Molecular dynamics algorithm for multiple time scales: Systems with disparate masses

Mark E. Tuckerman[a] and Bruce J. Berne
Department of Chemistry, Columbia University, New York, New York 10027

Angelo Rossi
IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598

(Received 30 July 1990; accepted 1 October 1990)

A frequently encountered problem in molecular dynamics is how to treat the long times that are required to simulate condensed systems consisting of mixtures of light and heavy particles. Standard methods require the choice of time step sufficiently small to guarantee stable solution for the low mass component with the consequence that these simulations require a very large number of central processing unit cycles to treat the relaxation of the heavier component. In this note, we present a new method that allows one to use a time step appropriate for the heavy particles. This method uses a similar idea to numerical analytical propogator algorithm, an algorithm we invented to treat high frequency oscillators interacting with low frequency baths and is based on a choice of a reference systems for the light particle motions. The method is applied to the case of a liquid containing 864 Lennard-Jones spheres, 824 of these particles having a mass, $M = 100$ and 40 spheres picked at random have a mass $m = 1$. It is shown that molecular dynamics using the new algorithm runs seven to ten times faster than standard methods and this approach as well as suitable generalizations should be very useful for future simulations of quantum and classical condensed matter systems.

I. INTRODUCTION

Consider a system consisting of a mixture of light (mass $= m$) and heavy spheres (mass $= M$). In such systems, there is a disparity in the molecular dynamic time scales. If one wishes to simulate such systems using the standard integrators of molecular dynamics, then the maximum time step that can be used to integrate the equations of motion must be chosen to insure accurate integration of the low mass component with the consequence that a very small time step is needed. When a large disparity in time scales exists, a very large number of central processing unit (CPU) cycles will be required to allow the slow degrees of freedom to fluctuate enough to obtain converged time averages for the whole system.

In this paper, a method for accelerating the simulation of such systems is presented. This method, called RESPA (reference system propogator algorithm), is a variant of the numerical analytical propogator algorithm (NAPA), algorithm that we invented for treating the problem of high frequency oscillators coupled to low frequency oscillators.[1] The RESPA method is based on numerical solutions of the reference system equations. The gist of the method is to define a dynamical reference system for the fast motion and to derive equations of motion for the deviation $\delta(t)$ of the fast coordinates from the reference system coordinates. These deviations are coupled to the equations of motion of the slow coordinates. The fast dynamical system is integrated for n small time steps $n\delta t$ holding the slow coordinates fixed. The time dependence of the reference system is then fed into the coupled equations for $\delta(t)$ and the slow coordinates and the resulting equations are integrated for one large time step $\Delta t = n\delta t$. The initial conditions for each large time step are then chosen so that this deviation $\delta(t)$ is zero with the consequence that the deviation is always kept small. The only approximation in this algorithm springs from the numerical integrator used to integrate the equations of motion of the reference system and the coupled equations. Otherwise, the method is self-correcting and exact. For simplicity, the reference system is taken to be the Hamiltonian of the original system with the slow coordinates held fixed at their values at the beginning of the time step.

Teleman and Jönsson[2] have proposed a multiple time-step (TJMTS) method in which the forces are separated into slow and fast components. This separation yields a set of coupled equations of motion for the slow and fast degrees of freedom. TJMTS uses a small step δt to advance the fast degrees of freedom n steps holding the slow variables fixed. The slow degrees of freedom are then updated using a time step $\Delta t = n\delta t$. This method does not correct for the errors incurred in the approximate factorization of the equations of motion, a fact which shows up in poor energy conservation. This is well illustrated when we compare the results of RESPA, TJMTS, and velocity Verlet[3] (using a small time step). Swindoll and Haile[4] have proposed a more accurate multiple time-step method than Teleman and Jönsson, but their method requires high-order spatial derivatives of the potential and is therefore more computationally intensive than RESPA.

For simplicity, we apply this new method to the simulation of a mixture of Lennard-Jones spheres consisting of 824 heavy spheres of mass $M = 100$ and 40 light spheres of mass $m = 1$. For Lennard-Jones (LJ) spheres, the two time scales are $\Delta t_f = \sqrt{m\sigma_1^2/\epsilon_1}$ and $\Delta t_s = \sqrt{M\sigma_2^2/\epsilon_2}$, where σ_i and ϵ_i are the Lennard-Jones parameters for component i. For il-

[a] Ph. D. student in the Department of Physics, Columbia University.

