Numerical Simulation In Molecular Dynamics Numerics Algorithms Parallelization Applications

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Time Reversability, Computer Simulation, Algorithms, Chaos - William Graham Hoover 2012
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.
Computational Chemistry. Computer Simulation Techniques - Edward Timoshenko 2021-05-06
We describe the important role of the in-silico methods in modern Chemistry and Physics of complex systems and overview the major techniques. The Born-Oppenheimer approximation for electronic configurations is introduced. Classical treatment of the motion of nuclei is then considered. Potential energy surfaces, force fields, geometry optimization and energy minimisation methods are discussed. The Newton’s equations of motion and their numerical integration methods are presented with the Euler and Verlet algorithms. Calculation of various observable averages is considered in Molecular Dynamics techniques in the NVE, NVT and NPT ensembles. Brownian stochastic Dynamics and the use of random numbers generators are introduced. Equilibrium simulations based on the Monte Carlo importance sampling methods and the Metropolis algorithm are discussed. The variational approach for the Schrödinger equation and various modern Quantum Chemistry methods for the electronic configurations of atomic and molecular systems are reviewed.
Numerical Modeling of Coupled Phenomena in Science and Engineering - Mario César Suárez Arriaga 2008-12-01
Mathematics is a universal language. Differential equations, mathematical modeling, numerical methods and computation form the underlying infrastructure of engineering and the sciences. In this context mathematical modeling is a very powerful tool for studying engineering problems, natural systems and human society. This interdisciplinary book cont
Computational Nanoscience - Kálmán Varga 2011-04-14
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.
Foundations of Nanotechnology - Three Volume Set - A. K. Haghi 2015-05-30
Nanoscale science, engineering, and technology—commonly referred to collectively as nanotechnology—is believed by many to offer extraordinary economic and societal benefits. Nanotechnology is generally defined as the ability to create and use materials, devices, and systems with unique properties at the scale of approximately 1 to 100 nm. Nanotechnology offers society the promise of major benefits, but also raises questions of potential adverse effects. The first volume covers pore size in carbon-based nano-adsorbents, resulting in materials that exhibit unique sorptive properties with a general view of the recent activities on the study of pore structure control. The collection of topics in volume 2 reflects the diversity of recent advances in nanoelements formation and interactions in nanosystems with a broad perspective that will be useful for scientists and engineers as the use of nanotechnology in the consumer and industrial sectors is expected to increase significantly in the future. And the third volume discusses important issues and trends related to research strategy in mechanics of carbon nanotubes.
Foundations of Nanotechnology, Volume Two - Sabu Thomas 2014-10-24
The collection of topics in this book reflects the diversity of recent advances in nanoelements formation and interactions in nanosystems with a broad perspective that is useful for scientists as well as for graduate students and engineers. One of the main tasks in making nanocomposites is building the dependence of the structure and shape of the nanoelements, forming the basis for the composite of their sizes. This is because with an increase or a decrease in the specific size of nanoelements, their physical–mechanical properties such as the coefficient of elasticity, strength, and deformation parameter, vary by over one order. The calculations show that this is primarily due to a significant rearrangement of the atomic structure and the shape of the nanoelement. The investigation of the above parameters of the nanoelements is technically complicated and laborious because of their small sizes. When the characteristics of powder nanocomposites are calculated, it is also very important to take into account the interaction of the nanoelements since the changes in their original shapes and sizes in the interaction process and during the formation of the nanocomposite can lead to a significant change in its properties and a cardinal structural rearrangement. In addition, the studies show the appearance of the processes of the ordering and self-assembling leading to a more organized form of a nanosystem. The above phenomena play an important role in nanotechnological processes. They allow nanotechnologies to be developed for the formation of nanostructures by the self-assembling method (which is based on self-organizing processes) and building up complex spatial nanostructures consisting of different nanoelements. The study of the above dependences based on the mathematical modeling methods requires the solution of the aforementioned problem at the atomic level. This requires large computational aids and computational time, which makes the development of economical calculation methods urgent. The objective of this volume is the development of such a technique in various nanosystems.
Computational Materials Science - Kaoru Ohno 2018-04-14
This textbook introduces modern techniques based on computer simulation to study materials science. It starts from first principles calculations enabling to calculate the physical and chemical properties by solving a many-body Schroedinger equation with Coulomb forces. For the exchange-correlation term, the local density approximation is usually applied. After the introduction of the first principles treatment, tight-binding and classical potential methods are briefly introduced to indicate how one can increase the number of atoms in the system. In the second

