

# Time-resolved force distribution analysis

Bogdan I Costescu and Frauke Gräter

**Abstract—Background:** Biomolecules or other complex macromolecules undergo conformational transitions upon exposure to an external perturbation such as ligand binding or mechanical force. To follow fluctuations in pairwise forces between atoms or residues during such conformational changes as observed in Molecular Dynamics (MD) simulations, we developed Time-Resolved Force Distribution Analysis (TRFDA).

**Results:** The implementation focuses on computational efficiency and low-memory usage and, along with the wide range of output options, makes possible time series analysis of pairwise forces variation in long MD simulations and for large molecular systems. It also provides an exact decomposition of pairwise forces resulting from 3- and 4-body potentials and a unified treatment of pairwise forces between atoms or residues. As a proof of concept, we present a stress analysis during unfolding of ubiquitin in a force-clamp MD simulation.

**Conclusions:** TRFDA can be used, among others, in tracking signal propagation at atomic level, for characterizing dynamical intermolecular interactions (e.g. protein-ligand during flexible docking), in development of force fields and for following stress distribution during conformational changes.

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**Index Terms—**

## I. BACKGROUND

Many biomolecular systems or other complex macromolecules can dynamically visit a broad range of conformational states. External perturbations such as a molecular interaction or a mechanical force can cause a molecule to dynamically transit between these conformational states. While the conformational space of biomolecules is typically analyzed by coordinate-based methods such as the detection of correlated motions, Force Distribution Analysis (FDA) has been recently developed as an alternative approach to analyze structure and structural transitions [1]. The advantages of analyzing internal forces instead of coordinates are two-fold. First, forces between atoms or residues represent internal coordinates, which consequently do not require any structural fitting. Secondly, forces are a more sensitive measure, as they are able to reveal low-amplitude yet functionally important motions such as those in a stiff protein core [2]. Among others, internal forces obtained from FDA proved able to explain the mechanical robustness of immunoglobulin domains [3] and to reveal the pre-stress in ubiquitin [4].

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FDA has been applied so far to averaged dynamical data from Molecular Dynamics (MD) simulations. However, the dynamics of the force distribution within proteins or other 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.

## II. IMPLEMENTATION

### A. 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 [5], [6]) 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 [7], and VMD [8] plugins are provided for visualization. The implementation includes several notable improvements over FDA, which are discussed below.

### B. 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.

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**N. R. Shetty,L. M. Patnaik,N. H.  
Prasad,N. Nalini**



## **Paper Ieee Transactions 2on Communication:**

**Communication Satellites** Donald H. Martin, Paul Robert Anderson, Lucy Bartamian, 2007 Communication Satellites Fifth Edition chronicles the worldwide development of communication satellites over a period of more than four decades Descriptive text and tabular data are presented for experimental and operational satellites of communications and broadcasting systems of individual nations and international organizations Descriptions are enhanced by drawings of satellites communication subsystem block diagrams and coverage maps The book includes extensive references and a supplemental bibliography

**Multifaceted approaches for Data Acquisition, Processing & Communication** Chinmay Chakraborty, Manisha Guduri, B Sandhya, K Shyamala, 2024-06-24 The objective of the conference is to bring to focus the recent technological advancements across all the stages of data analysis including acquisition processing and communication Advancements in acquisition sensors along with improved storage and computational capabilities have stimulated the progress in theoretical studies and state of the art real time applications involving large volumes of data This compels researchers to investigate the new challenges encountered where traditional approaches are incapable of dealing with large complicated new forms of data

*Time Frequency Analysis* Boualem Boashash, 2003-10-16 Time Frequency Signal Analysis and Processing covers fundamental concepts principles and techniques treatment of specialised and advanced topics methods and applications including results of recent research This book deals with the modern methodologies key techniques and concepts that form the core of new technologies used in IT multimedia telecommunications as well as most fields of engineering science and technology It focuses on advanced techniques and methods that allow a refined extraction and processing of information allowing efficient and effective decision making that would not be possible with classical techniques The Author fellow of IEEE for Pioneering contributions to time frequency analysis and signal processing education is an expert in the field having written over 300 papers on the subject over a period of 25 years This is a REAL book not a mere collection of specialised papers making it essential reading for researchers and practitioners in the field of signal processing The most comprehensive text and reference book published on the subject all the most up to date research on this subject in one place Key computer procedures and code are provided to assist the reader with practical implementations and applications This book brings together the main knowledge of time frequency signal analysis and processing TFSAP from theory and applications in a user friendly reference suitable for both experts and beginners

