

macromolecules, e.g. in equilibrium, under a constant load, a load varying in time, or upon binding of another molecule, can only be characterized by following the changes of the internal forces in time, which cannot be easily achieved with the previous implementation of FDA. We here introduce a Time-Resolved Force Distribution Analysis (TRFDA) method, which adds a temporal component to FDA to enable the analysis of pairwise forces associated with conformational changes.

2. Implementation

2.1. Overview

Time-Resolved Force Distribution Analysis (TRFDA) is based on the same concept of using pairwise forces as FDA, but focuses on their evolution during the MD simulation as well as on the analysis of large molecular systems. To achieve these goals, it stores in memory pairwise forces from only one integration time step at a time, such that the memory usage is independent from the length of the simulation. It also saves output data in new file formats, which are well suited for time series analysis. Similar to FDA, atomic pairwise forces are computed for all types of bonded interactions as well as from Coulomb and Lennard-Jones potentials; long-range electrostatic interactions computed on a grid (e.g. Particle Mesh Ewald Darden et al. (1993); Essmann et al. (1995)) cannot be decomposed in atomic pairwise forces. As in the previous FDA implementation, an MD simulation is first performed to obtain a trajectory, which is then used as the basis for a rerun using the TRFDA code. The core code is completely rewritten for GROMACS 4.5.3 Hess et al. (2008), and VMD Humphrey et al. (1996) plugins are provided for visualization. The implementation includes several notable improvements over FDA, which are discussed below.

2.2. Decomposition of forces from 3- and 4-body potentials

While two-body potentials such as bonds, Coulomb and Lennard-Jones potentials, can be directly used for the analysis of pairwise forces, many-body potentials which act on more than two atoms need to be decomposed into pairwise forces. TRFDA introduces a complete decomposition of the forces resulting from 3- and 4-body potentials (angle, dihedral angle, cross bond-bond, cross bond-angle), as described in the Additional file 1. The pairwise forces resulting from this way of force decomposition can have any direction, *i.e.* do not align with the vector connecting the two atoms involved. To accommodate this, all pairwise forces are stored and handled internally as vectors and are transformed into scalar values only when written to a file, if desired by the user.

The decomposition rectifies the shortcomings of the previous FDA code, which used approximations for computing pairwise forces resulting from 3- or 4-body potentials. For an angle formed by atoms i , j and k (j between i and k), it considered no pairwise forces to act on atom j , and assumed the pairwise force between atoms i and k to act along the distance vector between the two atoms. A similar decomposition has been used for a dihedral angle formed by four atoms. In contrast to these approximations, the decomposition used in TRFDA correctly reproduces the distribution of angle and dihedral forces in a molecule.

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Hutchings,Snejina Michailova,Adrian Wilkinson,2024-01-18 This authoritative Guide provides 41 summaries of important theories used for research in HRM Each entry clearly defines a theory provides insight into the development of the theory demonstrates the application of the theory to HRM and discusses areas where the theory could be applied in future research projects Additionally the two introductory chapters overview HRM in relation to theory and explain the importance of theory in research and issues to consider when using theory *Artificial Intelligence, Medical Engineering and Education* Z.B.

Hu,Q. Zhang,M. He,2024-02-28 Artificial Intelligence AI is a rapidly developing field of computer science which now plays an increasingly important role in many disciplines A catalyst for significant change research into AI is of particular importance in fields such as medicine and education and as such has become an area to watch for many people worldwide This book presents the proceedings of AIMEE 2023 the 7th International Conference on Artificial Intelligence Medical Engineering and Education held on 9 and 10 November 2023 in Guangzhou China The conference brought together top international researchers from around the world to exchange research results and address open issues in AI medical engineering and education A total of 238 submissions were received for AIMEE 2023 of which 89 papers were selected for presentation and publication after a rigorous international peer review process The book is divided into 3 sections covering artificial intelligence and scientific methodology systems engineering and analysis concepts methods and applications and education reform and innovation Presenting papers which explore and discuss many novel concepts and methodologies contributing to the rapid evolution of artificial intelligence and its applications the book will be of interest to all those working in the relevant fields