half of the book, Monte Carlo simulation is discussed in detail. Problems and solutions are provided to facilitate understanding. Readers will gain sufficient knowledge to begin theoretical studies in modern materials research. This second edition includes a lot of recent theoretical techniques in materials research. With the computers power now available, it is possible to use these numerical techniques to study various physical and chemical properties of complex materials from first principles. The new edition also covers empirical methods, such as tight-binding and molecular dynamics.

Parallel Processing and Applied Mathematics - Roman Wyrzykowski 2012-07-03

This two-volume-set (LNCS 7203 and 7204) constitutes the refereed proceedings of the 9th International Conference on Parallel Processing and Applied Mathematics, PPAM 2011, held in Torun, Poland, in September 2011. The 130 revised full papers presented in both volumes were carefully reviewed and selected from numerous submissions. The papers address issues such as parallel/distributed architectures and mobile computing; numerical algorithms and parallel numerics; parallel non-numerical algorithms; tools and environments for parallel/distributed/grid computing; applications of parallel/distributed computing; applied mathematics, neural networks and evolutionary computing; history of computing.

Multiscale Modelling and Optimisation of Materials and Structures - Tadeusz Burczynski 2022-05-19

Addresses the very topical, crucial and original subject of parameter identification and optimization within multiscale modeling methods Multiscale Modelling and Optimization of Materials and Structures presents an important and challenging area of research that enables the design of new materials and structures with better quality, strength and performance parameters as well as the creation of reliable models that take into account structural, material and topological properties at different scales. The authors' approach is four-fold; 1) the basic principles of micro and nano scale modeling techniques; 2) the connection of micro and/or nano scale models with macro simulation software; 3) optimization development in the framework of multiscale engineering and the solution of identification problems; 4) the computer science techniques used in this model and advice for scientists interested in developing their own models and software for multiscale analysis and optimization. The authors present several approaches such as the bridging and homogenization methods, as well as the general formulation of complex optimization and identification problems in multiscale modelling. They apply global optimization algorithms based on robust bioinspired algorithms, proposing parallel and multi-subpopulation approaches in order to speed-up computations, and discuss several numerical examples of multiscale modeling, optimization and identification of composite and functionally graded engineering materials and bone tissues. Multiscale Modelling and Optimization of Materials and Structures is thereby a valuable source of information for young scientists and students looking to develop their own models, write their own computer programs and implement them into simulation systems. Describes micro and nano scale models developed by the authors along with case studies of analysis and optimization Discusses the problems of computing costs, efficiency of information transfer, effective use of the computer memory and several other aspects of development of multiscale models Includes real physical, chemical and experimental studies with modern experimental techniques Provides a valuable source of information for young scientists and students looking to develop their own models, write their own computer programs, and implement them into simulation systems.

Wavelets in Numerical Simulation - Karsten Urban 2012-12-06

Sapere aude! Immanuel Kant (1724-1804) Numerical simulations playa key role in many areas of modern science and technology. They are necessary in particular when experiments for the underlying problem are too dangerous, too expensive or not even possible. The latter situation appears for example when relevant length scales are below the observation level. Moreover, numerical simulations are needed to control complex processes and systems. In all these cases the relevant problems may become highly complex. Hence the following issues are of vital importance for a numerical simulation: - Efficiency of the numerical solvers: Efficient and fast numerical schemes are the basis for a simulation of 'real world' problems. This becomes even more important for realtime problems where the runtime of the numerical simulation has to be of the order of the time span required by the simulated process. Without efficient solution methods the simulation of many problems is not feasible. 'Efficient' means here that the overall cost of the numerical scheme remains proportional to the degrees of freedom, i. e. , the numerical approximation is determined in linear time when the problem size grows e. g. to upgrade accuracy. Of course, as soon as the solution of large systems of equations is involved this requirement is very demanding.

