quantum mechanics with related topics including ab initio methods and Spin and Pauli's principles Statistical Mechanics presents an introduction to statistical mechanics of systems in thermodynamic equilibrium as well as continuum mechanics, quantum mechanics, and molecular dynamics Each part of the book concludes with exercise sets that allow readers to test their understanding of the presented material. Key theorems and fundamental equations are highlighted throughout, and an extensive bibliography outlines resources for further study. Extensively class-tested to ensure an accessible presentation, An Introduction to Mathematical Modeling is an excellent book for courses on introductory mathematical modeling and statistical mechanics at the upper-undergraduate and graduate levels. The book also serves as a valuable reference for professionals working in the areas of modeling and simulation, physics, and computational engineering.
Despite the tremendous advances in the techniques and equipment for carrying out high-pressure crystallography, the application or exploration of the high-pressure variable in detailed structural studies remains rare. The chapters in this book provide a set of lecture notes and supplementary material for a course on high pressure crystallography. The material comprises state-of-the-art reviews of high-pressure experiments using X-ray and neutron diffraction techniques at synchrotron and neutron facilities and in the laboratory, as well as complementary experimental high-pressure techniques and theoretical methods for investigating matter at elevated pressures. The materials studies range from elemental solids and liquids to inorganic compounds, minerals, organic compounds, clathrates and pharmaceutical compounds, to large biological molecules such as proteins and viruses. The book provides a reference for workers in high-pressure science wishing to learn more about crystallography and for established crystallographers potentially interested in high pressure as a variable, as well as an introductory guide to new researchers in the field.
????:Principles of polymer processing

This book provides the reader with a solid understanding of the fundamental modeling of photovoltaic devices. After the material independent limit of photovoltaic conversion, the readers are introduced to the most well-known theory of "classical" silicon modeling. Based on this, for each of the most important PV materials, their performance under different conditions is modeled. This book also covers different modeling approaches, from very fundamental theoretic investigations to applied numeric simulations based on experimental values. The book concludes wth a chapter on the influence of spectral variations. The information is supported by providing the names of simulation software and basic literature to the field. The information in the book gives the user specific application with a solid background in hand, to judge which materials could be appropriate as well as realistic expectations of the performance the devices could achieve.

This book contains 99 of the papers that were presented at the 6th in the series of Symposia on Characterization of Porous Solids held in Alicante, Spain, May 2002. Written by leading international specialists in the subject, the contributions represent an up-to-date and authoritative account of recent developments around the world in the major methods used to characterize porous solids. The book is a useful work of reference for anyone interested in characterizing porous solids, such as MCM-41 mesoporous materials, pillared clays, etc. Papers on pore structure determination using gas adsorption feature strongly, together with papers on small angle scattering methods, mercury porosimetry, microcalorimetry, scanning probe microscopies, and image analysis.

A small army of physicists, chemists, mathematicians, and engineers has joined forces to attack a classic problem, the “reversibility paradox”, with modern tools. This book describes their work from the perspective of computer simulation, emphasizing the authors' approach to the problem of understanding the compatibility, and even inevitability, of the irreversible second law of thermodynamics with an underlying time-reversible mechanics. Computer simulation has made it possible to probe reversibility from a variety of directions and “chaos theory” or “nonlinear dynamics” has supplied a useful vocabulary and a set of concepts, which allow a fuller explanation of irreversibility than that available to Boltzmann or to Green, Kubo and Onsager. Clear illustration of concepts is emphasized throughout, and reinforced with a glossary of technical terms from the specialized fields which have been combined here to focus on a common theme. The book begins with a discussion, contrasting the idealized reversibility of basic physics against the pragmatic irreversibility of real life. Computer models, and simulation, are next discussed and illustrated. Simulations provide the means to assimilate concepts through worked-out examples. State-of-the-art analyses, from the point of view of dynamical systems, are applied to many-body examples from nonequilibrium molecular dynamics and to chaotic irreversible flows from finite-difference, finite-element, and particle-based continuum simulations. Two necessary concepts from dynamical-systems theory — fractals and Lyapunov instability — are fundamental to the approach. Undergraduate-level physics, calculus, and ordinary differential equations are sufficient background for a full appreciation of this book, which is intended for advanced undergraduates, graduates, and research workers. The generous assortment of examples worked out in the text will stimulate readers to explore the rich and fruitful field of study which links fundamental reversible laws of physics to the irreversibility surrounding us all. This expanded edition stresses and illustrates computer algorithms with many new worked-out

