

entropy
2021

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Welcome from the Chair

The concept of entropy emerges initially from the scope of physics, but it is now clear that entropy is deeply related to information theory and the process of inference. Today, entropic techniques have found a broad spectrum of applications in all branches of science.

The conference will be organized into six sessions, which reflect the inter-disciplinary nature of entropy and its applications:

- Statistical Physics
- Information Theory, Probability and Statistics
- Thermodynamics
- Quantum Information and Foundations
- Complex Systems
- Entropy in Multidisciplinary Applications

The inter-disciplinary and multi-disciplinary nature of contributions from both theoretical and applied perspectives are welcome, including papers addressing conceptual and methodological developments, as well as new applications of entropy and information theory.

The conference is sponsored by MDPI, the publisher of the open-access journal *Entropy* and follows the very successful meeting **Entropy 2018: From Physics to Information Sciences and Geometry** held in May 2018 in Barcelona, Spain.

We very much look forward to your participation.



Prof. Dr J. A. Tenreiro Machado
Conference Chair

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entropy

an Open Access Journal by MDPI

Entropy (ISSN 1099-4300; CODEN: ENTRFG) is an international and interdisciplinary peer-reviewed open access journal of entropy and information studies, published monthly online by MDPI. The International Society for the Study of Information (IS4SI) and Spanish Society of Biomedical Engineering (SEIB) are affiliated with Entropy and their members receive a discount on the article processing charge. Among other databases, Viruses is indexed by the Science Citation Index Expanded (Web of Science), MEDLINE (PubMed) and other databases. Full-text available in PubMed Central.

Journal Webpage: <https://www.mdpi.com/journal/entropy>

Impact factor: **2.494** (2019)

5-Year Impact Factor: 2.530 (2019)

Invited Speakers

Invited Speakers



Prof. Dr. Kevin H. Knuth
University at Albany (SUNY),
Albany, NY, USA



Prof. Dr. Miguel Rubi
University of Barcelona,
Barcelona, Spain



Prof. Dr. Philip Broadbridge
La Trobe University,
Melbourne, Australia



Dr. Remo Garattini
University of Bergamo,
Bergamo, Italy



Prof. Dr. Nihat Ay
Max Planck Institute for
Mathematics in the Sciences,
Leipzig, Germany



Prof. Dr. Abraham Marmur
Technion-Israel Institute of
Technology, Haifa, Israel



Dr. Rosario Lo Franco
Università di Palermo, Italy



**Prof. Dr. Miguel A. F.
Sanjuán** Universidad Rey
Juan Carlos, Madrid, Spain

Program at a Glance

Program Structure			
	Wednesday 5 May 2021	Thursday 6 May 2021	Friday 7 May 2021
Morning	Opening Ceremony Session 1 - <i>Entropy in Multidisciplinary Applications (Part 1)</i>	Session 1 - <i>Entropy in Multidisciplinary Applications (Part 4)</i>	Session 5 - <i>Complex Systems (Part 2)</i>
	Session 2 - <i>Information Theory, Probability and Statistics (Part 1)</i>	Session 4 - <i>Statistical Physics (Part 1)</i>	Session 1 - <i>Entropy in Multidisciplinary Applications (Part 6)</i>
	Session 1 - <i>Entropy in Multidisciplinary Applications (Part 2)</i>	Session 1 - <i>Entropy in Multidisciplinary Applications (Part 5)</i>	Session 5 - <i>Complex Systems (Part 3)</i>
	Posters Discussion (1A & 1B)	Session 5 - <i>Complex Systems (Part 1)</i>	
	Lunch break		
Afternoon	Session 3 - <i>Quantum Information and Foundations</i>	Session 2 - <i>Information Theory, Probability and Statistics (Part 2)</i>	Session 6 - <i>Thermodynamics</i>
	Session 1 - <i>Entropy in Multidisciplinary Applications (Part 3)</i>	Session 4 - <i>Statistical Physics (Part 2)</i>	Session 1 - <i>Entropy in Multidisciplinary Applications (Part 7)</i>
		Posters Discussion (2A & 2B)	Closing Remarks & Awards Ceremony

Conference Program

Day 1: Wednesday 5 May 2021

08:00-08:15 **Opening Ceremony**

08:15-08:45 **Philip Broadbridge** (Invited Speaker): Pushing the thermodynamics/information analogy: Entropy behaviour of PDEs

Session 1 - Entropy in Multidisciplinary Applications (Part 1)

Chair: Nidia Caetano/Didier Leibovici

09:00-09:15 **William Bruce Sherwin:** Do Entropic Biodiversity Methods Outcompete Alternatives?

09:15-09:30 **Ivan Kennedy, Migdat Hodzic:** Action and entropy in heat engines: An action revision of the Carnot cycle

09:30-09:45 **Noor Al-Qazzaz, Mohannad Sabir, Sawal Ali, Siti Anom Ahmad, Karl Grammer:** Electroencephalogram Brain Mapping for revealing the emotional changes over the brain regions using Entropy biomarker

Session 2 - Information Theory, Probability and Statistics (Part 1)

Chair: Miguel A. F. Sanjuan /Gil Ariel

10:00-10:15 **Monika Pinchas, Hagar Turgeman:** A Novel Technique for Achieving the Approximated ISI at the Receiver for a 16QAM Signal sent via a FIR Channel based only on the Received Information and Statistical Techniques

10:15-10:30 **Ronit Bustin:** On the CTW-based Entropy Estimator

10:30-10:45 **Second Bwanakare:** On Superstar-Generalized Statistical Regression

10:45-11:00 **Gil Ariel:** Estimating differential entropy using recursive copula splitting

Session 1 - Entropy in Multidisciplinary Applications (Part 2)

Chair: William Bruce Sherwin/Ivan Kennedy

11:15-11:30 **Anastasiia Bakhchina:** The sample entropy of inter spike-intervals as a possible measure of relations between neuronal activity and individuum behaviour

11:30-11:45 **Karsten Keller, Tim Gutjahr:** Ordinal pattern based analysis: From change probabilities to asymmetries

- 11:45-12:00 **Yair Neuman, Yochai Cohen:** Max Entropy through Natural Interactions
- 12:00-12:15 **Marina Barulina, Dmitry Kondratov:** Modeling the sensing element of pressure nanosensors as simply supported size-dependent rectangular plate
- 12:15-13:00 **Posters Discussion (Part 1)**
Chair: Geert Verdoolaege/Claudiu Vinte
- 13:00-14:00 **Lunch break**
- 14:00-14:30 **Rosario Lo Franco (Invited Speaker):** Robust entanglement preparation through spatial indistinguishability quantified by entropic measure

Session 3 - Quantum Information and Foundations

Chair: Rosario Lo Franco/Stephan Weis

- 14:45-15:00 **Ofir Flom, Asher Yahalom, Haggai Zilberberg, Lawrence Horwitz, Jacob Levitan:** Tunneling as a Source for Quantum Chaos
- 15:00-15:15 **Ilya Spitkovsky, Stephan Weis:** Analysis of generalized Gibbs states
- 15:15-15:30 **Thomas Dittrich, Óscar Rodríguez:** Quantum chaos and quantum randomness—paradigms of quantum entropy production
- 15:45-16:15 **Kevin H. Knuth (Invited Speaker):** Entropy: The Evolution of a Concept

Session 1 - Entropy in Multidisciplinary Applications (Part 3)

Chair: Yair Neuman/William R. Cannon

- 16:30-16:45 **Santiago Gómez-Guerrero, Miguel García-Torres, Gustavo Sosa-Cabrera, Emilio Sotto-Riveros, Christian E. Schaerer:** Classifying dengue cases using CatPCA in combination with the MSU correlation
- 16:45-17:00 **Edgar Olivares Mañas, Richard Donovan:** Correlating the entropy of a fluid with live collective behaviors.
- 17:00-17:15 **Andres Orozco, Juan Ugarte, Catalina Tobón:** Cross recurrence quantification analysis as a tool for detecting rotors in atrial fibrillation: an in silico study

- 17:15-17:30 **Andrés García-Medina:** Network Analysis of Multivariate Transfer Entropy of Cryptocurrencies in Times of Turbulence
- 17:30-17:45 **Givanildo Nascimento-Jr, Cristopher Freitas, Osvaldo Rosso, André Aquino:** Causal Entropy-Complexity Plane with Multivariate Probability Distribution
- 17:45-18:00 **Alexej Parchomenko, Dirk Nelen, Jeroen Gillabel, Karl Vrancken, Helmut Rechberger:** Electrification of the passenger car fleet and its effect on resource use – a Statistical Entropy Analysis perspective

Day 2: Thursday 6 May 2021

Session 1 - Entropy in Multidisciplinary Applications (Part 4)

Chair: Walter Lacarbonara/Ivan Kennedy

- 08:00-08:15 **Bilena Almeida, Mohamed Bahrudeen, Vatsala Chauhan, Cristina Palma, Ines Baptista, Suchintak Dash, Vinodh Kandavalli, Andre Ribeiro:** Information Entropy of Single-Gene Expression Responses During Genome Wide Perturbations
- 08:15-08:30 **Jesús Malo:** Information flow in Color Appearance Neural Networks
- 08:30-08:45 **Claudiu Vinte, Marcel Ausloos, Titus Furtună:** The Intrinsic Entropy as Substitute for the Market Volatility of Underlying Securities
- 09:00-09:30 **J. Miguel Rubi (Invited Speaker):** Entropic transport in confined soft-matter and biological systems

Session 4 - Statistical Physics (Part1)