Molecular Dynamics Algorithm For Multiple Time Scales

David Baud

Molecular Dynamics Algorithm For Multiple Time Scales:

Multiple Time Scales Jeremiah U. Brackbill,Bruce I. Cohen,2014-05-10 Multiple Time Scales presents various numerical methods for solving multiple time scale problems The selection first elaborates on considerations on solving problems with multiple scales problems with different time scales and nonlinear normal mode initialization of numerical weather prediction models Discussions focus on analysis of observations nonlinear analysis systems of ordinary differential equations and numerical methods for problems with multiple scales The text then examines the diffusion synthetic acceleration of transport iterations with application to a radiation hydrodynamics problem and implicit methods in combustion and chemical kinetics modeling The publication ponders on molecular dynamics and Monte Carlo simulations of rare events direct implicit plasma simulation orbit averaging and subcycling in particle simulation of plasmas and hybrid and collisional implicit plasma simulation models Topics include basic moment method electron subcycling gyroaveraged particle simulation and the electromagnetic direct implicit method The selection is a valuable reference for researchers interested in pursuing further research on the use of numerical methods in solving multiple time scale problems Classical And Quantum Dynamics In Condensed Phase Simulations: Proceedings Of The International School Of Physics Bruce J Berne,Giovanni Ciccotti,David F Coker,1998-06-17 The school held at Villa Marigola Lerici Italy in July 1997 was very much an educational experiment aimed not just at teaching a new generation of students the latest developments in computer simulation methods and theory but also at bringing together researchers from the condensed matter computer simulation community the biophysical chemistry community and the quantum dynamics community to confront the shared problem the development of methods to treat the dynamics of quantum condensed phase systems This volume collects the lectures delivered there Due to the focus of the school the contributions divide along natural lines into two broad groups 1 the most sophisticated forms of the art of computer simulation including biased phase space sampling schemes methods which address the multiplicity of time scales in condensed phase problems and static equilibrium methods for treating quantum systems 2 the contributions on quantum dynamics including methods for mixing quantum and classical dynamics in condensed phase simulations and methods capable of treating all degrees of freedom quantum mechanically Computational Molecular Dynamics: Challenges, Methods, Ideas Peter Deuflhard,Jan Hermans,Benedict Leimkuhler,Alan E. Mark,Sebastian Reich,Robert D. Skeel,2012-12-06 On May 21 24 1997 the Second International Symposium on Algorithms for Macromolecular Modelling was held at the Konrad Zuse Zentrum in Berlin The event brought together computational scientists in fields like biochemistry biophysics physical chemistry or statistical physics and numerical analysts as well as computer scientists working on the advancement of algorithms for a total of over 120 participants from 19 countries In the course of the symposium the speakers agreed to produce a representative volume that combines survey articles and original papers all refereed to give an impression of the present state of the art of Molecular Dynamics The 29 articles of the book reflect the main topics of the Berlin meeting which were i Conformational Dynamics ii Thermodynamic Modelling iii Advanced Time Stepping Algorithms iv Quantum Classical Simulations and Fast Force Field and v Fast Force Field Evaluation **Computer Simulations in Condensed Matter: From Materials to Chemical Biology. Volume 1** Mauro Ferrario,Giovanni Ciccotti,Kurt Binder,2007-03-09 This comprehensive collection of lectures by leading experts in the field introduces and reviews all relevant computer simulation methods and their applications in condensed matter systems Volume 1 is an in depth introduction to a vast spectrum of computational techniques for statistical mechanical systems of condensed matter Volume 2 is a collection of state of the art surveys on numerical experiments carried out for a great number of systems **Reaction Dynamics in Clusters and Condensed Phases** Joshua Jortner,R.D. Levine,A. Pullman,2012-12-06 The Twenty Sixth Jerusalem Symposium reflected the high standards of these distinguished scientific meetings which convene once a year at the Israel Academy of Sciences and Humanities in Jerusalem to discuss a specific topic in the broad area of quantum chemistry and biochemistry The topic at this year s Jerusalem Symposium was reaction dynamics in clusters and condensed phases which constitutes a truly interdisciplinary subject of central interest in the areas of chemical dynamics kinetics photochemistry and