Design Technics Zeynep Çelik Alexander, John May, 2020-01-21 Leading scholars historicize and theorize technology's role in architectural design Although the question of technics pervades the contemporary discipline of architecture there are few critical analyses on the topic Design Technics fills this gap arguing that the technical dimension of design has often been flattened into the broader celebratory rhetoric of innovation Bringing together leading scholars in architectural and design history the volume's contributors situate these tools on a broader epistemological and chronological canvas The essays here

construct histories some panoramic and others unfolding around a specific episode of seven techniques regularly used by the designer in the architectural studio today rendering modeling scanning equipping specifying positioning and repeating Starting with observations about the epistemological changes that have unfolded in the discipline in recent decades but seeking to offer a more expansive meaning for technics the volume casts new light on concepts such as form experience and image that have played central roles in historical architectural discourses Among the questions addressed How was the concept of form immanent in practices of scanning since the late nineteenth century What was the historical relationship between rendering and experience in Enlightenment discourses How did practices of specifying reconfigure the distinction between intellectual and manual labor What kind of rationality is inherent in the designer's constant clicking of the mouse in front of her screen In addressing these and other questions this engaging and timely collection thereby proposes technics as a site for historical and philosophical reflection not only for those engaged in architectural design but also for any scholar working in the humanities today Contributors Lucia Allais Edward Eigen Orit Halpern John Harwood Matthew C Hunter and Michael Osman *Report Number BMI-NLVP-TR-69-2 on Selected Space Goals and Objectives and Their Relation to National Goals, to National Aeronautics and Space Administration, Under Contract Number NASw-1146* G. E. Wukelic, 1969

*Satellite Communications Payload and System* Teresa M. Braun, 2012-08-06 This is the first book primarily about the satellite payload of satellite communications systems It represents a unique combination of practical systems engineering and communications theory It tells about the satellites in geostationary and low earth orbits today both the so called bent pipe payloads and the processing payloads The on orbit environment mitigated by the spacecraft bus is described The payload units e g antennas and amplifiers as well as payload integration elements e g waveguide and switches are discussed in regard to how they work what they do to the signal their technology environment sensitivity and specifications At a higher level are discussions on the payload as an entity architecture including redundancy specifications what they mean how they relate to unit specifications and how to verify and specification compliance analysis budgets with uncertainty Aspects of probability theory handy for calculating and using uncertainty and variation are presented The highest level discussions on the end to end communications system start with a practical introduction to physical layer communications theory Atmospheric effects and interference on the communications link are described A chapter gives an example of optimizing a multibeam payload via probabilistic analysis Finally practical tips on system simulation and emulation are provided The carrier frequencies treated are 1 GHz and above Familiarity with Fourier analysis will enhance understanding of some topics References are provided throughout the book for readers who want to dig deeper Payload systems engineers payload proposal writers satellite communications systems designers and analysts and satellite customers will find that the book cuts their learning time Spacecraft bus systems engineers payload unit engineers and spacecraft operators will gain insight into the overall system Students in systems engineering microwave engineering communications theory probability theory and