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growth Multinational Enterprise Management Strategies in Developing Countries is an authoritative reference source for the latest scholarly research on diverse opportunities and obstacles facing multinational corporations in emerging economies Highlighting innovative perspectives and real world examples this book is ideally designed for researchers practitioners upper level students and industry professionals interested in management approaches for achieving success in international corporations *Commerce America* ,1978-03-27 **Talent Development and the Global Economy** Fredrick. M. Nafukho,Khali Dirani,Beverly Irby,2017-08-01 Talent has been identified as the only differentiator for an organization s nations or any region s success in this uncertain complex competitive and global environment Ulrich 2008 defined talent as the equation of 3Cs Talent Competence x Commitment x Contribution Malaeb and Chanaron 2010 p 2 noted Competence means that employees have the skills and abilities today and in the future for required business results Commitment means that employees are involved and engaged while Contribution means that employees find personal abundance at occupation While Ulrich 2008 observed that commitment focused on meaning and identity and other restraints that tap employee s heart This book is unique in many ways which makes it extraordinary First unlike other books that have examined issues of change facing the global economy no book has examined the issue of talent development from the perspective of special interest groups including management international students women refugees refugees non governmental organizations for profit for benefit and nonprofit organizations Thus talent development world over has become one of the most important issues when it comes to developing human resources especially through education and training The book presents pertinent research and practice on talent development management and argues that the term talent development broadly refers to management and development of high performing and high potential individuals in society required to carry out critical organizational and society roles aimed at improving human development The contributors of the book chapters include individuals actively involved in research teaching and practice in higher education and in business and industry The chapters are based on empirical data including review of relevant literature The book also recognizes that talent development is more than just crisis management and includes best talent management practices shared governance meaningful reforms strategic planning transparency and accountability social justice and respect for human life and the need to develop humane organizations and humane communities The contributions take cognizance of the fact that talent development as a concept is facing fundamental changes in the global knowledge economy and especially with political changes taking place world over Contributors also take cognizance of the fact that one important source of change in society has been the accelerating speed of scientific and technological advancement driven by the power of the Internet hence the need to develop talent for the 21st century and beyond The book is basically an academic book for use by undergraduates and graduate students at universities for profit for benefit and non profit organizations policy makers and formulators in ministries of Education supra national organizations foreign organizations multilateral organizations non governmental organizations community based

organizations as well as development stakeholders and community organizers Liability of Multinational Corporations under International Law Menno T. Kamminga, Saman Zia-Zarifi, 2021-12-28 ECIE2015-10th European Conference on Innovation and Entrepreneurship Renata Paola Dameri, Roberto Garelli and Marina Resta, 2015-08-24 These proceedings represent the work of contributors to the 10th European Conference on Innovation and Entrepreneurship ECIE 2015 hosted this year by The University of Genoa Italy on the 17 18 September 2015 The Conference Chair is Prof Luca Beltrametti and the Programme Co chairs are Prof Renata Paola Dameri Prof Roberto Garelli and Prof Marina Resta all from the University of Genoa ECIE continues to develop and evolve Now in its 10th year the key aim remains the opportunity for participants to share ideas and meet the people who hold them The scope of papers will ensure an interesting two days The subjects covered illustrate the wide range of topics that fall into this important and growing area of research The opening keynote presentation is given by Marco Doria Mayor of Genoa on the topic of Innovation and entrepreneurship in Genoa past present and future A second keynote will be given by Flavia Marzano from the National board for innovation and Italian digital agenda on the topic of Innovation New visions not just new technologies The second day Keynote will be given by Roberto Santoro President of the European Society of Concurrent Engineering Network ESoCE Net on the topic of People Olympics for healthy and active living A people driven social innovation platform In addition to the main themes of the conference there are a number of specialist mini tracks on topics including Innovation and strategy Entrepreneurship education in action The theory and practice of collaboration in entrepreneurship and Challenges for entrepreneurship and innovation in the 21st Century With an initial submission of 275 abstracts after the double blind peer review process there are 88 Academic research papers 6 PhD research papers 1 Masters Research paper 4 work in progress papers and 1 Non academic paper published in these Conference Proceedings These papers represent research from Australia Brazil Bulgaria Colombia Croatia Cyprus Czech Republic Denmark Egypt Finland France Germany Ghana Greece Hungary India Iran Ireland Israel Italy Japan Kazakhstan Kuwait Lithuania Malaysia Mexico Netherlands New Zealand Nigeria Norway Poland Portugal Romania Romania Russia Russian Federation Saudi Arabia South Africa Spain Sweden Thailand Thailand UK and USA **Digital Technologies and the Law of Obligations** Zvonimir Slakoper, Ivan Tot, 2021-09-30 Digital Technologies and the Law of Obligations critically examines the emergence of new digital technologies and the challenges they pose to the traditional law of obligations and discusses the extent to which existing contract and tort law rules and doctrines are equipped to meet these new challenges This book covers various contract and tort law issues raised by emerging technologies including distributed ledger technology blockchain based smart contracts and artificial intelligence as well as by the evolution of the internet into a participative web fuelled by user generated content and by the rise of the modern day collaborative economy facilitated by digital technologies Chapters address these topics from the perspective of both the common law and the civil law tradition While mostly focused on the current state of affairs and recent debates and initiatives within the European Union regulatory