condensed matter chemical physics The main theme of the Symposium was built around the exploration of the interrelationship between the dynamics in large finite clusters and in infinite bulk systems The main issues addressed microscopic and macroscopic sol vation phenomena cluster and bulk spectroscopy photodissociation and vibrational predissociation cage effects interphase dynamics reaction dynamics and energy transfer in clusters dense fluids liquids solids and biophysical systems The interdisciplinary nature of this research area was deliberated by intensive and extensive interactions between modern theory and advanced experimental methods This volume provides a record of the invited lectures at the Symposium **Liquid Crystals and their Computer Simulations** Claudio Zannoni,2022-07-28 Standing as the first unified textbook on the subject Liquid Crystals and Their Computer Simulations provides a comprehensive and up to date treatment of liquid crystals and of their Monte Carlo and molecular dynamics computer simulations Liquid crystals have a complex physical nature and therefore computer simulations are a key element of research in this field This modern text develops a uniform formalism for addressing various spectroscopic techniques and other experimental methods for studying phase transitions of liquid crystals and emphasises the links between their molecular organisation and observable static and dynamic properties Aided by the inclusion of a set of Appendices containing detailed mathematical background and derivations this book is accessible to a broad and multidisciplinary audience Primarily intended for graduate students and academic researchers it is also an invaluable reference for industrial researchers working on the development of liquid crystal display technology *Wspc Reference On Organic Electronics, The: Organic Semiconductors (In 2 Volumes)* Seth R Marder,Jean-luc Bredas,2016-06-24 This 2 volume set provides the reader with a basic understanding of the foundational concepts pertaining to the design synthesis and applications of conjugated organic materials used as organic semiconductors in areas including organic photovoltaic devices light emitting diodes field effect transistors spintronics actuation bioelectronics thermoelectrics and nonlinear optics While there are many monographs in these various areas the emphasis here is both on the fundamental chemistry and physics concepts underlying the field of organic semiconductors and on how these concepts drive a broad range of applications This makes the volumes ideal introductory textbooks in the subject They will thus offer great value to both junior and senior scientists working in areas ranging from organic chemistry to condensed matter physics and materials science and engineering Number of Illustrations and Tables 168 b w illus 242 colour illus 13 tables **Multiscale Computational Methods in Chemistry and Physics** Achi Brandt,Jerzy Bernholc,Kurt Binder,2001 This book brings together interdisciplinary contributions ranging from applied mathematics theoretical physics quantum chemistry and molecular biology all addressing various facets of the problem to connect the many different scales that one has to deal with in the computer simulation of many systems of interest in chemistry e g polymeric materials biological molecules clusters surface and interface structure Particular emphasis is on the multigrid technique and its applications ranging from electronic structure calculations to the statistical mechanics of polymers *Long Time Scale Computer Simulations of Proteins* Peter Eastman,2000 **Theoretical Biophysics Technical Report** ,1991 **Multiple-time-scale Order Reduction for Stochastic Kinetics and Molecular Simluation of Crystallization** Ethan Allen Sturman Mastny,2007 □□□□□ □□□□ 1953, Dissertation Abstracts International ,2008 **Bridging the Time Scales** Peter. Nielaba,Michel Mareschal,Giovanni Ciccotti,2014-01-15 **SIAM Journal on Scientific Computing** ,2003 Monte Carlo and Molecular Dynamics of Condensed Matter Systems Kurt Binder,Giovanni Ciccotti,1996 **Bridging the Time Scales** Peter Nielaba,Michel Mareschal,Giovanni Ciccotti,2002-12-19 The behaviour of many complex materials extends over time and lengthscales well beyond those that can normally be described using standard molecular dynamics or Monte Carlo simulation techniques As progress is coming more through refined simulation methods than from increased computer power this volume is intended as both an introduction and a review of all relevant modern methods that will shape molecular simulation in the forthcoming decade Written as a set of tutorial reviews the book will be of use to specialists and nonspecialists alike ACS Directory of Graduate Research 1993 American Chemical Society. Committee on Professional Training,1993 **5th International Conference on Multibody Systems, Nonlinear Dynamics, and Control** ,2005 Pacific Symposium on Biocomputing ,1996