Error Control and Adaptivity in Scientific Computing - Haydar Bulgak 2012-12-06

One of the main ways by which we can understand complex processes is to create computerised numerical simulation models of them. Modern simulation tools are not used only by experts, however, and reliability has therefore become an important issue, meaning that it is not sufficient for a simulation package merely to print out some numbers, claiming them to be the desired results. An estimate of the associated error is also needed. The errors may derive from many sources: errors in the model, errors in discretization, rounding errors, etc. Unfortunately, this situation does not obtain for current packages and there is a great deal of room for improvement. Only if the error can be estimated is it possible to do something to reduce it. The contributions in this book cover many aspects of the subject, the main topics being error estimates and error control in numerical linear algebra algorithms (closely related to the concept of condition numbers), interval arithmetic and adaptivity for continuous models.

Numerical Simulation in Molecular Dynamics - Michael Griebel 2007-08-16

This book details the necessary numerical methods, the theoretical background and foundations and the techniques involved in creating computer particle models, including linked-cell method, SPME-method, tree codes, amd multipol technique. It illustrates modeling, discretization, algorithms and their parallel implementation with MPI on computer systems with distributed memory. The text offers step-by-step explanations of numerical simulation, providing illustrative code examples. With the description of the algorithms and the presentation of the results of various simulations from fields such as material science, nanotechnology, biochemistry and astrophysics, the reader of this book will learn how to write programs capable of running successful experiments for molecular dynamics.

Handbook of Collective Robotics - Serge Kernbach 2013-05-29

This book is devoted to mechatronic, chemical, bacteriological, biological, and hybrid systems, utilizing cooperative, networked, swarm, self-organizing, evolutionary and bio-inspired design principles and targeting underwater, ground, air, and space applications. It addresses issues such as open-ended evolution, self-replication, self-development, reliability, scalability, energy foraging, adaptivity, and artificial sociality. The book has been prepared by 52 authors from world-leading research groups in 14 countries. This book covers not only current but also future key technologies and is aimed at anyone who is interested in learning more about collective robotics and how it might affect our society.

Parallel Computing Technologies - Victor Malyshkin 2009-08-04

This book constitutes the proceedings of the 10th International Conference on Parallel Computing Technologies, PaCT 2009, held in Novosibirsk, Russia on August 31-September 4, 2009. The 34 full papers presented together with 2 invited papers and 7 poster papers were carefully reviewed and selected from 72 submissions. The papers are organized in topical sections on models of parallel computing, methods and algorithms, fine-grained parallelism, parallel programming tools and support, and applications.

Supercomputing for Molecular Dynamics Simulations - Alexander Heinecke 2015-03-30

This work presents modern implementations of relevant molecular dynamics algorithms using ls1 mardyn, a simulation program for engineering applications. The text focuses strictly on HPC-related aspects, covering implementation on HPC architectures, taking Intel Xeon and Intel Xeon Phi clusters as representatives of current platforms. The work describes distributed and shared-memory parallelization on these platforms, including load balancing, with a particular focus on the efficient implementation of the compute kernels. The text also discusses the software-architecture of the resulting code.

Computer Simulations of Surfaces and Interfaces - Burkhard Dünweg 2013-03-07

Studies of surfaces and interactions between dissimilar materials or phases are vital for modern technological applications. Computer simulation methods are indispensable in such studies and this book contains a substantial body of knowledge about simulation methods as well as the theoretical background for performing computer experiments and analyzing the data. The book is self-contained, covering a range of

topics from classical statistical mechanics to a variety of simulation techniques, including molecular dynamics, Langevin dynamics and Monte Carlo methods. A number of physical systems are considered, including fluids, magnets, polymers, granular media, and driven diffusive systems. The computer simulation methods considered include both standard and accelerated versions. The simulation methods are clearly related to the fundamental principles of thermodynamics and statistical mechanics.

Route Choice Modelling and Runtime Optimisation for Simulation of Building Evacuation - Armel Ulrich Kemloh Wagoum 2013

Advanced Computational Methods for Knowledge Engineering - Ngoc Thanh Nguyen 2013-03-22

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.

