



Atomistic Computer Simulations A Practical Guide

Vladimir I. Nekorkin



Atomistic Computer Simulations A Practical Guide:

Atomistic Computer Simulations Veronika Brázdová, David R. Bowler, 2013-04-16 Many books explain the theory of atomistic computer simulations this book teaches you how to run them This introductory how to title enables readers to understand plan run and analyze their own independent atomistic simulations and decide which method to use and which questions to ask in their research project It is written in a clear and precise language focusing on a thorough understanding of the concepts behind the equations and how these are used in the simulations As a result readers will learn how to design the computational model and which parameters of the simulations are essential as well as being able to assess whether the results are correct find and correct errors and extract the relevant information from the results Finally they will know which information needs to be included in their publications This book includes checklists for planning projects analyzing output files and for troubleshooting as well as pseudo keywords and case studies The authors provide an accompanying blog for the book with worked examples and additional material and references <http://www.atomisticsimulations.org> *Atomistic Computer Simulations* Veronika Brázdová, David R. Bowler, 2013-04-16 Many books explain the theory of atomistic computer simulations this book teaches you how to run them This introductory how to title enables readers to understand plan run and analyze their own independent atomistic simulations and decide which method to use and which questions to ask in their research project It is written in a clear and precise language focusing on a thorough understanding of the concepts behind the equations and how these are used in the simulations As a result readers will learn how to design the computational model and which parameters of the simulations are essential as well as being able to assess whether the results are correct find and correct errors and extract the relevant information from the results Finally they will know which information needs to be included in their publications This book includes checklists for planning projects analyzing output files and for troubleshooting as well as pseudo keywords and case studies The authors provide an accompanying blog for the book with worked examples and additional material and references <http://www.atomisticsimulations.org> *Big Practical Guide To Computer Simulations (2nd Edition)* Alexander K Hartmann, 2015-01-29 This book teaches you all necessary problem independent tools and techniques needed to implement and perform sophisticated scientific numerical simulations Thus it is suited for undergraduate and graduate students who want to become experts in computer simulations in Physics Chemistry Biology Engineering Computer Science and other fields **Modeling Biomaterials** Josef Málek, Endre Süli, 2022-01-21 The investigation of the role of mechanical and mechano chemical interactions in cellular processes and tissue development is a rapidly growing research field in the life sciences and in biomedical engineering Quantitative understanding of this important area in the study of biological systems requires the development of adequate mathematical models for the simulation of the evolution of these systems in space and time Since expertise in various fields is necessary this calls for a multidisciplinary approach This edited volume connects basic physical biological and physiological concepts to methods for the mathematical

modeling of various materials by pursuing a multiscale approach from subcellular to organ and system level Written by active researchers each chapter provides a detailed introduction to a given field illustrates various approaches to creating models and explores recent advances and future research perspectives Topics covered include molecular dynamics simulations of lipid membranes phenomenological continuum mechanics of tissue growth and translational cardiovascular modeling Modeling Biomaterials will be a valuable resource for both non specialists and experienced researchers from various domains of science such as applied mathematics biophysics computational physiology and medicine

Multiscale Modeling for Process Safety Applications Arnab Chakrabarty, Sam Mannan, Tahir Cagin, 2015-11-29 Multiscale Modeling for Process Safety Applications is a new reference demonstrating the implementation of multiscale modeling techniques on process safety applications It is a valuable resource for readers interested in theoretical simulations and or computer simulations of hazardous scenarios As multi scale modeling is a computational technique for solving problems involving multiple scales such as how a flammable vapor cloud might behave if ignited this book provides information on the fundamental topics of toxic fire and air explosion modeling as well as modeling jet and pool fires using computational fluid dynamics The book goes on to cover nanomaterial toxicity QPSR analysis on relation of chemical structure to flash point molecular structure and burning velocity first principle studies of reactive chemicals water and air reactive chemicals and dust explosions Chemical and process safety professionals as well as faculty and graduate researchers will benefit from the detailed coverage provided in this book Provides the only comprehensive source addressing the use of multiscale modeling in the context of process safety Bridges multiscale modeling with process safety enabling the reader to understand mapping between problem detail and effective usage of resources Presents an overall picture of addressing safety problems in all levels of modeling and the latest approaches to each in the field Features worked out examples case studies and a question bank to aid understanding and involvement for the reader