examples, and includes considerable new material on shockwaves, Lyapunov instability and fluctuations. Sample Chapter(s) Chapter 1: Time Reversibility, Computer Simulation, Algorithms, Chaos (1,908 KB) Contents:Time Reversibility, Computer Simulation, Algorithms, ChaosTime-Reversibility in Physics and ComputationGibbs' Statistical MechanicsIrreversibility in Real LifeMicroscopic Computer SimulationShockwaves RevisitedMacroscopic Computer SimulationChaos, Lyapunov Instability, FractalsResolving the Reversibility ParadoxAfterword — a Research Perspective Readership: Students of statistical physics and computer simulation. Keywords:Time Reversibility;Computer Simulation;Algorithms;ChaosKey Features:Provides comprehensive resource for simulation and analysis of classical equilibrium and nonequilibrium systems, both small and largeClear and thorough exposition of latest algorithms and techniques for research in simulationHands-on algorithms, clear analysis of recent developments, assessment of the state-of-the-artReviews: “Bill and Carol Hoover have teamed up to produce this greatly expanded new edition of Bill's earlier book grappling with one of the oldest problems in physics — reconciling the irreversibility of thermodynamics with the reversibility of Newtonian mechanics. It represents a personal account of a lifetime of research, including insights provided by advances in chaos, fractals, and computer simulation. It is the best source for anyone seeking a deep understanding of these seemingly paradoxical basic laws of physics.” Julien Clinton Sprott Emeritus Professor of Physics, University of Wisconsin – Madison Author of Chaos and Time-Series Analysis and Elegant Chaos “The second edition with over 100 pages of new material, gives an up-to-date and distinctive treatment of physical issues, emphasizing the need for a holistic view incorporating theory, simulation and experiment … It provides rich inspiration and insight for graduate students and more experienced researchers alike. This work challenges philosophers and mathematicians to engage with the latest numerical and experimental findings, and practitioners of quantum chaos and nanotechnology to incorporate and extend the underpinning classical irreversibility.” Dr Carl Dettmann University of Bristol “Many remarks and asides are very informative and will be of interest to a broad range of physicists. I was pleasantly surprised by the overall ambition, breadth and scope of this excellent book. ” Contemporary Physics Review of the First Edition: “The author has written a lively, informal, and somewhat personal review of a branch of statistical physics that he has helped develop over the past two decades or so.” Mathematical Reviews

This book represents the final reports of the scientific projects funded within the DFG-SPP1466 and, hence, provides the reader with the possibility to familiarize with the leading edge of VHCF research. It draws a balance on the existing knowledge and its enhancement by the joint research action of the priority program. Three different material classes are dealt with: structural metallic materials, long-fiber-reinforced polymers and materials used in micro-electro-mechanical systems. The project topics address the development of suitable experimental techniques for high-frequency testing and damage monitoring, the characterization of damage mechanisms and damage evolution, the development of mechanism-based models and the transfer of the obtained knowledge and understanding into engineering regulations and applications.

Volume Two of this two-volume sequence presents a comprehensive overview of protein structure prediction methods and includes protein threading, De novo methods, applications to membrane proteins and protein complexes, structure-based drug

design, as well as structure prediction as a systems problem. A series of appendices review the biological and chemical basics related to protein structure, computer science for structural informatics, and prerequisite mathematics and statistics.