communications simulation and modelling will find examples to supplement theoretical texts     Emerging Research in Computing, Information, Communication and Applications N. R. Shetty, L. M. Patnaik, N. H. Prasad, N. Nalini, 2017-11-15 This book presents the proceedings of International Conference on Emerging Research in Computing Information Communication and Applications ERCICA 2016 ERCICA provides an interdisciplinary forum for researchers professional engineers and scientists educators and technologists to discuss debate and promote research and technology in the upcoming areas of computing information communication and their applications The book discusses these emerging research areas providing a valuable resource for researchers and practicing engineers alike     *IEICE Transactions on Communications , 3DTV Content Capture, Encoding and Transmission* Daniel Minoli, 2010-12-28 The First to Present 3D Technology as Applied to Commercial Programming for the Consumer This is the first book to provide an overview of the technologies standards and infrastructure required to support the rollout of commercial real time 3 Dimension Television 3 Dimension Video 3DTV 3DV services It reviews the required standards and technologies that have emerged or are just emerging in support of such new services with a focus on encoding mechanisms formats and the buildout of the transport infrastructure While there is a lot of academic interest in various intrinsic aspects of 3DTV service providers and consumers ultimately tend to take a system level view 3DTV stakeholders need to consider the overall architectural system level view of what it will take to deploy an infrastructure that is able to reliably and cost effectively deliver a commercial grade quality bundle of multiple 3DTV content channels to paying customers with high expectations This text therefore takes such a system level view revealing how to actually deploy the technology Presented in a self contained tutorial fashion the book begins with a review of 3DTV in the marketplace and the opportunities and challenges therein Recent industry events related to 3D are also discussed From there the fundamental visual concepts supporting stereographic perception of 3DTV 3DV are explained as are encoding approaches Readers will understand frame mastering and compression for conventional stereo video CSV and more advanced methods such as video plus depth V D multi view video plus depth MV D and layered depth video LDV Next the elements of an end to end 3DTV system are covered from a satellite delivery perspective with explanations of digital video broadcasting DVB and DVB handheld Transmission technologies are assessed for terrestrial and IPTV based architecture IPv6 is reviewed in detail Finally the book presents 3DTV 3DV standardization and related activities which are critical to any type of broad deployment System planners the broadcast TV industry satellite operators Internet service providers terrestrial telecommunication carriers content developers design engineers venture capitalists and students and professors are among those stakeholders in these services and who will rely on this volume to discover the latest 3D advances market opportunities and competing technologies     Report of NRL Progress Naval Research Laboratory (U.S.), 1973     11th International Conference on Magnet Technology (MT-11) T. Sekiguchi, S. Shimamoto, 2012-12-06 Over the years the aim of the International Conference on Magnet Technology has been the exchange of information on the design construction and

operation of magnets for a variety of applications such as high energy physics fusion electrical machinery and others The aim has included advances in materials for magnet conductors insulators and supporting structures Since its inception the focus of the International Conference on Magnet Technology has gradually shifted to superconducting magnets Now almost all papers are related to superconductivity The 11th International Conference on Magnet Technology MT 11 was organized by the combined efforts of the Institute of Electrical Engineers of Japan the Association for Promotion of Electrical Electronic and Information Engineering and the Tokyo Section of the IEEE The Conference was held at the Tsukuba University Hall Tsukuba Japan from 28 August to 1 September 1989 courtesy of the University of Tsukuba The Tsukuba University Hall was large enough to host invited talks parallel sessions poster sessions and industrial exhibitions 461 participants from 19 countries registered for MT 11 and 280 invited and contributed papers were presented The papers were reviewed not only by the Program Committee but also by foreign participants Working sessions and social events were characterized by a truly international atmosphere Scientific as well as cultural excursions were organized so that foreign visitors could experience the spirit of modern Japan 26 companies of which 8 were from Western countries participated in the industrial exhibition which featured diverse products and services of interest to the magnet community

**Essays on Coding Theory** Ian F. Blake, 2024-03-14 Brief informal introductions to coding techniques developed for the storage retrieval and transmission of large amounts of data

**Mobile Networks and Management** Ramón Agüero, Thomas Zinner, Rossitza Goleva, Andreas Timm-Giel, Phuoc Tran-Gia, 2015-02-27 This book constitutes the post proceedings of the 6th International ICST Conference on Mobile Networks and Management MONAMI 2014 held in Würzburg Germany in September 2014 The 22 revised full papers presented were carefully reviewed and selected from 30 submissions In addition MONAMI 2014 hosted a workshop on enhanced living environments which also featured 10 papers The volume is organized thematically in six parts covering LTE networks virtualization and software defined networking self organizing networks energy awareness in wireless networks wireless networks algorithms and techniques and applications and context awareness The workshop on enhanced living environments is organized in thematic sessions on ambient assisted living architectures human interaction technologies devices and mobile cloud