Computer Simulation of Liquids - M. P. Allen 2017

A first in its field, this book is both an introduction to computer simulation of liquids for upper level undergraduates and a how-to guide for specialists. The authors discuss the latest simulation techniques of molecular dynamics and the Monte Carlo methods as well as how to avoid common programming pitfalls. Theoretical concepts and practical programming advice are amply reinforced with examples of computer simulation in action and samples of Fortran code. The authors have also included a wide selection of programs and routines on microfiche to aid chemists, physicists, chemical engineers, and computer scientists, as well as graduate and advanced students in chemistry.

Dynamics of Engineered Artificial Membranes and Biosensors - William Hoiles 2018-05-03

Learn about the state of the art in building artificial membranes and synthetic biological devices, and in constructing mathematical models for their dynamics at multiple time and spatial scales with this comprehensive book. Drawing on recent advances in bioengineering and biochemistry, it describes how to engineer tethered bilayer lipid membranes, bioelectronic interfaces, high-resolution biosensors, and diagnostic devices for non-invasive cellular measurements and electroporation. Multi-physics models combining atomistic (molecular dynamics and coarse-grained molecular dynamics), mesoscopic (Poisson–Nernst–Planck), and macroscopic (reaction-rate theory) dynamics provide a complete structure-to-function description of these devices. Experiments and dynamic models explain how anti-microbial peptides penetrate membranes, how molecular machine biosensors built out of artificial membranes can detect femtomolar concentrations, and how electroporation can be controlled. Supported by atomistic simulation code online, this is essential reading for researchers, students and professionals in bioengineering, chemical engineering, biophysics, applied mathematics, and electrical engineering.

Fundamentals of Friction and Wear on the Nanoscale - Enrico Gnecco 2014-11-05

This book provides an updated review on the development of scanning probe microscopy and related techniques, and the availability of computational techniques not even imaginable a few decades ago. The 36 chapters cover instrumental aspects, theoretical models and selected experimental results, thus offering a broad panoramic view on fundamental issues in nanotribology which are currently being investigated. Compared to the first edition, several topics have been added, including triboluminescence, graphene mechanics, friction and wear in liquid environments, capillary condensation, and multiscale friction modeling. Particular care has been taken to avoid overlaps and guarantee the independence of the chapters. In this way, our book aims to become a key reference on this subject for the next five to ten years to come.

Practical Guide to Computer Simulations - Alexander K. Hartmann 2009

This book presents all the computational techniques and tools needed to start doing scientific research using computer simulations. After working through this book, the reader will possess the necessary basic background knowledge, from program design, programming in C, fundamental algorithms and data structures, random numbers, and debugging, all the way to data analysis, presentation and publishing. In each of these fields, no preliminary knowledge is assumed. The reader will be equipped to successfully perform complete projects from the first idea until the final publication. All techniques are explained using many examples in C; these C codes, as well as the solutions to exercises, are readily available in the accompanying CD-ROM. The techniques in this book are independent of the fields of research, and hence they are suitable for conducting research projects in physics, chemistry, computer science, biology and engineering. This also means that no problem-dependent algorithms are introduced; therefore, this book does NOT explain molecular dynamics, Monte Carlo, finite elements and other special-purpose techniques, which would be beyond the scope of a general-purpose book. There has been no similar comprehensive book written so far. Currently, one needs many different books to learn all the necessary elements. With this book, however, one basically needs only a second book on field-specific algorithms in order to be fully equipped to perform computer simulations research.

Physics and Chemistry of Classical Materials - Ewa Klodzinska 2014-11-21

This book provides a comprehensive presentation of the concepts, properties, and applications of classical materials. It also provides the first unified treatment for the broad subject of classical materials. The authors use a fundamental approach to define the structure and properties of a wide range of solids on the basis of the local chemical bonding and atomic order present in the material. Emphasizing the physical and chemical origins of different material properties, this important volume focuses on the most technologically important materials being utilized and developed by scientists and engineers. This new book: • Provides a collection of chapters that highlight some important areas of current interest in polymer products and chemical processes •Focuses on topics with more advanced methods • Emphasizes precise mathematical development and actual experimental details • Analyzes theories to formulate and prove the physicochemical principles • Provides an up-to-date and thorough exposition of the present state of the art of complex materials • Familiarizes the reader with new aspects of the techniques used in the examination of polymers, including chemical, physicochemical, and purely physical methods of examination • Describes the types of techniques now available to the chemist and technician and discusses their capabilities, limitations, and applications This book presents peer-reviewed chapters and survey articles on review, research, and development in the fields of classical materials. The wide coverage makes this book an excellent reference book for researchers and graduate students on the subject. The new topics covered in this book will be an excellent resource for industries and academic researchers as well.