Chair: Eugenio Vogel/Asher Yahalom

- 09:45-10:00 **Frank Lad:** A stunning realisation: the touted defiance of Bell's inequality by quantum probabilities derives from a mathematical error
- 10:00-10:15 **Alberto Megías, Andrés Santos:** Kullback-Leibler Divergence of a Freely Cooling Granular Gas of Inelastic Hard Disks and Spheres
- 10:15-10:30 **Jan Korbel, Simon Lindner, Rudolf Hanel, Stefan Thurner:** Thermodynamics of systems with emergent molecule structures

Session 1 - Entropy in Multidisciplinary Applications (Part 5)

Chair: Philip Broadbridge/Claudiu Vinte

- 10:45-11:00 **Renata Rychtáriková, Georg Steiner, Gero Kramer, Michael Fischer, Dalibor Štys:** Application of Rényi entropy-based 3D electromagnetic centroids to segmentation of fluorescing objects in tissue sections
- 11:00-11:15 **Didier Leibovici, Christophe Claramunt, Shaun Quegan:** Evaluating spatial and temporal fragmentation of a categorical variable using new metrics based on entropy: example of vegetation land cover
- 11:15-11:30 **Miguel Garcia Torres, Federico Divina, Francisco A. Gómez Vela, José Luis Vázquez Noguera:** A Fast Multivariate Symmetrical Uncertainty based heuristic for high dimensional feature selection
- 11:30-11:45 **Kranti Navare, Karl Vrancken, Karel Van Acker:** Statistical entropy analysis to evaluate cascading use of wood

Session 5 - Complex Systems (Part1)

Chair: Nihat Ay/Adam Gadomski

- 12:00-12:15 **Thomas Tarenzi, Marta Rigoli, Raffaello Potestio:** Information routing in proteins: the case of a therapeutic antibody
- 12:15-12:30 **Tim Gutjahr, Karsten Keller:** Conditional permutation entropy as a measure for the complexity of dynamical systems
- 12:30-12:45 **Raffaello Potestio:** Representation and information in molecular modelling
- 12:45-13:00 **Matthew Morena, Kevin Short:** Chaotic Entanglement: Entropy and Geometry

13:00-14:00 **Lunch break**

- 14:00-14:30 **Miguel Sanjuán (Invited Speaker):** Basin Entropy: A new Method to Measure Unpredictability in Physical Systems

Session 2 - Information Theory, Probability and Statistics (Part 2)

Chair: Geert Verdoolae/Gil Ariel

- 14:45-15:00 **Themis Matsoukas:** Thermodynamics Beyond Molecules: Statistical Mechanics of Probability Distributions and Stochastic Processes
- 15:00-15:15 **Themis Matsoukas:** Entropy, Statistical Thermodynamics and Stochastic Processes

- 15:15-15:30 **Santiago Gómez-Guerrero, Gustavo Sosa-Cabrera, Miguel García-Torres, Inocencio Ortiz-Samudio, Christian E. Schaerer:** Multivariate Symmetrical Uncertainty as a measure for interaction in categorical patterned datasets
- 15:30-15:45 **Pedro Pessoa, Felipe Costa, Ariel Caticha:** Entropic dynamics on Gibbs statistical manifolds
- 15:45-16:00 **Shayan Hundrieser, Marcel Klatt, Axel Munk:** Entropic Optimal Transport on Countable Spaces: Statistical Theory and Asymptotics
- 16:00-16:15 **Francisco J Valverde-Albacete, Carmen Peláez Moreno:** Informational harmoniums

Session 4 - Statistical Physics (Part 2)

Chair: Miguel Rubi/Eugenio Vogel

- 16:30-16:45 **Oscar Negrete, Francisco Peña, Patricio Vargas, Eugenio Vogel, Gonzalo Saravia:** New parameters and extensive methodology to describe the three phase transitions in the q-states clock model
- 16:45-17:00 **Alma Mendez:** The fundamental diagram in vehicular traffic
- 17:00-17:15 **Guillermo Chacón-Acosta:** Entropy production of reaction-diffusion systems under confinement
- 17:15-18:00 **Posters Discussion (Part 2)**

Chair: Federico Fogolari/Nikos Karayiannis

Day 3: Friday 7 May 2021

Session 5 - Complex Systems (Part 2)

Chair: Adam Gadomski/Nataliya Stankevich

- 08:00-08:15 **Nataliya Stankevich:** Different scenarios leading to hyperchaos development in radiophysical generators
- 08:15-08:30 **Adam Gadomski:** Walking down over the spatiotemporal scales in a particular nonequilibrium-thermodynamics dissipative phenomenon called friction
- 08:30-08:45 **Miguel Herranz, Pablo Ramos, Katerina Foteinopoulou, Nikos Karayiannis, Manuel Laso:** Simulation Studies of Entropy-Driven Crystallization in Athermal Chain Packings in the Bulk and Under Confinement

09:00-09:30 **Nihat Ay (Invited Speaker):** Information Geometry & Complexity Science

Session 1 - Entropy in Multidisciplinary Applications (Part 6)

Chair: Andre Ribeiro/Karsten Keller

- 09:45-10:00 **Frank van Ruitenbeek, Jasper Goseling, Wim Bakker, Kim Hein:** Shannon entropy and hydrothermal processes
- 10:00-10:15 **Arnas Survyla, Benas Kemesi, Renaldas Urniežius:** Entropy Measure for Planning, Prediction and Online Estimation in Biotechnological Processes
- 10:15-10:30 **Silvin Knight, Louise Newman, John O'Connor, Rose Anne Kenny, Roman Romero-Ortuno:** Approximate entropies of resting state continuous neurocardiovascular physiological signals are associated with physical frailty in older adults
- 10:30-10:45 **Antonio Davalos, Meryem Jabloun, Olivier Buttelli, Philippe Ravier:** On the Implementation of Downsampling Permutation Entropy variants in the detection of Bearing Faults in Rotatory Machines
- 11:00-11:30 **Remo Garattini (Invited Speaker):** Aspects of Gravity's Rainbow in Black Hole Entropy

Session 5 - Complex Systems (Part 3)

Chair: Nikos Karayiannis/Nataliya Stankevich

- 11:45-12:00 **Carlotta Langer, Nihat Ay:** Complexity as causal information integration
- 12:00-12:15 **Miguel Aguilera, S. Amin Moosavi, Hideaki Shimazaki:** An information geometry approach for unifying mean field theories of asymmetric kinetic Ising systems
- 12:15-12:30 **Stanisław Niepostyn:** Entropy in Software Architecture
- 12:30-12:45 **Roberto Menichetti:** On the search of minimum information loss in coarse-grained modelling of biomolecules
- 12:45-13:45 **Lunch break**
- 13:45-14:15 **Abraham Marmur (Invited Speaker):** The mathematical state of equations of state

Session 6 - Thermodynamics

Chair: Abraham Marmur/Federico Fogolari

- 14:30-14:45 **Federico Fogolari:** Conformational and translational-rotational entropy from molecular ensembles
- 14:45-15:00 **Róbert Kovács, Patrizia Rogolino:** Analysis of the nonlinear Maxwell-Cattaneo-Vernotte equation
- 15:00-15:15 **Julian Gonzalez-Ayala, Alejandro Medina Dominguez, Jose Miguel Mateos Roco, Antonio Calvo Hernández:** Stability under limited control in weakly dissipation cyclic heat engines
- 15:15-15:30 **R. Leticia Corral-Bustamante:** The Entropy of Supermassive Black Holes during its Evaporation Time
- 15:30-15:45 **Gian Paolo Beretta:** The Fourth Law of Thermodynamics: every nonequilibrium state is characterized by a metric in state space with respect to which its spontaneous attraction towards stable equilibrium is along the path of steepest entropy ascent

Session 1 - Entropy in Multidisciplinary Applications (Part 7)

Chair: Kevin Knuth/William R. Cannon

- 16:00-16:15 **Xavier Zamora, Angel Cuadras:** Entropy Measurements with Infrared Sensors
- 16:15-16:30 **Ellis Scharfenaker:** Quantal Response Statistical Equilibrium: A New Class of Maximum Entropy Distributions
- David Galas, James Kunert-Graf, Nikita Sakhanenko:** Developing an information theory of quantitative genetics
- 16:30-16:45 **Juan Ugarte, Catalina Tobón, Antonio Mendes Lopes, Jose Tenreiro Machado:** The atrial resting potential distribution within a fibrotic zone and its effects on the conduction on non-fibrotic zones: A simulation study
- 16:45-17:00 **William R. Cannon, Sam Britton, Mark Alber:** Cracking the Code of Metabolic Regulation in Biology using Maximum Entropy/Caliber and Reinforcement Learning
- 17:30-18:00 **Closing Remarks & Awards Ceremony**

Poster Lists

5 May 2021

Information Theory, Probability and Statistics (Posters 1A)

- 29156 **Rémi Besson, Erwan Le Pennec, Stéphanie Allasonnière:** A Model-Based Reinforcement Learning Approach for a Rare Disease Diagnostic Task
- 29276 **Andreia Teixeira, André Souto, Luís Antunes:** On Conditional Tsallis Entropy
- 30038 **Marco Wilhelm, Gabriele Kern-Isberner:** Predicting Human Responses to Syllogism Tasks Following the Principle of Maximum Entropy
- 30222 **Maria Ribeiro, Teresa Henriques, Luísa Castro, Andreia Teixeira, André Souto, Luís Antunes, Cristina Costa-Santos:** The Entropy Universe
- 30229 **Masayuki Henmi:** Information Geometry of Estimating Functions in Parametric Statistical Models
- 30271 **Hiroshi Matsuzoe:** Gauge freedom of entropies on q-Gaussian distributions
- 30295 **João S. Resende, Marco Almeida, Rolando Martins, Luís Antunes:** A Kolmogorov Complexity for multidisciplinary domains
- 43535 **Anastasia Malashina:** Entropy analysis of n-grams and estimation of the number of meaningful language texts
- 43584 **Francesco Buono:** A Dual Measure of Uncertainty: The Deng Entropy
- 44156 **Federica Parisi, Tiziano Squartini, Diego Garlaschelli:** Generalized inference for the efficient reconstruction of weighted networks
- 44173 **Andrea Somazzi, Diego Garlaschelli:** Constraint choice and model selection in the generalized maximum entropy principle