framework contributors also discuss the central themes from the perspective of the national law of obligations examining the adaptability of existing legal doctrines to contemporary challenges addressing the occasional legislative attempts to deal with the private law aspects of these challenges and pointing to issues where legislative interventions would be most welcomed Case studies are drawn from the United States Singapore and other parts of the common law world Digital Technologies and the Law of Obligations will be of interest to legal scholars and researchers in the fields of contract law tort law and digital law as well as to legal practitioners and members of law reform bodies

International Arbitration in the Energy

Sector Maxi Scherer, 2018-02-22 Disputes in the energy and natural resources sector are at the heart of international arbitration With more arbitrations arising in the international energy sector than in any other sector it is not surprising that the highest valued awards in the history of arbitration come from energy related arbitrations Energy disputes often involve complex and controversial issues relating to security sovereignty and public welfare International Arbitration in the Energy Sector puts international energy disputes into a global context providing broad coverage of different forms and systems of dispute resolution across both renewable and non renewable sectors With contributions from leading arbitrators academics and industry experts from across the globe the twenty chapters in the book enable readers to compare the approaches to and learnings from energy arbitrations across various legal systems and geographic regions After outlining the international energy arbitration legal framework in Part I the text delves into a detailed analysis of the problems which regularly arise in practice These include among other things commercial disputes in Part II e g over the upstream oil sector and long term gas supply contracts investor state disputes in Part III e g under the Energy Charter Treaty and public international law disputes in Part IV e g concerning international boundaries and the distribution of natural resources Alongside recent developments in the international energy sector attention is given to climate and sustainable development disputes which raise important questions about enforcing sustainability objectives on individuals corporations and states Backed by analyses of arbitral awards national court and international tribunal decisions treaties and other international legal instruments as well as current events and news in the energy industry this text offers a unique contribution to international energy literature and provides insightful commentary on the prevalent issues in the field It is essential reading for any practitioner or researcher in the energy and natural resources sector

Commercial Library Operating Procedures Guide ,1990

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Ali, Zolman Bin Hari, Meng Chew Leow, 2024-07-13 This book is a compilation of conference papers presented at the International Conference on Advancing and Redesigning Education 2023 ICARE 23 It covers four main topics including Technology Enhanced Learning Innovative Curriculum and Program Offering Learning Beyond Classroom and Digital Campus This book presents the recent innovations and the authors practical experiences in teaching and learning and helps educational practitioners to enhance their teaching and learning

Encyclopedia of Organizational Knowledge,

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Industrial Engineering and Management Innovation Ershi Qi, 2015-10-12 The 6th International Asia Conference on Industrial Engineering and Management Innovation is sponsored by the Chinese Industrial Engineering Institution and organized by Tianjin University The conference aims to share and disseminate information on the most recent and relevant researches theories and practices in industrial and system engineering to promote their development and application in university and enterprises

Field Guide to Intercultural Research David S. A. Guttormsen, Jakob Luring, Malcolm

Chapman, 2021-01-29 This informative Field Guide to Intercultural Research is specifically designed to be used in the field guiding the reader away from pitfalls and towards best practice It shares valuable fieldwork challenges and experiences as well as insights into key methodological debates and practical recommendations relevant to both new and seasoned researchers

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