Molecular Dynamics Algorithm For Multiple Time Scales Book Review: Unveiling the Power of Words

In some sort of driven by information and connectivity, the energy of words has be more evident than ever. They have the capacity to inspire, provoke, and ignite change. Such may be the essence of the book **Molecular Dynamics Algorithm For Multiple Time Scales**, a literary masterpiece that delves deep in to the significance of words and their effect on our lives. Compiled by a renowned author, this captivating work takes readers on a transformative journey, unraveling the secrets and potential behind every word. In this review, we shall explore the book is key themes, examine its writing style, and analyze its overall affect readers.

Table of Contents Molecular Dynamics Algorithm For Multiple Time Scales

Molecular Dynamics Algorithm For Multiple Time Scales Introduction

In the digital age, access to information has become easier than ever before. The ability to download Molecular Dynamics Algorithm For Multiple Time Scales has revolutionized the way we consume written content. Whether you are a student looking for course material, an avid reader searching for your next favorite book, or a professional seeking research papers, the option to download Molecular Dynamics Algorithm For Multiple Time Scales has opened up a world of possibilities. Downloading Molecular Dynamics Algorithm For Multiple Time Scales provides numerous advantages over physical copies of books and documents. Firstly, it is incredibly convenient. Gone are the days of carrying around heavy textbooks or bulky folders filled with papers. With the click of a button, you can gain immediate access to valuable resources on any device. This convenience allows for efficient studying, researching, and reading on the go. Moreover, the cost-effective nature of downloading Molecular Dynamics Algorithm For Multiple Time Scales has democratized knowledge. Traditional books and academic journals can be expensive, making it difficult for individuals with limited financial resources to access information. By offering free PDF downloads, publishers and authors are enabling a wider audience to benefit from their work. This inclusivity promotes equal opportunities for learning and personal growth. There are numerous websites and platforms where individuals can download Molecular Dynamics Algorithm For Multiple Time Scales. These websites range from academic databases offering research papers and journals to online libraries with an expansive collection of books from various genres. Many authors and publishers also upload their work to specific websites, granting readers access to their content without any charge. These platforms not only provide access to existing literature but also serve as an excellent platform for undiscovered authors to share their work with the world. However, it is essential to be cautious while downloading Molecular Dynamics Algorithm For Multiple Time Scales. Some websites may offer pirated or illegally obtained copies of copyrighted material. Engaging in such activities not only violates copyright laws but also undermines the efforts of authors, publishers, and researchers. To ensure ethical downloading, it is advisable to utilize reputable websites that prioritize the legal distribution of content. When downloading Molecular Dynamics Algorithm For Multiple Time Scales, users should also consider the potential security risks associated with online platforms. Malicious actors may exploit vulnerabilities in unprotected websites to distribute malware or steal personal information. To protect themselves, individuals should ensure their devices have reliable antivirus software installed and validate the legitimacy of the websites they are downloading from. In conclusion, the ability to download Molecular Dynamics Algorithm For Multiple Time Scales has transformed the way we access information. With the convenience, cost-effectiveness, and accessibility it offers, free PDF downloads have become a popular choice for students, researchers, and book lovers worldwide. However, it is crucial to engage in ethical downloading practices and prioritize personal security when utilizing online platforms. By doing so, individuals can make the most of the vast array of free PDF resources available and embark on a journey of continuous learning and intellectual growth.