Basic Concepts in Computational Physics - Benjamin A. Stickler 2016-03-21

This new edition is a concise introduction to the basic methods of computational physics. Readers will discover the benefits of numerical methods for solving complex mathematical problems and for the direct simulation of physical processes. The book is divided into two main parts: Deterministic methods and stochastic methods in computational physics. Based on concrete problems, the first part discusses numerical differentiation and integration, as well as the treatment of ordinary differential equations. This is extended by a brief introduction to the numerics of partial differential equations. The second part deals with the generation of random numbers, summarizes the basics of stochastics, and subsequently introduces Monte-Carlo (MC) methods. Specific emphasis is on MARKOV chain MC algorithms. The final two chapters discuss data analysis and stochastic optimization. All this is again motivated and augmented by applications from physics. In addition, the book offers a number of appendices to provide the reader with information on topics not discussed in the main text. Numerous problems with worked-out solutions, chapter introductions and summaries, together with a clear and application-oriented style support the reader. Ready to use C++ codes are provided online.

Computational Granular Dynamics - Thorsten Pöschel 2005-12-06

Computer simulations not only belong to the most important methods for the theoretical investigation of granular materials, but provide the tools that have enabled much of the expanding research by physicists and engineers. The present book is intended to serve as an introduction to the application of numerical methods to systems of granular particles. Accordingly emphasis is on a general understanding of the subject rather

than on the presentation of latest advances in numerical algorithms. Although a basic knowledge of C++ is needed for the understanding of the numerical methods and algorithms in the book, it avoids usage of elegant but complicated algorithms to remain accessible for those who prefer to use a different programming language. While the book focuses more on models than on the physics of granular material, many applications to real systems are presented.

Parallel Algorithms in Computational Science - Dieter Heermann 1991-02-12

Mathematics of Computing -- Parallelism.

Advanced Machining Processes - Angelos P. Markopoulos 2017-11-23

Modeling and machining are two terms closely related. The benefits of the application of modeling on machining are well known. The advances in technology call for the use of more sophisticated machining methods for the production of high-end components. In turn, more complex, more suitable, and reliable modeling methods are required. This book pertains to machining and modeling, but focuses on the special aspects of both. Many researchers in academia and industry, who are looking for ways to refine their work, make it more detailed, increase their accuracy and reliability, or implement new features, will gain access to knowledge in this book that is very scare to find elsewhere.

Atomistic Simulation Methods in Solid Mechanics - Zhiping Xu 2018-07-01

Many exciting problems in mechanics are multiscale in nature. For example, the failure of materials involves breaking of chemical bonds at the atomic scale and crack spreading at larger scales. Mechanics of the cell as a material is defined by the cytoskeleton networks and membrane, as built up from proteins and lipids at the molecular level. To solve these problems, one must be equipped with techniques that are able to address the multiphysics nature at different space and time scales and successfully bridging them. Recently, rapid progresses in micro-, nanomechanics and mechanics of biological materials urges the development of theoretical models and numerical techniques within this scenario. The goal of this book is to bring a pedestrian introduction and in-depth discussion on the key ideas and challenges. In this book, we aim to present the developing field of atomistic simulation methods and their applications in solid mechanics, in a self-contained way. The first part (the algorithm) will cover basics in quantum, classical and statistical mechanics knowledge, also basic concepts and physics of solid mechanics. With this background, the algorithm of molecular dynamics and relative methods such as Monte-Carlo methods are introduced as well. The second part of the book focuses on a number of hot topics in the current mechanics community, from failure of materials, nanomechanics, to mechanics of biological materials. In the third part, extended discussion on novel methods for solving multiscale solid mechanics problems are introduced. Some of them are fresh and still under development at the time the manuscript is prepared and are believed by the authors to be the future direction in this field. The book addresses theoretical issues, and detailed numeric algorithms as well. The readers are assumed to have basic knowledge in engineering mechanics and college physics. Some experience with physical chemistry or solid-state physics will be helpful. Illustrative examples and problems are prepared after many chapters for self-study purposes.