Traffic Systems Reviews and Abstracts United States. Federal Highway Administration, 1968

**Selected papers from the 2019 IEEE International Workshop on Metrology for AeroSpace** Pasquale Daponte, Eulalia Balestrieri, 2021-04-21 This book is devoted to recent developments of instrumentation and measurement techniques applied to the aerospace field It includes 23 selected papers from the 2019 IEEE International Workshop on Metrology for AeroSpace Measurements are essential for obtaining a deeper knowledge of a phenomenon or an asset as well as for making proper decisions and proposing new and efficient solutions and this is especially true in environments as complex as aerospace The research contributions included in the book can raise the interest of a wide group of researchers operators and decision makers from metrology and aerospace fields by presenting the most innovative

solutions in this field from the scientific and technological points of view      *Imaging and Vision Systems* Jacques Blanc-Talon, 2001 *Imaging Vision Systems Theory Assessment Applications Advances in Computation Theory Practice Volume 9*      **Advances in Computer Communications and Networking**, 1979      **The Transactions of the Institute of Electronics and Communications Engineers of Japan** Denshi Tsūshin Gakkai, 1985      High Speed Networks and Multimedia Communications Zoubir Mammeri, Pascal Lorenz, 2004-09-21 Nowadays networks and telecommunications are two of the most active fields. Research and development in these areas have been going on for some time reaching the stage of products. The objectives of HSNMC 2004 International Conference on High Speed Networks and Multimedia Communications were to promote research and development activities and to encourage communication between academic researchers and engineers throughout the world in the areas related to high speed networks and multimedia communications. The seventh edition of HSNMC was held in Toulouse France on June 30 July 2 2004.

There were 266 submissions to HSNMC this year from 34 countries which were evaluated by program committee members assisted by external viewers. Each paper was reviewed by several reviewers. One hundred and one papers were selected to be included in these proceedings. The quality of submissions was high and the committee had to decline some papers worthy for publication. The papers selected in this book illustrate the state of the art, current discussions and development trends in the areas of networks, telecommunication and multimedia applications. The contributions published in this book underline the international importance of the related field of research. They cover a variety of topics such as QoS in Diff-Serv networks, QoS analysis and measurement, performance modelling, TCP modelling and analysis, MPLS for QoS provision, scheduling and resource allocation, routing, multicast, security and privacy issues, peer-to-peer applications, video applications, software and middleware for networks, mobile networks, mobility, satellite, mobile IP, wireless networks, WLAN, ad hoc networks, 3G, UMTS, IEEE 802.

**Coding Theory and Applications** Angela Barbero, 2008-08-26 It is a pleasure to welcome you to the proceedings of the second International Castle Meeting on Coding Theory and its Applications held at La Mota Castle in Medina del Campo. The event provided a forum for the exchange of results and ideas which we hope will foster future collaboration. The first meeting was held in 1999 and encouraged by that experience we now intend to hold the meeting every three years. Springer kindly accepted to publish the proceedings volume you have in your hands in their LNCS series. The topics were selected to cover some of the areas of research in Coding Theory that are currently receiving the most attention. The program consisted of a mixture of invited and submitted talks with the focus on quality rather than quantity. A total of 34 papers were submitted to the meeting. After a careful review process conducted by the scientific committee aided by external reviewers we selected 14 of these for inclusion in the current volume along with 5 invited papers. The program was further augmented by the remaining invited papers in addition to papers on recent results printed in a separate volume. We would like to thank everyone who made this meeting possible by helping with the practical and scientific preparations, the organization committee, the scientific

committee the invited speakers and the many external reviewers who shall remain anonymous I would especially like to mention the General Advisor of the meeting yvind Ytrehus Finally I extend my gratitude to all the authors and participants who contributed to this meeting



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