

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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Corporate Environmental Accountability in International Law Elisa Morgera,2020-09-03 This fully updated second edition of Corporate Accountability in International Environmental Law examines systematically all international sources of corporate accountability standards with specific reference to environmental protection and elaborates on their theoretical and practical implications for international environmental law The book argues that although international environmental law does not bind multinational corporations and other business entities growing practice points to the emergence and consolidation of international legal standards These standards allow adapting and translating inter State obligations embodied in international environmental law into specific normative benchmarks to determine the legitimacy of the conduct of the private sector against internationally recognized values and rules The role of international organizations who in the absence of State intervention identify and promote the application of selected international environmental standards is analyzed in depth This analysis demonstrates how these international organizations are a driving force in establishing and

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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 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 Proceedings of the International Conference on Advancing and Redesigning Education 2023 Mohd Fakhizan bin Romlie, Siti Haryani Shaikh 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, Administration, and Technology

Khosrow-Pour D.B.A., Mehdi, 2020-09-29 For any organization to be successful it must operate in such a manner that knowledge and information human resources and technology are continually taken into consideration and managed effectively Business concepts are always present regardless of the field or industry in education government healthcare not for profit engineering hospitality tourism among others Maintaining organizational awareness and a strategic frame of mind is critical to meeting goals gaining competitive advantage and ultimately ensuring sustainability The Encyclopedia of Organizational Knowledge Administration and Technology is an inaugural five volume publication that offers 193 completely new and previously unpublished articles authored by leading experts on the latest concepts issues challenges innovations and opportunities covering all aspects of modern organizations Moreover it is comprised of content that highlights major breakthroughs discoveries and authoritative research results as they pertain to all aspects of organizational growth and development including methodologies that can help companies thrive and analytical tools that assess an organization s internal health and performance Insights are offered in key topics such as organizational structure strategic leadership information technology management and business analytics among others The knowledge compiled in this publication is designed for entrepreneurs managers executives investors economic analysts computer engineers software programmers human resource departments and other industry professionals seeking to understand the latest tools to emerge from this field and who are looking to incorporate them in their practice Additionally academicians researchers and students in fields that include but are not limited to business management science organizational development entrepreneurship sociology corporate psychology computer science and information technology will benefit from the research compiled within this publication

Proceedings of the 6th International Asia Conference on 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

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