Stochastic Numerics for Mathematical Physics - Grigori N. Milstein 2021-12-03

This book is a substantially revised and expanded edition reflecting major developments in stochastic numerics since the first edition was published in 2004. The new topics, in particular, include mean-square and weak approximations in the case of nonglobally Lipschitz coefficients of Stochastic Differential Equations (SDEs) including the concept of rejecting trajectories; conditional probabilistic representations and their application to practical variance reduction using regression methods; multi-level Monte Carlo method; computing ergodic limits and additional classes of geometric integrators used in molecular dynamics; numerical methods for FBSDEs; approximation of parabolic SPDEs and nonlinear filtering problem based on the method of characteristics. SDEs have many applications in the natural sciences and in finance. Besides, the employment of probabilistic representations together with the Monte Carlo technique allows us to reduce the solution of multi-dimensional problems for partial differential equations to the integration of stochastic equations. This approach leads to powerful computational mathematics that is presented in the treatise. Many special schemes for SDEs are presented. In the second part of the book numerical methods for solving complicated problems for partial differential equations occurring in practical applications, both linear and nonlinear, are constructed. All the methods are presented with proofs and hence founded on rigorous reasoning, thus giving the book textbook potential. An overwhelming majority of the methods are accompanied by the corresponding numerical algorithms which are ready for implementation in practice. The book addresses researchers and graduate students in numerical analysis, applied probability, physics, chemistry, and engineering as well as mathematical biology and financial mathematics.

Multiscale Molecular Methods in Applied Chemistry - Barbara Kirchner 2012-01-25

First-Principles-Based Multiscale, Multiparadigm Molecular Mechanics and Dynamics Methods for Describing Complex Chemical Processes, by A. Jaramillo-Botero, R. Nielsen, R. Abrol, J. Su, T. Pascal, J. Mueller and W. A. Goddard.- Dynamic QM/MM: A Hybrid Approach to Simulating Gas–Liquid Interactions, by S. Yockel and G. C. Schatz.- Multiscale Modelling in Computational Heterogeneous Catalysis, by F. J. Keil.- Real-World Predictions from Ab Initio Molecular Dynamics Simulations, by B. Kirchner, P. J. di Dio and J. Hutter.- Nanoscale Wetting Under Electric Field from Molecular Simulations, by C. D. Daub, D. Bratko and A. Luzar.- Molecular Simulations of Retention in Chromatographic Systems: Use of Biased Monte Carlo Techniques to Access Multiple Time and Length Scales, by J. L. Rafferty, J. I. Siepmann, M. R. Schure.- Thermodynamic Properties for Applications in Chemical Industry via Classical Force Fields, by G. Guevara-Carrion, H. Hasse and J. Vrabec.- Multiscale Approaches and Perspectives to Modeling Aqueous Electrolytes and Polyelectrolytes, by L. Delle Site, C. Holm and N. F. A. van der Vegt.- Coarse-Grained Modeling for Macromolecular Chemistry, by H. A. Karimi-Varzaneh and F. Müller-Plathe.-

Rock Characterisation, Modelling and Engineering Design Methods - Xia-Ting Feng 2013-05-17

Rock Characterisation, Modelling and Engineering Design Methods contains the contributions presented at the 3rd ISRM SINOROCK Symposium (Shanghai, China, 1820 June 2013). The papers contribute to the further development of the overall rock engineering design process through the sequential linkage of the three themes of rock characterisation, model

Quantum Transport Calculations for Nanosystems - Kenji Hirose 2014-04-11

As electric devices become smaller and smaller, transport simulations based on the quantum mechanics become more and more important. There are currently numerous textbooks on the basic concepts of quantum transport, but few present calculation methods in detail. This book provides various quantum transport simulation methods and shows applications for transport properties of nanometer-scale systems. It starts with a short review of quantum transport, followed by various calculation methods based on scattering approaches, non-equilibrium Green’s function (NEGF), master equation, and time-dependent wave-packet diffusion (TD-WPD). With these tools, transport properties of various nanosystems are then explored.