Entropy in Multidisciplinary Applications (Posters 1B)

- 28896 **Takuya Yamano:** Fisher information of Landau states and relative information against the lowest level
- 30218 **Luísa Castro, Filipa Barros, Sandra Soares, Susana Brás:** ECG and EDA information transfer on emotion evaluation
- 32537 **Alexandre Carvalho, José Príncipe:** Hellinger Entropy Concept: multidisciplinary applications.
- 43475 **Caroline Roithner, Helmut Rechberger:** Statistical entropy opens a new way to assess the recyclability of products

- 44112 **Kazuko Sugimoto, Tsuneyoshi Sugimoto:** Detection of internal defects in concrete and evaluation of a healthy part of concrete by non-contact acoustic inspection using normalized spectral entropy
- 44153 **Gustavo Bertoli, Guilherme Koga, Fernanda Puosso, Amy Clarke, Claudio Kiminami, Francisco Coury:** Design of high-C Cr-Co-Ni medium entropy alloy for tribological applications
- 44174 **Angel Rico, Angel Cuadras:** Near Zero Energy Buildings Entropy Performance
- 44177 **Martí Garcia-Corominas, Angel Cuadras:** Battery Charge and Discharge Strategies in Terms of Entropy Production
- 44181 **Mirjana Platiša, Nikola Radovanović, Goran Milašinović, Siniša Pavlović:** Sample entropy approach to the examination of cardio-respiratory coupling in response to cardiac resynchronization therapy
- 44191 **José María López Belinchón, Miguel Ángel López Guerrero, Raúl Alcaraz Martínez:** On the estimation the probability of cardiovascular and cerebrovascular events in hypertensive patients using nonlinear analysis, time and frequency domain methods.
- 44198 **Nesma Houmani, Majd Abazid, Jerome Boudy, Bernadette Dorizzi:** Epoch-based Entropy : A Statistical EEG Marker for Alzheimer's Disease Detection
- 44208 **Marzio Di Vece, Tiziano Squartini, Diego Garlaschelli:** From Network Reconstruction to Network Econometrics: unbiased estimation of average effects
- 44214 **Tommaso Radicioni, Tiziano Squartini, Fabio Saracco:** Analysing discursive communities and semantic networks on Twitter: an entropy-based approach
- 44218 **Ana Paula Rocha, Helder Pinto, Celestino Amado, Maria Eduarda Silva, Riccardo Pernice, Michal Javorka, Luca Faes:** Assessing Transfer Entropy in cardiovascular and respiratory time series: A VARFI approach
- 44245 **Yasunari Zempo, Satoru Kano:** Maximum Entropy Method Applied to Time-series Data in Real-time Time-Dependent Density Functional Theory

6 May 2021

Statistical Physics (Posters 2A)

- 28983 **Charles Roberto Telles:** Work sharing as a metric and productivity indicator for administrative workflows
- 30294 **Ana Laura Garcia-Perciante, Marco Alvarez, Alma Mendez:** A kinetic model for pedestrian evacuation in a corridor with an aggressive sparse countercurrent.

- 30300 **Guillermo Chacón-Acosta, Ana García-Perciante, Alma Sagaceta-Mejía:** On the relation of Eckart and Landau-Lifshitz reference frames for higher orders in the dissipative fluxes couplings
- 43622 **Oleksandr Kliushnichenko, Sergey Lukyanets:** Nonlinear dynamical screening effects and strong local fluctuations of drag forces in collective scattering of particle streams on impurity ensembles
- 44158 **Tiziano Squartini, Joey de Mol, Frank den Hollander, Diego Garlaschelli:** Breaking of ensemble equivalence in networks
- 29138 **Eugenio Vogel, Julian Riccardo, José Riccardo, Pedro Pasinetti, Antonio Ramirez-Pastor:** Adsorption of long straight rigid rods on two-dimensional lattices: study of orientational surface phase transitions from entropic considerations

Information Theory, Probability and Statistics (Posters 2A)

- 32529 **Khoder Makkawi, Nourdine AIT-TMAZIRTE, Maan El Badaoui El Najjar, Nazih Moubayed:** General entropy-based framework for a robust and fail-safe multi-sensor data fusion

Complex Systems (Posters 2A)

- 29275 **Rafael M Gutierrez, Chandrashekhar U Murade, Jianfeng Guo, George Shubeita:** Entropy and entropic forces to model biological fluids
- 29325 **Javier Benito, Oscar Parreño, Miguel Herranz, Pablo Ramos, Nikos Karayiannis, Manuel Laso:** Confined Polymers as Self-Avoiding Random Walks on Restricted Lattices
- 30055 **Marta Rigoli:** Investigating the structure-dynamics-function relationship in antibodies
- 30064 **Marco Giuliani:** Measurement and minimisation of the Mapping Entropy of a Coarse-Grained biomolecular system
- 30110 **Laura Angioletti, Michela Balconi:** Complexity inside and outside the brain: how to manage internal (interoceptive) and external (domotics) environment during adaptive inter-actions
- 30251 **Maria Ribeiro, Luísa Castro, Luís Antunes, Cristina Costa-Santos, Teresa Henriques:** Complexity as cardiorespiratory coupling measure in neonates with different gestational ages
- 44171 **Daniel Martínez-Fernández, Clara Pedrosa, Miguel Herranz, Katerina Foteinopoulou, Nikos Karayiannis, Manuel Laso:** Entropy-driven Phase Transition of Semiflexible Hard-Sphere Polymer Packings in Two and Three Dimensions
- 44201 **Vassilios Gavriil, Alkiviadis-Constantinos Cefalas, Zoe Kollia, Evangelia Sarantopoulou:** Chaotic and thermodynamic interplay in nanocavities

Entropy in Multidisciplinary Applications (Posters 2B)

- 29112 **Qiang Li, Emmanuel Johnson, Jose Juan Esteve-Taboada, Valero Laparra, Jesús Malo:** Computing variations of entropy and redundancy under nonlinear mappings not preserving the signal dimension: quantifying the efficiency of V1 cortex
- 29203 **Andreia F. Gaudêncio, Mirvana Hilal, Pedro G. Vaz, João M. Cardoso, Anne Humeau-Heurtier:** Bi-dimensional colored fuzzy entropy applied to melanoma dermoscopic images
- 29249 **Johannes Bleher, Thomas Dimpfl:** Estimation of Relative Entropy Measures based on Quantile Regression
- 29286 **Juan Luis Crespo Mariño, Ricardo Monge-Gapper:** Preliminary study of entropy-based indicators to discriminate cancer-related characteristics.
- 29311 **Raimundo Real, Alba Estrada:** A stepwise assessment of parsimony and entropy in species distribution modelling
- 29348 **Dalibor Štys, Stefan Tangl, Renata Rychtáriková:** Superresolved light microscopy information on the structure of the stained dental tissue section obtained by point divergence gain analysis
- 29521 **Omar Velazquez Martinez, Annukka Santasalo-Aarnio, Markus Reuter, Rodrigo Serna-Guerrero:** Case studies of Statistical Entropy Analysis in Recycling Processes: A tool in Support of a Circular Economy
- 29885 **João Carvalho, Susana Brás, Armando Pinho:** Entropy-Based ECG Biometric Identification
- 30175 **Migdat Hodzic, Ivan Kennedy:** Entropy of Vostok Ice Core Data and Kalman Filter Harmonic Bank Climate Predictor
- 32526 **Qiang Li:** Measuring Functional Connectivity of Human Intra-Cortex Regions with Total Correlation
- 44132 **Walter Legnani, Marco Baldiviezo, Camila Bontempo, Yanina Corsaro, Juan Fernandez Biancardi, Adrian Paglia, Masia Hernando, Matías Rodriguez:** Evaluation of the performance of permutation entropy variants for classifying auditory evoked potentials
- 44154 **Diego Santana, Kayque Santos, Claudio Kiminami, Francisco Coury:** Design and characterization of Cr_{29.7}Co_{29.7}Ni_{35.4}Al_{4.0}Ti_{1.2} precipitation hardened high entropy alloy
- 44185 **Jordao Oliveira, Ivonete Avila, Marcelo Pinheiro, Carlos Maciel:** Entropy: from Thermodynamics to Information Theory

Thermodynamics (Posters 2B)

- 28919 **Ilias Tyrovolas:** New Explanation for the Mpemba effect

- 29657 **Francisco Peña, Patricio Vargas, Oscar Negrete:** Quasistatic and quantum-adiabatic Otto engine for a two-dimensional material: The case of a graphene quantum dot
- 30309 **Peter Ván:** Dissipative extension of Electrodynamics
- 44169 **Ruth Estephania Gonzalez Narvaez, Federico Vazquez Hurtado, Mariano López de Haro:** The minimum entropy production principle and heat transport in solids with internal structure
- 44184 **Ricardo T Páez-Hernández, Juan Carlos Chimal-Eguía, Juan Carlos Pacheco-Paez:** Comparative performance analysis of a Brownian Carnot cycle from the perspective of a stochastic model against the Linear Irreversible Thermodynamics theory.
- 44190 **Luis Eduardo Vidal-Miranda, Juan Carlos Chimal-Eguía, Juan Carlos Pacheco-Paez, Ricardo Teodoro Páez-Hernández:** Efficiency of an arrangement in series of irreversible thermal engines working at maximum power.