FAQs About Molecular Dynamics Algorithm For Multiple Time Scales Books

What is a Molecular Dynamics Algorithm For Multiple Time Scales PDF? A PDF (Portable Document Format) is a file format developed by Adobe that preserves the layout and formatting of a document, regardless of the software, hardware, or operating system used to view or print it. **How do I create a Molecular Dynamics Algorithm For Multiple Time Scales PDF?** There are several ways to create a PDF: Use software like Adobe Acrobat, Microsoft Word, or Google Docs, which often have built-in PDF creation tools. Print to PDF: Many applications and operating systems have a "Print to PDF" option that allows you to save a document as a PDF file instead of printing it on paper. Online converters: There are various online tools that can convert different file types to PDF. **How do I edit a Molecular Dynamics Algorithm For Multiple Time Scales PDF?** Editing a PDF can be done with software like Adobe Acrobat, which allows direct editing of text, images, and other elements within the PDF. Some free tools, like PDFescape or Smallpdf, also offer basic editing capabilities. **How do I convert a Molecular Dynamics Algorithm For Multiple Time Scales PDF to another file format?** There are multiple ways to convert a PDF to another format: Use online converters like Smallpdf, Zamzar, or Adobe Acrobats export feature to convert PDFs to formats like Word, Excel, JPEG, etc. Software like Adobe Acrobat, Microsoft Word, or other PDF editors may have options to export or save PDFs in different formats. **How do I password-protect a Molecular Dynamics Algorithm For Multiple Time Scales PDF?** Most PDF editing software allows you to add password protection. In Adobe Acrobat, for instance, you can go to "File" -> "Properties" -> "Security" to set a password to restrict access or editing capabilities. Are there any free alternatives to Adobe Acrobat for working with PDFs? Yes, there are many free alternatives for working with PDFs, such as: LibreOffice: Offers PDF editing features. PDFsam: Allows splitting, merging, and editing PDFs. Foxit Reader: Provides basic PDF viewing and editing capabilities. How do I compress a PDF file? You can use online tools like Smallpdf, ILovePDF, or desktop software like Adobe Acrobat to compress PDF files without significant quality loss. Compression reduces the file size, making it easier to share and download. Can I fill out forms in a PDF file? Yes, most PDF viewers/editors like Adobe Acrobat, Preview (on Mac), or various online tools allow you to fill out forms in PDF files by selecting text fields and entering information. Are there any restrictions when working with PDFs? Some PDFs might have restrictions set by their creator, such as password protection, editing restrictions, or print restrictions. Breaking these restrictions might require specific software or tools, which may or may not be legal depending on the circumstances and local laws.

Find Molecular Dynamics Algorithm For Multiple Time Scales :

sideways a novel by rex pickett
seinfeld and pandis second edition
signals and systems oppenheim 2nd edition solution
section 20 1 review species interactions answers
seu sonho tem futuro livro de candice pascoal
sequentronic an automated transmission from mercedes benz
~~seismic design aids for nonlinear pushover analysis of reinforced concrete and steel bridges advances in earthquake engineering~~
science explorer grade 7 guided reading and study workbook answers
~~silvercrest wireless doorbell manual~~
~~singer engineering mechanics solutions manualpdf~~
sindh police jobs as inspector sho asi constable
scott 2009 standard postage stamp catalogue
siempre pienso en ti
shreve s chemical process industries 5th edition by g t auston
sch3u grade 11 gases and atmospheric chemistry unit overview

Molecular Dynamics Algorithm For Multiple Time Scales :

Fundamentals of Nursing: Human Health and Function All-new, richly illustrated concept maps , ideal for visual learners, apply the nursing process and critical thinking to the chapter-opening case scenarios. Fundamentals of Nursing - Wolters Kluwer Jan 22, 2020 — ... nursing process framework that clarifies key capabilities, from promoting health to differentiating between normal function and dysfunction ... Fundamentals of Nursing: Human Health and Function This book cover everything u need to get you through your fundamental course , it is very thorough , an amazing book , it's easy to real and totally helpful , ... Fundamentals of nursing : human health and function What is Culture? Communication in the Nurse-