Recent Advances in Computational and Experimental Mechanics, Vol—I - D. Maity 2022-01-01

This book (Vol. - I) presents select proceedings of the first Online International Conference on Recent Advances in Computational and Experimental Mechanics (ICRACEM 2020) and focuses on theoretical, computational and experimental aspects of solid and fluid mechanics. Various topics covered are computational modelling of extreme events; mechanical modelling of robots; mechanics and design of cellular materials; mechanics of soft materials; mechanics of thin-film and multi-layer structures; meshfree and particle based formulations in continuum mechanics; multi-scale computations in solid mechanics, and materials; multiscale mechanics of brittle and ductile materials; topology and shape optimization techniques; acoustics including aero-acoustics and wave propagation; aerodynamics; dynamics and control in micro/nano engineering; dynamic instability and buckling; flow-induced noise and vibration; inverse problems in mechanics and system identification; measurement and analysis techniques in nonlinear dynamic systems; multibody dynamical systems and applications; nonlinear dynamics and control; stochastic mechanics; structural dynamics and earthquake engineering; structural health monitoring and damage assessment; turbomachinery noise; vibrations of continuous systems, characterization of advanced materials; damage identification and non-destructive evaluation; experimental fire mechanics and damage; experimental fluid mechanics; experimental solid mechanics; measurement in extreme environments; modal testing and dynamics; experimental hydraulics; mechanism of scour under steady and unsteady flows; vibration measurement and control; bio-inspired materials; constitutive modelling

of materials; fracture mechanics; mechanics of adhesion, tribology and wear; mechanics of composite materials; mechanics of multifunctional materials; multiscale modelling of materials; phase transformations in materials; plasticity and creep in materials; fluid mechanics, computational fluid dynamics; fluid-structure interaction; free surface, moving boundary and pipe flow; hydrodynamics; multiphase flows; propulsion; internal flow physics; turbulence modelling; wave mechanics; flow through porous media; shock-boundary layer interactions; sediment transport; wave-structure interaction; reduced-order models; turbo-machinery; experimental hydraulics; mechanism of scour under steady and unsteady flows; applications of machine learning and artificial intelligence in mechanics; transport phenomena and soft computing tools in fluid mechanics. The contents of these two volumes (Volumes I and II) discusses various attributes of modern-age mechanics in various disciplines, such as aerospace, civil, mechanical, ocean engineering and naval architecture. The book will be a valuable reference for beginners, researchers, and professionals interested in solid and fluid mechanics and allied fields.

Computational Multiscale Modeling of Fluids and Solids - Martin Oliver Steinhauser 2007-10-28

Devastatingly simple, yet hugely effective, the concept of this timely text is to provide a comprehensive overview of computational physics methods and techniques used for materials modeling on different length and time scales. Each chapter first provides an overview of the physical basic 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.

Parallel Computing - Roman Trobec 2009-06-18

The use of parallel programming and architectures is essential for simulating and solving problems in modern computational practice. There has been rapid progress in microprocessor architecture, interconnection technology and software devel- ment, which are in?uencing directly the rapid growth of parallel and distributed computing. However, in order to make these bene?ts usable in practice, this dev- opment must be accompanied by progress in the design, analysis and application aspects of parallel algorithms. In particular, new approaches from parallel num- ics are important for solving complex computational problems on parallel and/or distributed systems. The contributions to this book are focused on topics most concerned in the trends of today’s parallel computing. These range from parallel algorithmics, progr- ming, tools, network computing to future parallel computing. Particular attention is paid to parallel numerics: linear algebra, differential equations, numerical integ- tion, number theory and their applications in computer simulations, which together form the kernel of the monograph. We expect that the book will be of interest to scientists working on parallel computing, doctoral students, teachers, engineers and mathematicians dealing with numerical applications and computer simulations of natural phenomena.

Scientific Computing and Algorithms in Industrial Simulations - Michael Griebel 2017-10-30

The contributions gathered here provide an overview of current research projects and selected software products of the Fraunhofer Institute for Algorithms and Scientific Computing SCAI. They show the wide range of challenges that scientific computing currently faces, the solutions it offers, and its important role in developing applications for industry. Given the exciting field of applied collaborative research and development it discusses, the book will appeal to scientists, practitioners, and students alike. The Fraunhofer Institute for Algorithms and Scientific Computing SCAI combines excellent research and application-oriented development to provide added value for our partners. SCAI develops numerical techniques, parallel algorithms and specialized software tools to support and optimize industrial simulations. Moreover, it implements custom software solutions for production and logistics, and offers calculations on high-performance computers. Its services and products are based on state-of-the-art methods from applied mathematics and information technology.