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Abstracts

Oral Presentations

Pushing the Thermodynamics/Information Analogy: Entropy Behaviour of PDEs

sciforum-029536

Philip Broadbridge

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It is easily seen that the heat-flow statement of 2nd law of thermodynamics is equivalent to information irreversibility when $p(x,t)$ satisfies a general nonlinear 2nd order diffusion equation. In many situations the viscosity solution of a nonlinear wave equation is that which maintains a specified conservation law and maximizes the entropy jump at a shock. There are some systems in which information is not monotonic and yet it would be helpful to view entropy as predominantly increasing: (i) Heat and mass transport in the plasma universe cannot be represented by classical diffusion with unbounded speed of propagation. The simplest phenomenological correction to the hyperbolic diffusion equation is predominantly irreversible. (ii) A pure quantum state satisfying the Schrödinger equation. By the Hopf-Cole transformation this is equivalent to the momentum equation of the irrotational Madelung fluid. However interventionist measurement induces vorticity in the fluid, which dissipates along with entropy increase during collapse to an eigen-state. While vorticity is present a full description requires a vector potential as well as the Schrödinger potential. (iii) So-called fourth-order diffusion is information-irreversible only for an identified class of nonlinear diffusivities.



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Do Entropic Biodiversity Methods Outcompete Alternatives?

sciforum-029220

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The journal 'Entropy' is full of elegant entropy/information approaches for all aspects of biology and medicine, from molecular interactions to landscape diversity. But do these methods work as well as (or better than) alternative methods? Often this is not evaluated by either simulation or empirical data, with some exceptions (e.g., [1]); here I concentrate on two newer evaluations:

Assessing frequency differentiation between groups, times or locations; I focus on the very popular Bray-Curtis measure and its entropic competitors. I assess Bray-Curtis' fit to several groups of criteria. First, it fits many basic requirements for any diversity measure. Secondly, I examine its independence from confounding effects. Finally, I look at its sensitivity to natural changes, threats, or management that affect underlying dispersal, adaptation, random change, or generation of novelty. If we can forecast a measure such as Bray-Curtis under various conditions, then we can evaluate effects of past events, and forecast effects of future management. I show that Bray-Curtis can be forecast from underlying biological processes, but that the forecasting ability is improved by converting it into closely related entropy/information measures.

Incorporating functional differences between the variants (e.g., DNA sequence, expression, morphology) into biodiversity measures. Past methods have met counterintuitive stumbling-blocks, such as negative diversity, and apparent differentiation depending heavily on variability within-group. Attempts to minimise these problems have resulted in measures with poor sensitivity to functional differences between variants – which the method was supposed to incorporate! A novel approach, based on three related entropy measures, avoids these counterintuitive problems [2].

References

1. Sherwin, W.B.; Chao, A.; Jost, L.; Smouse, P.E. Information theory broadens the spectrum of molecular ecology and evolution. *Trends Ecol. Evol.* **2017**, *32*, 948–963.
2. Chao, A.; Chiu, C.H.; Villéger, S.; Sun, I.F.; Thorn, S.; Lin, Y.C.; Chiang, J.M.; Sherwin, W.B. An attribute-diversity approach to functional diversity, functional beta diversity, and related (dis) similarity measures. *Ecol. Monogr.* **2019**, *89*, e01343.



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Action and Entropy in Heat Engines: An Action Revision of the Carnot Cycle

sciforum-030162

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Action (@) is a state property with physical dimensions of angular momentum ($mr\dot{v} = mr^2\dot{\omega}$). But it is scalar, rather than a vector, with a finite phase angle for change ($mr^2\omega\delta\theta$). We have shown (*Entropy* 21454) that molecular entropy (s) is a logarithmic function of mean values of action ($s = k\ln[e^u(@_t/\hbar)^3(@_r/\hbar)^{2.3}(@_v/\hbar)]$), where k is Boltzmann's constant, $\hbar$ Planck's quantum of action, u the kinetic molecular freedom; mean action values for translation ($@_t$), rotation ($@_r$) and vibration ($@_v$) are easily calculated from molecular properties. This is a novel development from statistical mechanics, mindful of Nobel laureate Richard Feynman's favored principle of least action. The heat flow powering each engine cycle is reversibly partitioned between external mechanical work with compensating internal changes in the action and chemical potential of the working fluid. Equal entropy changes at the high temperature source and the low temperature sink match equal action and entropy changes in the working fluid. Asymmetric variations in quantum states with volume occur isothermally but constant action ($mr^2\omega$) is maintained during the adiabatic or isentropic phases. The maximum work possible per reversible cycle ($-\Delta G$) is the net variation in the configurational Gibbs function of the working fluid between the source and sink temperatures. The engine's inertia compensates so that external kinetic work performed adiabatically in the expansion phase is restored to the working fluid during the adiabatic compression, allowing its enthalpy to return to the same value, as claimed by Carnot. Restoring Carnot's non-sensible heat or *calorique* as action as a basis for entropy will be discussed in the context of designing more efficient heat engines, including that powering the Earth's climate cycles where we introduce the concept of vortical entropy for cyclones and anticyclones.



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Electroencephalogram Brain Mapping for Revealing the Emotional Changes over the Brain Regions Using Entropy Biomarker

sciforum-030186

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Developing a brain mapping for emotional changes over the brain regions remains a crucial goal for improving the process of emotional recognition. The EEGs of forty volunteer individuals were gotten while the individuals were shown seven, short video clips (i.e., anger, anxiety, disgust, happiness, sadness, surprise and neutral). The motivation of this work is twofold. First, it aims to propose the brain electrical activity mapping using the effectiveness of the multiscale fuzzy entropy () feature. Second, it aims to detect the optimal EEG channels for anger, anxiety, disgust, happiness, sadness, surprise and neutral emotional states over the brain regions (i.e., frontal, temporal, parietal and occipital) using the differential evolution-based channel selection algorithm (DEFS_Ch). The results revealed that the frontal region was statistically significant from temporal, parietal and occipital. Moreover, anger emotional state was significantly different from the other emotional states. Furthermore, the anger, sadness and anxiety were significantly different from disgust, happiness, surprise and neutral at the occipital region. For more inspection, DEFS_Ch algorithm has been used to select the most effective emotional channels over the brain regions, anger and anxiety were shared the channels in the frontal, temporal and occipital regions. Disgust was identified by the frontal, temporal, parietal and occipital channels. Sadness and disgust were identified by the channels from the frontal and temporal regions. Surprise and happiness were identified by the left frontal, parietal and occipital channels. Finally, the neutral emotional states were identified by the channels from the lateral regions of the brain particularly in right and left frontal and temporal regions. The main novelty of this study was in building up an EEG brain mapping over the brain regions for different emotional changes to help the clinician for improving the procedure of emotional recognition from the EEG signals.



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A Novel Technique for Achieving the Approximated ISI at the Receiver for a 16QAM Signal Sent via a FIR Channel Based Only on the Received Information and Statistical Techniques

sciforum-029318

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Let us consider for a moment the digital communication case where during transmission, a source signal undergoes a convoluted distortion between its symbols and the channel impulse response. This distortion is referred to as inter-symbol interference (ISI) which causes harmful distortions and presents a major difficulty in the recovery process. A Single-input-multiple-output (SIMO) channel is obtained from the use of an array of antennas in the receiver where the same information is transmitted through different sub-channels, all received sequences will be distinctly distorted versions of the same message. The ISI level from each sub-channel is unknown up to now to the receiver. Thus, even when one or more sub-channels cause heavy ISI, the whole information from all the sub-channels was still considered in the receiver. Obviously, if we know the approximated ISI of each sub-channel, we would use in the receiver only those sub-channels with the lowest ISI level to get improved system performance. In this talk we present a systematic way for getting the approximated ISI from each sub-channel modeled as a finite-impulse-response (FIR) channel with real-valued coefficients for a 16QAM (16 quadrature amplitude modulation, a modulation using $\pm\{1,3\}$ levels for in-phase and quadrature components) source signal transmission. The approximated ISI is based on the Maximum Entropy density approximation technique, on the Edgeworth Expansion up to order six, on the Laplace integral method and on the generalized Gaussian distribution (GGD). Although the approximated ISI was derived for the noiseless case, it was tested successfully for signal to noise ratio (SNR) of SNR = 30 dB and SNR = 20 dB as well.



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On the CTW-Based Entropy Estimator

sciforum-029344

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Estimating the entropy of a sequence of discrete observations is a problem that raises in many different fields. There are numerous different applications of it, specifically in neuroscience, where entropy has been adopted as the main measure for describing the amount of information transmitted between neurons (see Gao et al., 2008 and reference therein). Gao et al., 2008 conducted a thorough comparison of the performance of the most popular and effective entropy estimators. They have shown that the context tree weighted (CTW) based estimator, which uses the probability estimation produced by the CTW lossless compression algorithm by Willems et al., 1995, repeatedly and consistently provides the most accurate results. The motivation for using the CTW probability for estimating the entropy is the well-known Shannon-McMillan-Breiman (SMB) result. However, the CTW probability is a result of a “twice universal” approach, meaning it is a weighted combination of the estimated probabilities of the sequence, over all possible bounded memory tree models (up to a predetermined maximum memory).

Motivated by this we examine the CTW based estimator from the view point of the CTW algorithm redundancy performance analysis (Willems et al., 1995). We define the SMB entropy as the normalized logarithm of the true probability, assuming a specific model for the source. We consider this finite length quantity to be the best possible estimator of the entropy given a specific model. By defining a random variable distributed over all possible bounded memory tree models we extend this definition and define the conditional SMB entropy. We bound the over estimation of the CTW-based estimator compared to both the conditional SMB entropy as well as the SMB entropy of a specific model. In both cases we show that the over estimation approaches zero according to $O(\log T / T)$, where T is the length of the sequence.