Patient Relationship. Values, Ethics, and Legal Issues. Nursing Research and Evidence-Based ... Nursing Fundamentals Fundamentals of Nursing: The Art and Science of Nursing Care. Text, Study Guide and Video Guide to Clinical Nursing Skills Set on CD-ROM Package. $150.45. Fundamentals of Nursing: Human Health and Function ... Ruth F. The Fourth Edition of this comprehensive text provides an introduction to the broad range of the discipline of nursing, including theory, the nursing ... Fundamentals of Nursing: Human Health and Function ... Fundamentals of Nursing: Human Health and Function (Enhanced with Media) 7th Edition is written by Ruth Craven and published by Lippincott Williams & Wilkins. Fundamentals of Nursing: Human Health And Function ... Johnson, Joyce Young; Vaughans, Bennita W.; Prather-Hicks, Phyllis ... Synopsis: This study guide includes chapter overviews, critical thinking case studies, and ... Fundamentals of nursing : human health and function ... Spiritual health. Ch. 1. The changing face of nursing -- Ch. 2. Community-based nursing and continuity of care -- Ch. 3. The profession of nursing -- Ch. 4. Fundamentals of nursing: Human health and function Download Citation | Fundamentals of nursing: Human health and function: Seventh edition | This groundbreaking text emphasizes critical thinking by weaving ... Essentials of Epidemiology in Public Health: 9781284128352 Essentials of Epidemiology in Public Health, Fourth Edition combines theory and practice in presenting traditional and new epidemiologic concepts. Essentials of Epidemiology in Public Health Essentials of Epidemiology in Public Health, Fourth Edition combines theory and practice in presenting traditional and new epidemiologic concepts. Navigate eBook Access for Essentials of Epidemiology in ... Navigate eBook Access to Essentials of Epidemiology in Public Health, Fourth Edition is a digital-only, eBook with 365 day access. Essentials of Epidemiology in Public Health Up-to-date examples from the epidemiologic literature on diseases of public health importance are provided throughout the book. The Third Edition is a thorough ... Essentials of Epidemiology in Public Health, 2nd Edition Successfully tested in the authors' courses at Boston University and Harvard University, this text combines theory and practice in presenting traditional ... Essentials of Epidemiology in Public Health Essentials of Epidemiology in Public Health, Second Edition will familiarize readers with terminology and key concepts in the design, analysis, and ... (PDF) ESSENTIALS OF FOURTH EDITION | Chelsea Gould These criticisms assume that epidemiology is a system of knowledge about health and disease, based on observation. In fact, consensus on the definition of the ... Third Edition of 'Essentials of Epidemiology in Public ... The best-selling “Essentials of Epidemiology in Public Health” has been used in more than 100 graduate programs across the country. It was co-authored by George ... Essentials of Epidemiology in Public Health Essentials of Epidemiology in Public Health, Fourth Edition combines theory and practice in presenting traditional and new epidemiologic concepts. Essentials of Epidemiology in Public Health Essentials of Epidemiology in Public Health, Fourth Edition combines theory and practice in presenting traditional and new epidemiologic concepts. Transformation of the Heart: Stories by Devotees of Sathya ... This wonderful book is a collection of stories by people whose lives have been transformed by Sathya Sai Baba. Written with warmth and compassion, ... Transformation of the Heart:

Stories By Devotees of Sri ... This wonderful book is a collection of stories by people whose lives have been transformed by Sathya Sai Baba. Written with warmth and compassion, ... Transformation of the Heart: Stories by Devotees of Sathya Sai ... This wonderful book is a collection of stories by people whose lives have been transformed by Sathya Sai Baba. Written with warmth and compassion, ... Stories by Devotees of Sathya Sai Baba: 9780877287162 - ... This wonderful book is a collection of stories by people whose lives have been transformed by Sathya Sai Baba. Written with warmth and compassion, ... Stories By Devotees of Sri Sathya Sai Baba, Judy (e Item Number. 185181693182 ; Book Title. Transformation of the Heart: Stories By Devotees of Sri Sathya Sa ; Author. Judy (editor) Warner ; Accurate description. Stories by Devotees of Sathya Sai Baba Jul 1, 1990 — This wonderful book is a collection of stories by people whose lives have been transformed by Sathya Sai Baba. Stories By Devotees of Sri Sathya Sai Baba by Judy (Editor) ... Transformation of the Heart: Stories By Devotees of Sri Sathya Sai Baba. by Judy (Editor) Warner, Judy (Compiled, Edited By) Warner ... Transformation of the Heart: Stories By Devotees of Sri ... Home tuckerstomes Transformation of the Heart: Stories By Devotees of Sri Sathya Sai Baba ; Or just $17.81 ; About This Item. Andhra Pradesh India: Sri Sathya Sai ... Transformation of the Heart - Books Transformation of the Heart ; ISBN · 978-81-7208-768-5 ; Publisher · Sri Sathya Sai Sadhana Trust, Publications Division ; Content · Quantity 1 Book ; Length · 8.000 " Transformation of the Heart – By Sai Charan Swami had symbolically H-Transformed a sinner into a saint! Another story is that of an American, who did not believe in Swami's Divinity. His wife though, ...