Computer Simulation of Liquids - M. P. Allen 1989

Computer simulation is an essential tool in studying the chemistry and physics of liquids. Simulations allow us to develop models and to test them against experimental data. This book is an introduction and practical guide to the molecular dynamics and Monte Carlo methods.

Computer Simulation in Physics and Engineering - Martin Oliver Steinhauser 2013-01-01

This work is a needed reference for widely used techniques and methods of computer simulation in physics and other disciplines, such as materials science. The work conveys both: the theoretical foundations of computer simulation as well as applications and "tricks of the trade", that often are scattered across various papers. Thus it will meet a need and fill a gap for every scientist who needs computer simulations for his/her task at hand. In addition to being a reference, case studies and exercises for use as course reading are included.

Euro-Par 2015: Parallel Processing Workshops - Sascha Hunold 2015-12-17

This book constitutes the thoroughly refereed post-conference proceedings of 12 workshops held at the 21st International Conference on Parallel and Distributed Computing, Euro-Par 2015, in Vienna, Austria, in August 2015. The 67 revised full papers presented were carefully reviewed and selected from 121 submissions. The volume includes papers from the following workshops: BigDataCloud: 4th Workshop on Big Data Management in Clouds - Euro-EDUPAR: First European Workshop on Parallel and Distributed Computing Education for Undergraduate Students - Hetero Par: 13th International Workshop on Algorithms, Models and Tools for Parallel Computing on Heterogeneous Platforms - LSDVE: Third Workshop on Large Scale Distributed Virtual Environments - OMHI: 4th International Workshop on On-chip Memory Hierarchies and Interconnects - PADAPS: Third Workshop on Parallel and Distributed Agent-Based Simulations - PELGA: Workshop on Performance Engineering for Large-Scale Graph Analytics - REPPAR: Second International Workshop on Reproducibility in Parallel Computing - Resilience: 8th Workshop on Resiliency in High Performance Computing in Clusters, Clouds, and Grids - ROME: Third Workshop on Runtime and Operating Systems for the Many Core Era - UCHPC: 8th Workshop on UnConventional High Performance Computing - and VHPC: 10th Workshop on Virtualization in High-Performance Cloud Computing.

Physical-Chemical Mechanics of Disperse Systems and Materials - Eugene D. Shchukin 2015-12-02

Physical–Chemical Mechanics of Disperse Systems and Materials is a novel interdisciplinary area in the science of the disperse state of matter. It covers the broad spectrum of objects and systems with dimensions ranging from nanometers to millimeters and establishes a fundamental basis for controlling and tuning the properties of these systems as well as the processes taking place in them. Physical–chemical mechanics focuses on the analysis of the complex physical–chemical interfacial phenomena taking place both in the transition of a dispersed system into a material, such as in the course of pressing, sintering, hydration hardening, and sol-gel transitions, and in the course of the dispersion of bulk materials taking place in milling, mechanical treatment, friction and wear, and fracturing. These studies are based on thorough experimental investigation of contact interactions between particles in these processes. The book is divided into two sections. The first section covers basic principles of the formation, stability and rupture of contacts between particles in different media and in surfactant solutions, as well as the properties of coagulation structures and their rheology. The second section covers surface phenomena taking place in solid-like structures with phase contacts and in compact bodies with an emphasis on several applications and processes as well as the special role of the Rehbinder effect. Where appropriate and relevant, the book presents essays on specific significant and principal studies, such as the damageability of crystal and glass surfaces, the strength of industrial catalysts, the nano-mechanisms of cement hardening, the role of the structure-mechanical barrier in the stabilization of fluorinated systems, and contact interactions in papermaking. It also devotes attention to experimental methods used in physical–chemical mechanics, the direct measurement of contact strength, and relevant instrumentations. The book utilizes the content used over many years in lecture courses and includes fundamental material on colloid and surface chemistry, the strength of materials, rheology, and tensors, which makes it well suited for novices and experts in the field.