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On Superstar-Generalized Statistical Regression

sciforum-029363

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Recent academic literature has confirmed the existence of robust structures characterizing most of many real world systems described by the power law(PL). Intuitively, PL becomes more legible at the level of high frequency series fluctuations in their upper part (thus an asymptotic law), knowing that for certain phenomena the lower part could be generated by this same law. In phenomenological terms, fluctuations in the upper part of natural or social series generally lead to the criticality point at the eve of phase change (e.g., change in physical properties and behavior of matter at a certain temperature human eccentric behavior under the effect of higher emotion, financial crash, etc.). The present proposal goes beyond the traditional statistical methodology mainly based on the Central Limit Theorem(CLT) which presents serious limits when dealing with complex dynamic phenomena. In front of such endogenous methodological problem, a large community of statisticians instead try to find out new techniques fundamentally within the traditional CLT. In line with recent research, this paper recall and extends the fundamentals of a recent approach of non-extensive cross-entropy econometrics (NCEE) (Bwanakare 2019). Equivalently, and to honor Rosen (see Rosen 1981, Gabaix 2009) who, for the first time, used the expression of “Economics of Superstars” to exemplify the presence of PL in the case of artistic earnings (stars inclusively), we propose here the expression of Superstars Generalized statistical regression (SGSR). Thus, this paper proposes a theoretical, power law-based simultaneous regression equation to be estimated through the q-generalised Kullback-Leibler statistical theory of information.



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Estimating Differential Entropy Using Recursive Copula Splitting

sciforum-029577

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We present a new method for estimating the Shannon differential entropy of multidimensional random variables using independent samples. The method is based on decomposing the distribution into a product of the marginal distributions and the joint dependency, also known as the copula. The entropy of marginals is estimated using one-dimensional methods. The entropy of the copula, which always has a compact support, is estimated recursively by splitting the data along statistically dependent dimensions. The method can be applied both for distributions with compact and non-compact supports, which is imperative when the support is not known or of mixed type (in different dimensions). At high dimensions (larger than 20), numerical examples demonstrate that our method is not only more accurate, but also significantly more efficient than existing approaches. We apply the new method to estimate the entropy of several statistical physics model showing out of equilibrium dynamics. The models show a phase transition in which the structure become hyper-uniform. We show that the phase transition can be detected by studying the entropy of particle configurations.



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The Sample Entropy of Inter Spike-Intervals as a Possible Measure of Relations between Neuronal Activity and Individuum Behaviour

sciforum-030268

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Relations between the non-linear structure of neuronal activity and the way that neurons are involved in the behaviour were studied. To describe the non-linear structure of neuronal activity, the complexity of inter-spike intervals sequences was assessed calculating the sample entropy (SampEn). The experimental data used in analyses consisted of recordings of singular neuronal activity in the cingulate cortex of rabbits performing cyclic appetitive operant behaviour. All neurons were divided into two groups: specialized cells ($N = 29$) and cells with nonspecific activity ($N = 84$). The specialization of a neuron in relation to a defined behaviour is assessed via the probability of activation in behavioral acts. Neuronal activity and behaviour were recorded during the first and the second week after rabbits reach the learning criterion (10 right behaviour cycles performance one after another).

SampEn of inter-spike intervals was significantly lower in the group of specialized cells than in the group of cells with nonspecific activity (Mann–Whitney test; $p = 0.01$). Concurrently, the average frequency of spikes didn't differentiate between groups ($p = 0.33$). In the whole set of cells, SampEn didn't differ significantly between the first and the second weeks of training sessions ($p = 0.34$). Yet the group of specialized cells performed lower SampEn during the second week of training than the first week ($p = 0.03$). The group of cells with nonspecific activity showed higher SampEn during the second week of training than the first week ($p = 0.02$).

The results can reflect the difference in the constancy of relations between neurons in the group. Specialized cells have a more constant set and links between each other than cells that have unidentified specialization in the experiment. Their activity is less constant in the observed behaviour and they are more changeable in the set and the structure of links.

Supported by RSF Grant №18-78-10114.



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Ordinal Pattern Based Analysis: From Change Probabilities to Asymmetries

sciforum-030270

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The analysis of ordinal pattern distributions provides a relatively new and interesting approach to nonlinear time series analysis leading, for example, to the concept of permutation entropy. Data analysis methods based on ordinal patterns have been applied in different fields of research such as biomedicine, econophysics and engineering. Main reasons for the increasing success of these analysis methods are that ordinal patterns contain intrinsic information on the dynamical structure of a system and that ordinal pattern-based methods are robust and simple from a computational viewpoint.

Whereas some nice asymptotic results have been found for pattern length going to infinity, in practical data analysis short patterns describing certain features of data and models behind them are of some special interest. We demonstrate this point by discussing some statistics based on counting monotone changes and on considering asymmetries in ordinal pattern distributions. The data analysis methods obtained on this base are illustrated by considering some real world data.



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Max Entropy through Natural Interactions

sciforum-043176

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The Principle of Maximum Entropy, suggests that when one tries to predict the shape of a distribution, then among all possible distributions available for his choice, he should choose the one that maximizes the entropy of the distribution under some few chosen constraints expressing his limited knowledge of the situation. This principle has deep meaning for human and non-human organisms alike, but it is hard to imagine how it is taken place in natural environments under bounded rationality [1]. The context of the current talk is the way natural cognitive processes may be modeled through entropy and bounded rationality (e.g., [2,3]). More specifically, we would like to present a novel idea [4] describing the way in which the entropy of a predicted distribution increases through a structured process of natural interaction that builds on three principles only: Zipf's [5] principle of least effort, Laplace's principle of indifference, and The Copernican principle, suggesting no observer occupy a special place in the universe. This process will be presented, illustrated and supported by simulations never presented before.

References

1. Simon, H.A. *Models of Man*; Wiley: New York, NY, USA, 1957.
2. Neuman, Y.; Vilenchik, D. Modeling small systems through the relative entropy lattice. *IEEE Access* **2019**, *7*, 43591–43597.
3. Neuman, Y.; Cohen, Y.; Tamir, B. Short-term prediction through ordinal patterns. *R. Soc. Open Sci.* **2021**, *8*, 201011.
4. Neuman, Y. *How Small Social Systems Work: From Soccer Teams to Families and Jazz Trios*; Springer: New York, NY, USA, 2021.
5. Zipf, G.K. *Human Behavior and the Principle of Least Effort: An Introduction to Human Ecology*; Ravenio Books: 2016.



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Modeling the Sensing Element of Pressure Nanosensors as Simply Supported Size-Dependent Rectangular Plate

sciforum-030276

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The study of the dynamics of the nanoelectromechanical sensor (NEMS) is currently relevant since they are the next step in the evolution and miniaturization of sensors. Due to the nanosized of sense elements and other components of NEMS, they need in non-classical approaches for the study of their dynamics. Furthermore, the development of these non-classical approaches is a fundamental problem, and many scientists are working on its resolving. One more significant problem is the application of these non-classical approaches to components of the different kinds of NEMS and the obtainment the mathematical models are ready to use for a practical purpose.

In the paper, the mathematical model of the sensing element of pressure nanosensors was constructed based on the new modified couple-stress theory and the third-order plate theory. The sensing element was considered as a simply supported rectangular nanoplate under the distributed force at the bottom of the plate. The dynamic version of the principle of virtual displacements was used for obtaining the differential equations of motion and natural boundary conditions.

A series of computational experiments were carried out for an orthotropic nanoplate. Some combinations of parameters of the mathematical model are found for which chaotic motion is possible.



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Robust Entanglement Preparation through Spatial Indistinguishability Quantified by Entropic Measure

sciforum-030166

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Initialization of composite quantum systems into highly entangled states is important to enable their use for quantum technologies. However, unavoidable noise in the preparation stage makes the system state mixed, hindering the achievement of this goal. We address this problem in the context of identical particle systems adopting the operational framework of spatially localized operations and classical communication (sLOCC). After a brief description of the formalism, we define the entanglement of formation for an arbitrary state (pure or mixed) of two identical qubits, valid for both bosons and fermions. We then introduce an entropic measure of spatial indistinguishability as an information resource, tunable by the shapes of spatial wave functions. We finally apply these tools to a situation of experimental interest, that is noisy entangled state preparation. We find that spatial indistinguishability, even partial, can be a property shielding nonlocal entanglement from preparation noise, independently of the exact shape of spatial wave functions. These results prove that quantum indistinguishability is an inherent control for noise-free entanglement generation.



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Tunneling as a Source for Quantum Chaos

sciforum-029093

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Classical chaos is generally defined as exponential divergence of nearby trajectories causing instability in the orbits with respect to initial conditions. The wave function may be thought of as representing an ensemble of points in phase space and a fast spreading of the wave packet can be compared with a rapid or exponential separation of neighboring trajectories in the classical case. We use an one dimensional model of a square barrier embedded in an infinite potential well to demonstrate that tunneling leads to a complex behavior of the wave function and that the degree of complexity may be quantified by use of the spatial entropy function defined by $S = - \int |\Psi(x,t)|^2 \ln |\Psi(x,t)|^2 dx$.

Chaos is supposed to imply increase of the entropy and a rapid rise of the entropy function can be understood as the burst of chaotic behavior. There is no classical counterpart to tunneling but a decrease in the tunneling may be interpreted as an approach of a quantum system to a classical system.

We show that changing the square barrier with barriers of increasing height/breadth not only decrease the tunneling but also slows down the rapid rise of the entropy function which for a low/thin barrier for small times is a fluctuating function around a smooth almost constant asymptotic value.