Large-Scale Quantum-Mechanical Enzymology Greg Lever, 2015-06-06 This work establishes linear scaling density functional theory DFT as a powerful tool for understanding enzyme catalysis one that can complement quantum mechanics molecular mechanics QM MM and molecular dynamics simulations The thesis reviews benchmark studies demonstrating techniques capable of simulating entire enzymes at the ab initio quantum mechanical level of accuracy DFT has transformed the physical sciences by allowing researchers to perform parameter free quantum mechanical calculations to predict a broad range of physical and chemical properties of materials In principle similar methods could be applied to biological problems However even the simplest biological systems contain many thousands of atoms and are characterized by extremely complex configuration spaces associated with a vast number of degrees of freedom The development of linear scaling density functional codes makes biological molecules accessible to quantum mechanical calculation but has yet to resolve the complexity of the phase space Furthermore these calculations on systems containing up to 2 000 atoms can capture contributions to the energy that are not accounted for in QM MM methods for which the Nobel

prize in Chemistry was awarded in 2013 and the results presented here reveal profound shortcomings in said methods

Introduction to Nonlinear Oscillations Vladimir I. Nekorkin, 2016-05-02 A systematic outline of the basic theory of oscillations combining several tools in a single textbook The author explains fundamental ideas and methods while equally aiming to teach students the techniques of solving specific practical or more complex problems Following an introduction to fundamental notions and concepts of modern nonlinear dynamics the text goes on to set out the basics of stability theory as well as bifurcation theory in one and two dimensional cases Foundations of asymptotic methods and the theory of relaxation oscillations are presented with much attention paid to a method of mappings and its applications With each chapter including exercises and solutions including computer problems this book can be used in courses on oscillation theory for physics and engineering students It also serves as a good reference for students and scientists in computational neuroscience

Advances in Computer Simulation Studies on Crystal Growth Hiroki Nada, 2018-11-16 This book is a printed edition of the Special Issue Advances in Computer Simulation Studies on Crystal Growth that was published in Crystals

Computational Modelling of Nanomaterials Panagiotis Grammatikopoulos, 2020-09-30 Due to their small size and their dependence on very fast phenomena nanomaterials are ideal systems for computational modelling This book provides an overview of various nanosystems classified by their dimensions 0D nanoparticles QDs etc 1D nanowires nanotubes 2D thin films graphene etc 3D nanostructured bulk materials devices Fractal dimensions such as nanoparticle agglomerates percolating films and combinations of materials of different dimensionalities are also covered e g epitaxial decoration of nanowires by nanoparticles i e 0D 1D nanomaterials For each class the focus will be on growth structure and physical chemical properties The book presents a broad range of techniques including density functional theory molecular dynamics non equilibrium molecular dynamics finite element modelling FEM numerical modelling and meso scale modelling The focus is on each method s relevance and suitability for the study of materials and phenomena in the nanoscale This book is an important resource for understanding the mechanisms behind basic properties of nanomaterials and the major techniques for computational modelling of nanomaterials Explores the major modelling techniques used for different classes of nanomaterial Assesses the best modelling technique to use for each different type of nanomaterials Discusses the challenges of using certain modelling techniques with specific nanomaterials

Global Arsenic Hazard Nabeel Khan Niazi, Irshad Bibi, Tariq Aftab, 2022-12-02 This book provides a plethora of information about global arsenic As contamination and the challenges for environment Arsenic is a naturally occurring metalloid that is widely distributed in water soil air and biota from natural and anthropogenic sources Arsenic has been found in drinking water in over 100 countries worldwide which caused a major public health issue including cardiovascular disorders diabetes and cancers of various organs these are some of the general health effects of As exposure Exposure of plants to As even at very low concentrations can cause many morphological physiological and biochemical changes The recent research on As in the water soil plant human systems indicates that As

toxicity to plants varies with As speciation in plants type of plant species and with other soil factors controlling As accumulation in plants In recent years the development of efficient green chemistry methods for detoxification of trace metal poisoning has become a major focus of researchers It has been investigated in order to find an eco friendly and recyclable technique for the removal of As contamination from the natural resources Understanding the significance of As hazard and roles of sustainable or eco friendly approaches in its mitigation we intend to bring forth a comprehensive volume Global Arsenic Hazard Ecotoxicology and Remediation highlighting the various prospects involved in current scenario We are hopeful that this comprehensive volume will furnish the requisite of all those who are working or have interest in the proposed topic