Also the mean square width of the wave packet shows a rapid rise for a low/thin barrier before entering a steady asymptotic mean.

We conclude that the complex behavior associated with tunneling and the rapid rise of entropy is similar to that expected from a chaotic dynamical system. We therefore suggest that the rapid spread of the wave function can be used as a definition for quantum chaos.



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Analysis of Generalized Gibbs States

sciforum-030286

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An exponential family is a manifold of generalized Gibbs state of the form $\exp(H)/\text{Tr}(\exp(H))$, where H belongs to a vector space of (possibly non-commutative) hermitian matrices. Generalized Gibbs states are important in small-scale thermodynamics, they represent equilibrium states regarding several conserved quantities that admit novel operations without heat dissipation [1]. Quantum information theory and condensed matter physics consider a space of local Hamiltonians acting on spins. The entropy distance from this exponential family is a measure of many-body complexity [2–4].

This talk is concerned with the geometry and topology of an exponential family and its entropy distance [5]. The maximum-entropy inference map parametrizes the exponential family. This map is continuous in the interior of its domain, the joint numerical range [6]. We describe the points of discontinuity in terms of open mapping theorems and eigenvalue crossings. Because of the discontinuity, the inference map and the entropy distance cannot be approximated through interior points. Instead, it is necessary to study faces (flat portions on the boundary) of the joint numerical range. With local Hamiltonians, this requires studying the faces of the set of quantum marginals.

References

1. Lostaglio, M.; Jennings, D.; Rudolph, T. Thermodynamic resource theories, non-commutativity and maximum entropy principles. *New J. Phys.* **2017**, *19*, 043008.
2. Ay, N.; Olbrich, E.; Bertschinger, N.; Jost, J. A geometric approach to complexity. *Chaos* **2011**, *21*, 037103.
3. Niekamp, S.; Galla, T.; Kleinmann, M.; Gühne, O. Computing complexity measures for quantum states based on exponential families. *J. Phys. A-Math. Gen.* **2013**, *46*, 125301.
4. Zeng, B.; Chen, X.; Zhou, D.-L.; Wen, X.-G. *Quantum Information Meets Quantum Matter*; Springer: New York, NY, USA, 2019.
5. Weis, S. Information topologies on non-commutative state spaces. *J. Convex Anal.* **2014**, *21*, 339–399.
6. Rodman, L.; Spitkovsky, I.M.; Szkoła, A.; Weis, S. Continuity of the maximum-entropy inference: Convex geometry and numerical ranges approach. *J. Math. Phys.* **2016**, *57*, 015204.



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Quantum Chaos and Quantum Randomness— Paradigms of Quantum Entropy Production

sciforum-032099

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Quantum chaos and quantum measurement have one constitutive feature in common: They capture information at the smallest scales to lift it to macroscopic observability, thus generating classical facts. Fundamental bounds of the information content of closed quantum systems with finite-dimensional Hilbert space restrict their entropy production to a finite timescale. Only in open systems where fresh entropy infiltrates from the environment, quantum dynamics (partially) recovers sustained entropy production as in classical chaos.

This interpretation opens a novel perspective also on randomness in quantum measurement, where a macroscopic apparatus observes a quantum system. Notably in spin measurements, their results involve an element of fundamental unpredictability. The analogy with quantum chaos suggests that random outcomes of quantum measurements could, in a similar manner, reveal the entropy generated through the coupling to a macroscopic environment, which is required anyway to explain a crucial feature of quantum measurement that becomes manifest in the collapse of the wavepacket: decoherence. However, the subsequent step from a set of probabilities to specific individual measurement outcomes (the “second collapse”) still evades a proper understanding in terms of microscopic models. Could it be explained by the exchange of entropy between macroscopic apparatus and measured system?

I explore this hypothesis in the case of spin measurements. The model of quantum measurement proposed by Zurek and others is combined with a unitary approach to decoherence using heat baths that comprise only a finite number N of modes, as recently proposed in quantum chemistry and quantum optics. For large $N \gg 1$, the dynamics of the measured spin is expected to exhibit a scenario of episodes of significant spin polarization in either direction of increasing length, alternating with spin flips, determined by the initial condition of the apparatus. I present preliminary analytical and numerical results which support this expectation.



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Entropy: The Evolution of a Concept

sciforum-030409

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Entropy has been, and continues to be, one of the most misunderstood of physical concepts. This is because entropy is a quantification of one's state of ignorance about a system rather than a quantification of some aspect of a system itself. In this talk I will begin by looking back at the history of entropy tracking the evolution of thought from Carnot's generalized heat engine, Lord Kelvin's temperature scale, Clausius' entropy, to Boltzmann's counting of microstates. This evolution in thought then took significant leaps as the concept of Shannon's information was introduced and Jaynes, realizing that this was a matter of inductive inference, introduced the principle of maximum entropy. The concept of entropy continues to evolve as demonstrated by the relation between entropy and the relevance of questions. As a result, the future holds great promise as information-theoretic and entropic methods are justifiably and confidently applied to new problems in new domains far beyond those involving thermodynamics, statistical mechanics and communication theory. And we will see entropic techniques employed in new technologies, such as question-asking machines.



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Classifying Dengue Cases Using CatPCA in Combination with the MSU Correlation

sciforum-030030

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Dengue is a mosquito-borne viral infection that is a leading cause of serious illness and death among children and adults in many countries across the world. In Paraguay, dengue incidence has been increasing especially in urban areas, becoming endemic and epidemic in the last few years.

This work seeks to understand what factors are responsible for the epidemic and hemorrhagic varieties of dengue. Considering that collected data are of mixed nature (nominal and continuous), Categorical Principal Components Analysis (CatPCA) is adopted as a first tool. However, interpretation of CatPCA output can be challenging, partly because the same variable may appear throughout several of the principal components.

Multivariate Symmetrical Uncertainty (MSU), an entropy-based similarity measure, allows quantifying correlations in a multivariate environment and detecting both linear and nonlinear associations. In this work, the MSU measure is used in combination with CatPCA to obtain greater insight regarding the relevance of each variable.

We apply the two techniques combined in stages, using nation-wide data collected by the country's Sanitary Surveillance Department from nearly 200,000 suspected and confirmed cases throughout 5 years. The first few runs of CatPCA help to discard the less relevant attributes. A subsequent run of CatPCA provides principal components that account for a high percentage of the total variance. Working with the attribute sets identified by CatPCA, MSU finds n -way interactions and correlations, and groups those attributes for further selection. Segregation of attributes in disjoint groups can be done at this stage; this allows for an easier interpretation of groupings including those containing the key linear and nonlinear correlations.

The outcomes from this combined approach are better than the CatPCA alone, identifying individual and grouped variables that contribute to the behavior of the class.



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Correlating the Entropy of a Fluid with Live Collective Behaviors

sciforum-030074

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Given a group of individuals inside a fluid flow (e.g., air or water) that behaves as a collective to some degree, factors like the shape of a group or the distance between its individuals can affect the forces that each individual inside the group may notice, such as drag or lift forces. Bird flocks, swarms or cycling riders are just some group behavior examples where the topology of fluid flow and information exchange affects the aerodynamics of the whole group, and may also interact with other groups or external individuals.

This group dynamics and interaction can be numerically correlated by entropy. The fundamental basis of the most of Computational Fluid Dynamics (CFD) problems is the Navier–Stokes (NS) equations, which define many single-phase fluid flows with some multi-phase flow extensions. NS equations are written as a function of the fluid velocity and pressure (in addition to other variables that describe the fluid properties), but they can also be re-written as a function of entropy. However, it is not easy to find a direct methodology that relates the entropy of a system, the fluid dynamics and the collective behavior of a system inside this fluid.

In this work we propose a method to easily calculate the entropy of a CFD solution by computing the pixels of its image based on Shannon entropy. Using the results obtained, we study the relation between information mechanics, fluid dynamics and fluid forces.



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Cross Recurrence Quantification Analysis as a Tool for Detecting Rotors in Atrial Fibrillation: An In Silico Study

sciforum-030227

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Atrial fibrillation is a cardiac arrhythmia characterized by rapid and irregular heartbeats that could be sustained by repetitive and cyclic activations around a core, known as rotors. Intracardiac electrograms studies have related the occurrence of a signal waveform pattern, called complex fragmented atrial electrograms (CFAE), with the surroundings of the rotor core.

Recurrence quantification analysis (RQA) has been proposed as a tool to detect CFAE. In RQA, the phase space trajectories are computed from the signal and the appropriate time delay embedding. In this work, we propose the computation of cross RQA (cRQA) using two distinct electrograms. We hypothesized that there is low recurrence rate when cRQA is estimated from a signal recorded near a rotor core and another in an adjacent point around the core.

We test the sample entropy, RQA and cRQA in five 2D in-silico simulations of atrial fibrillation sustained by different mechanisms: (i) a single stable rotor, (ii) a figure-of-eight re-entry with two stable rotors, (iii) a figure-of-eight re-entry with two meandering rotors, (iv) a single stable rotor and multiple propagating waves, (v) semi-stable rotors, meandering rotors and multiple propagating waves. Unipolar electrograms are simulated for each fibrillatory episode.

Our results show that, by applying sample entropy, the core of stable rotors, meandering rotors and multiple waves collision are associated with, by applying RQA the core of stable rotors and some areas with multiple waves collision exhibit low recurrence rates, notwithstanding meandering rotors were not detected. Differently, by applying cRQA only the cores of stable rotors are detected through low recurrence rates. These results suggest that cRQA could be a useful tool for stable rotors detection with high specificity. Future studies should include real electrograms recorded from patients with atrial fibrillation.