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a four quadrant or multiple quadrant operation is required in industrial as well as commercial applications these applications require both driving and braking i e motoring and generating capability some of these applications include electric traction systems cranes and lifts cable laying winders and engine test loading systems

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speed control of a machine is the most vital and important part in any industrial organization this paper is designed to develop a four quadrant speed control system for a dc motor using microcontroller the motor is operated in four quadrants i e clockwise counter clock wise forward brake and reverse brake

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paper proposes a way to govern the rate and route control of a dc motor with the help of a 4 quadrant dc dc chopper the speed under the base velocity may be controlled by way of armature voltage manage technique mosfets are used for the switching operation of the chopper the gates of those mosfets are given pwm

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the four quadrant chopper block represents a four quadrant controlled chopper for converting a fixed dc input to a variable dc output the block contains two bridge arms each bridge arm each has two switching devices options for the type of

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3 four quadrant operation of dc motor four quadrant operation or mode of any dc motor means that machine operate in four quadrants they are forward breaking mode forward motoring mode reverse breaking or stop mode and reverse motoring mode a motor operates in two modes motoring and breaking a motor drive capable of

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this paper gives a control for three phase brushless dc bldc motor in all four quadrant operation the control system in this paper is capable to detect and identify the rotor position by sensor signal 1 in this paper behaviour of bldc motor is studied in all four quadrant operations through simulation model

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may 11 2021 a four quadrants dc chopper fqdc has been developed to work with a series motor for the application of dc drive electric vehicle in previous work capable of operating in such driving conditions and offers several types of chopper operation modes such as driving and reverse regenerative and resistive braking generator mode field weakening

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aug 8 2020 1 answer sorted by 1 you can think of the first quadrant operation as being a buck converter down from the supply to the motor you can think of the second quadrant as being a boost converter from the motor s generated low voltage up to the supply voltage

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put simply the four quadrants that the controller can work in are 1 motor going clockwise controller applying clockwise drive 2 motor going anti clockwise controller applying anti clockwise drive 3 motor going clockwise controller applying anti clockwise drive 4 motor going anti clockwise controller applying clockwise drive

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sep 11 2019 four quadrants drive dc chopper for series motor full size image this modes of operation can be controlled by ai controllers such as expert system fuzzy logic self tuning fuzzy 10 11 12 13 14 15 16 neural network as well as anfis but this paper focused only on the circuit operation of generator mode

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four quadrant operation of dc motor means that the machine operates in four quadrants they are forward braking forward motoring reverse motoring and reverse braking a motor operates in two modes motoring and braking

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1 to observe the four quadrant operation of a dc motor 2 to control a motor under torque control 3 to couple the speed control motor and torque controlled motor and observe the effect of a stepped torque 6 2 four quadrant operation of a dc motor the four quadrant operation is performed by giving an alternating reference speed command to

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aug 16 2021 the four quadrant operation of the motor can be described as follows quadrant i in the first quadrant the developed power by the motor is positive thus the motor operates in motoring mode and converts electrical energy into mechanical energy therefore the operation of the motor in first quadrant is called forward motoring quadrant ii

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the control of bldc motor in four quadrants is very crucial in this paper bldc motor is controlled in all the four quadrants without any wastage of power during regenerative braking period power generated is being stored in the chargeable battery

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aug 3 2019 introduction in this experiment four quadrant operation of a dc motor is simulated as well as run in real time the speed and current control model developed in the previous experiment is used to emulate the four regions of operation theoretical background consider an elevator system shown in figure below

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jan 1 2018 doi org 10 1016 j matpr 2017 11 261 get rights and content this paper proposes a method that designs a simulation model of four quadrant operation of bldc motor drive and to reduce the torque ripples in the developed model the characteristics of speed torque back emf are effectively monitored and analyzed

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four quadrant operation of a pm dc motor 5 1 objective the objective of this activity is to analyze the four quadrant operation of a permanent magnet dc pm dc motor this activity was derived from those developed and distributed by the university of minnesota umn 5 2 review of four quadrant operation