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Network Analysis of Multivariate Transfer Entropy of Cryptocurrencies in Times of Turbulence

sciforum-044128

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We investigate the effects of the recent financial turbulence of 2020 on the market of cryptocurrencies taking into account the hourly price and volume of transactions from December 2019 to April 2020. The data were subdivided into time frames and analyzed the directed network generated by the estimation of the multivariate transfer entropy. The approach followed here is based on a greedy algorithm and multiple hypothesis testing. Then, we explored the clustering coefficient and the degree distributions of nodes for each subperiod. It is found the clustering coefficient increases dramatically in March and coincides with the most severe fall of the recent worldwide stock markets crash. Further, the log-likelihood in all cases bent over a power-law distribution, with a higher estimated power during the period of major financial contraction. Our results suggest the financial turbulence induce a higher flow of information on the cryptocurrency market in the sense of a higher clustering coefficient and complexity of the network. Hence, the complex properties of the multivariate transfer entropy network may provide early warning signals of increasing systematic risk in turbulence times of the cryptocurrency markets.



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Causal Entropy-Complexity Plane with Multivariate Probability Distribution

sciforum-044240

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We propose a multivariate causality entropy-complexity plane by using a multivariate probability distribution function (PDF) and adapting the Normalized Permutation Entropy H and Statistical Complexity C .

Alongside the standard embedding dimension D for ordinal patterns of length $D!$, we considered sub-patterns of embedding dimensions that get more information in the phase space, since the order patterns do not always detect sensory changes in the time series. This level of complexity can capture details of the probability distribution of the system that are not discriminated by measures of randomness, such as entropy, thus the multivariate causality entropy-complexity plan is adopted.

In this application, the plane was used to analyze complex time series and the results indicate robustness in the distinction between chaotic systems, even after the insertion of noise in each of the chaotic time series that defines the system. Thus, the multivariate plan is more objective to extract the structure of a system and, thus, to characterize it.



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Electrification of the Passenger Car Fleet and Its Effect on Resource Use—A Statistical Entropy Analysis Perspective

sciforum-030177

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The European automotive sector undergoes a severe transformation that is driven by the increasing uptake of alternative drivetrains. In the year 2050 it is expected that 40–80% of new vehicles entering the vehicle stock will be electric (Hill and Bates, 2018). Even though the electrification of the vehicle stock may contribute positively to reaching the EU climate targets, the transformation will also create costs, not only monetary, but also in terms of efforts and losses of functionality. On the one hand substantial efforts will be needed to extract, concentrate and refine materials to produce components and vehicles with new drivetrain technology. On the other hand considerable efforts will be related to restoring functionality losses that result from the large-scale exchange of the vehicle fleet. To assess the effect of the vehicle stock transformation on resource use a dynamic material flow analysis (MFA) is employed and five possible future scenarios of the mobility transition are modelled for the EU until 2050. In a second step the results of the MFA are evaluated through the method of Statistical Entropy Analysis (SEA). The SEA results show that the changes in the vehicle stock, its renewal rate, as well as the adaptation of the reuse, remanufacturing-, and recycling- system, need to be aligned to the pace of the transition to minimize the loss of functionality and reduce the efforts involved. The study demonstrates how SEA can be used to evaluate future socio-technological transitions of larger systems like the European automotive system and identify the best combinations of resource management strategies. It is shown that SEA provides insights that allow to quantify hotspots of functionality loss and determine the most effective combinations of product stock and materials management interventions, contributing to more sustainable use of resources and existing stocks.



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Information Entropy of Single-Gene Expression Responses during Genome Wide Perturbations

sciforum-029111

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Transcription factors (TF) are known to drive gene-to-gene interaction dynamics under optimal growth conditions, but lesser is known about how much they affect the dynamics of gene regulatory networks (GRN) at the global level, due to the contribution of many other variables.

We investigate how TF interactions of the GRN of *E. coli* affects the global entropy of single-genes response dynamics, during a genome-wide perturbation caused by a shift in RNA polymerase (RNAP) concentrations.

For this, we classified genes based on their number of (known) input TFs. Also, we assigned a value to each TF input (−1 for repression and +1 for activation) and classified genes based on the sum of its input interactions. For both classification schemes, we estimated the information entropy of the single-gene input interactions of each class.

Next, we measured by RNA-seq the fold changes of each gene due to weak, medium, and strong perturbations of RNAP concentration, from which we quantified the information entropy of single-gene responses of each class.

We found that the information entropy of the fold changes of the classes of genes increases (non-linearly) with the magnitude of the perturbation, in a manner that is consistent with the information entropy of the sum of the input interactions of individual genes, rather than their number of inputs.

Overall, we argue that, in the event of genome wide perturbations, asymmetries in input functions of TFs partially control the propagation of information between genes of the GRN of *E. coli*.



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Information Flow in Color Appearance Neural Networks

sciforum-029113

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Color Appearance Models are biological neural networks that consist of a cascade of linear + nonlinear layers that transform the measurements at the retina into an internal representation of color that correlates with psychophysical experience. The basic layers of these networks include: (1) chromatic adaptation (normalization of the mean and covariance of the color manifold), (2) change to opponent color channels (PCA-like rotation), and (3) saturating nonlinearities to get perceptually Euclidean color representations (dimension-wise equalization). The Efficient Coding Hypothesis in neuroscience argues that these transforms should emerge from information theory [Barlow Proc.Nat.Phys.Lab.59, Barlow Network 01]. In the specific case of color vision there are a number of evidences of this [Buschbaum Proc.Roy.Soc.83, Twer Network 01, Laparra&Malo Neural Comp. 12, Laparra&Malo Front.Human.Neurosci.15]. The question for these color networks is, what is the coding gain due to the different mechanisms in the networks?

In this work, representative Color Appearance Models are analyzed in terms of how they modify the statistical redundancy along the network and how much information is transferred from the input to the noisy response. The proposed information-theoretic analysis is done using methods and data that were not available before: (1) new statistical tools to estimate (multivariate) information-theoretic quantities between multidimensional sets based on Gaussianization [Laparra&Malo IEEE Trans.Neur.Nets.11, Johnson, Laparra & Malo ICML 19], and (2) new colorimetrically calibrated scenes in different CIE illuminations for proper evaluation of chromatic adaptation [Gutmann,Laparra, Hyvarinen & Malo PLOS 14].

Results identify the psychophysical mechanisms critically responsible for gains in chromatic information transference: opponent channels and their nonlinear nature are more important than chromatic adaptation at the retina. Moreover, our visual neural pathway allocates at least 70% of the information capacity for spatial information as opposed to only 30% devoted to color.



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The Intrinsic Entropy as Substitute for the Market Volatility of Underlying Securities

sciforum-029151

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Grasping the market volatility of underlying securities, and accurately estimating it in particular, are ones of the salient preoccupations of those involved in the securities industry and derivative instruments pricing.

This paper presents the results of employing the intrinsic entropy model as substitute for the market volatility of underlying securities. Diverging from the widely used volatility models that take into account only elements of the traded prices, namely Open, High, Low, Close prices of a trading day (OHLC), the intrinsic entropy model quantifies in as well the volumes traded during the considered time frame. We adjust the intraday intrinsic entropy model that we introduced earlier for the exchange-traded securities, in order to connect daily OHLC prices with the ratio of the corresponding daily volume to the overall volume traded in the considered period. The intrinsic entropy model conceptualizes this ratio as entropy probability or market credence associated to the corresponding price level.

The intrinsic entropy is computed using historical daily data for traded market indices (S&P 500, Dow 30, NYSE Composite, NASDAQ Composite, Russell 2000, DAX Performance-Index, CAC 40, Hang Seng Index and Nikkei 225). We compare the results produced by the intrinsic entropy model with the volatility obtained for the same data sets using industry widely employed volatility estimators such as Parkinson (HL), Garman-Klass (OHLC), Rogers-Satchell (OHLC), Garman-Klass Yang-Zhang extension (OHLC) and Yang-Zhang (OHLC).

We consequently study the efficiency of the intrinsic entropy and volatility estimates by comparing them with the volatility of the standard close to close estimate. The intrinsic entropy model proves to consistently deliver a minimal estimation error for various time frames we experimented with, along with its peculiar indication regarding the market inclination toward either buying or selling the underlying security.



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Entropic Transport in Confined Soft-Matter and Biological Systems

sciforum-043100

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Transport in small-scale biological and soft-matter systems typically occurs under confinement conditions in which particles proceed through obstacles and irregularities of the boundaries that may significantly alter their trajectories. A transport model that assimilates the confinement to the presence of entropic barriers provides an efficient approach to quantify its effect on the particle current and the diffusion coefficient. We review the main peculiarities of entropic transport and treat two cases in which confinement effects play a crucial role, with the appearance of emergent properties. The presence of entropic barriers modifies the mean first-passage time distribution and therefore plays a very important role in ion transport through micro- and nano-channels. The functionality of molecular motors, modeled as Brownian ratchets, is strongly affected when the motor proceeds in a confined medium that may constitute another source of rectification. The interplay between ratchet and entropic rectification gives rise to a wide variety of dynamical behaviors, not observed when the Brownian motor proceeds in an unbounded medium. Entropic transport offers new venues of transport control and particle manipulation and new ways to engineer more efficient devices for transport at the nanoscale.



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A Stunning Realisation: The Touted Defiance of Bell's Inequality by Quantum Probabilities Derives from a Mathematical Error

sciforum-029125

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I shall display the mathematical error in the currently accepted derivation of the expected value of Bell's quantity " s " in the context of a gedankenexperiment on a single pair of photons in CHSH form. The fact that this mistaken value exceeds 2 supports the touted conclusion of quantum theorists that quantum probabilities defy Bell's inequality if the principle of local realism is presumed. The error is based on the neglect of four symmetric functional relations among the four components of s in a thought experiment designed to assess this principle. The expectation of the linear combination defining s is *not* twice the square root of 2 as is widely supposed, but rather is found to be an interval rounded to (1.1213, 2.0] when calculated via linear programming procedures. There are four dimensions of freedom in the coherent expectation polytope. I shall display the slices of this polytope as it passes through 3-D space. A comment on the maximum entropy distribution within this polytope will conclude the presentation. I shall introduce the contents of four papers relevant to the issue, which are available on Researchgate: Quantum violation of Bell's inequality: a misunderstanding based on a mathematical error of neglect; The GHSZ argument: a gedankenexperiment requiring more denken; Resurrecting the principle of local realism and the prospect of supplementary variables; More Hoojums than Boojums: quantum mysteries for no one. The GHSZ article has been published in *Entropy*.



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Kullback-Leibler Divergence of a Freely Cooling Granular Gas of Inelastic Hard Disks and Spheres

sciforum-028911

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The velocity distribution function (f_{HCS}) of a granular gas modeled by inelastic hard d -spheres in the Homogenous Cooling State (HCS) is still unknown. Deviations from a Maxwellian distribution (f_{M}) at the system temperature by means of an infinite expansion in terms of Sonine polynomials is the typical approach. In the quest of finding the Lyapunov functional related to this system, the Kullback-Leibler divergences $D_{\text{KL}}[f|f_{\text{HCS}}]$ and $D_{\text{KL}}[f|f_{\text{M}}]$ of the time-dependent velocity distribution function (f) with respect to the HCS and Maxwellian distributions, respectively, are proposed and studied. Kinetic theory results for inelastic hard disks and spheres [1] are supported by Molecular Dynamics (MD) simulations. Whereas $D_{\text{KL}}[f|f_{\text{M}}]$ may present a non-monotonic behavior with time, it is observed that $D_{\text{KL}}[f|f_{\text{HCS}}]$ seems to be a valid candidate for a Lyapunov functional, as proposed in [2]. Interestingly, $D_{\text{KL}}[f_{\text{HCS}}|f_{\text{M}}]$ exhibits a non-monotonic dependence on the coefficient of restitution. Moreover, for a more complete description of the problem, fourth- and sixth-order cumulants are revisited, MD simulation results being compared with kinetic-theory predictions for a wide range of values of the coefficient of restitution. Finally, in some simulations, and after a first freely cooling period, a sort of Maxwell's demon acts by reversing the instantaneous velocity of each particle in an attempt to return to the initial configuration. Although an initial ordering is apparently reached by the elastic system (Loschmidt's paradox), the complete reverted evolution is flatly rejected in the inelastic case since time reversal symmetry and detailed balance are broken down in that case, both results being in accordance with [3].

References

1. Santos, A.; Montanero, J.M. The second and third Sonine coefficients of a freely cooling granular gas revisited. *Granular Matter* **2009**, *11*, 157–168.
2. De Soria MI, G.; Maynar, P.; Mischler, S.; Mouhot, C.; Rey, T.; Trizac, E. Towards an H-theorem for granular gases. *J. Stat. Mech. Theory Exp.* **2015**, *2015*, P11009.
3. Orban, J.; Bellemans, A. Velocity-inversion and irreversibility in a dilute gas of hard disks. *Phys. Lett. A* **1967**, *24*, 620–621.



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Thermodynamics of Systems with Emergent Molecule Structures

sciforum-029206

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Boltzmann entropy is defined as the logarithm of state multiplicity. For multinomial multiplicities, it results in the ordinary Boltzmann-Gibbs-Shannon entropy. However, for non-multinomial systems, we obtain different expressions for entropy. This is the case of complex systems, particularly the case of systems with emergent structures. Probably the most prominent examples of such systems are provided by the chemical reactions with long-range interactions, i.e., where every particle can interact with each other. Based on the original ideas of L. Boltzmann, we calculate the entropy of a system with emergent molecule states. It turns out that the corresponding entropy is the Boltzmann-Gibbs entropy plus a correction that can be interpreted as a structural entropic force. The corresponding thermodynamics is an alternative for the grand-canonical ensemble that correctly counts the number of states. We demonstrate this approach on several examples, including chemical reactions of the type $2X \rightarrow X_2$, phase transitions in a magnetic gas, and the fully connected Ising model. For the fully-connected Ising model, the presence of molecule states shifts the Curie temperature down and changes the order of the phase transition from the second-order to the first order. For systems with short-range interactions, we recover the ordinary Boltzmann-Gibbs entropy and derive the well-known relation between chemical potential and concentration.



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Application of Rényi Entropy-Based 3D Electromagnetic Centroids to Segmentation of Fluorescing Objects in Tissue Sections

sciforum-029346

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The understanding of the physico-chemical basis of the intracellular processes requires determination of local concentrations of cell chemical constituents. For that, light microscopy is the irreplaceable method. Using an example of a (auto)fluorescent tissue, we clarify some still ignored aspects of image build-up in the light microscope for maximal extraction of information from the 3D microscopic experiments. We introduce an algorithm based on the Rényi entropy approach, namely on the Point Divergence Gain (see Entropy 20(2), p. 106):

$$\text{PDG}_{\alpha}^{l-m} = 1/(1 - \alpha) \log_2 \{[(n_l - 1)^\alpha - n_l + (n_m + 1)^\alpha - n_m]/C_\alpha + 1\},$$

where α is the Rényi coefficient; and n_l and n_m are frequencies of occurrence of phenomena (intensity) l in the 1st matrix (digital image) and of phenomena (intensity) m in the 2nd matrix (digital image). The digital images are optical cuts consecutive in a stack obtained along the microscope optical path between which weighted frequencies of occurrences of all phenomena (intensities) in the 1st matrix (digital we exchange a pixel of intensity l for a pixel of intensity m). The term C_α is a sum of α -image).

We removed an image background using $\text{PDG}_{50}^{l-m} = 0$ which is an approximation to $\text{PDG}_{\infty}^{l-m} = 0$ (analogy to min entropy). Then, we sought voxels (3D pixels) called 3D electromagnetic centroids that corresponded to $\text{PDG}_2^{l-m} = 0$ (i.e., multifractality approximation to subtraction of two images consecutive in a z-stack). This localized the information about the object independently of the size of this voxel (see Ultramicroscopy 179, pp. 1–14) and gave us cores of the objects' images. At $\text{PDG}_{10}^{l-m} = 0$, we obtained extended 3D images of the observed objects called spread functions.

This approach enables us to localize positions of individual fluorophores and their general spectral properties and, consequently, to make approximative conclusions about intracellular biochemistry.



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Evaluating Spatial and Temporal Fragmentation of a Categorical Variable Using New Metrics Based on Entropy: Example of Vegetation Land Cover

sciforum-029459

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Associated with climate change and/or land use pressure, forest fragmentation is a spatio-temporal shrinking process that reduces the sizes of forest patches. This breaks up forest patches so increasing their number before the small ones progressively disappear. Fragmentation can be assessed spatially as a level of the current status of the fragmented spatial configuration and temporally as the level of the speed of the fragmentation process itself. Among the different landscape metrics based on patches as indicative measures for fragmentation, the Shannon entropy of the observed spatial distribution of categories has been of particular interest. Based on a recently suggested spatio-temporal entropy framework focusing on patch size and shape distributions, this paper shows how to derive useful fragmentation metrics at local and global levels, spatially, temporally or both. Moreover, it shows that using fully symmetric approaches between space, time and category within this framework, can lead to more sensitive fragmentation metrics as well as providing complementary local approach for cartographic representation. Land cover data simulations from land surface modelling to a 2100 horizon are used to illustrate the proposed fragmentation metrics.



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A Fast Multivariate Symmetrical Uncertainty Based Heuristic for High Dimensional Feature Selection

sciforum-029531

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In classification tasks the increase in the number of dimensions of a data makes the learning process harder. In this context feature selection usually allows to induce simpler classifier models while keeping the accuracy. However, some factors, such as the presence of irrelevant and redundant features, make the feature selection process challenging. Symmetrical Uncertainty (SU) is an entropy-based measure widely used to identify subsets of useful features for the classification task. However, SU is a bivariate measure and, so, it ignores possible dependencies among more than two features. In order to overcome this issue, SU has been extended to the multivariate case. This extension, called Multivariate Symmetrical Uncertainty (MSU), is time-consuming and may become impracticable when evaluating larger subsets of features during the search. In this work we propose a MSU based Feature Selection (MSUFS) heuristic to address feature selection on high-dimensional data. In order to design MSUFS, the concept of Approximate Markov Blanket is redefined to take into account the MSU measure. The performance of MSUFS is tested on high-dimensional datasets from different domains and its results where compared with popular and competitive techniques. Results show that MSUFS is capable of identifying possible correlations and interaction among features and, therefore, it achieves competitive results. Finally, the proposed strategy is also applied to a case study regarding melanoma skin cancer.

Acknowledgments: This work is partially supported by the research project PINV15-0257 from CONACyT-Paraguay. Authors are also thankful to the Andalusian Scientific Computer Science Centre (CICA) for allowing us to use their computing infrastructures.



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Statistical Entropy Analysis to Evaluate Cascading Use of Wood

sciforum-030178

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Biological materials are biodegradable in nature. Consequently, it is harder to preserve their material value. Recycling these materials to its original form is difficult. Hence the material is cascaded down in its application. Cascading use implies a system in which biomass progresses through a series of uses before finally being burned to recover energy. The aim is to preserve the material quality and prioritize the use based on the maximum added value that can potentially be generated from it. For instance, sawn wood should preferably be used for building, furniture and other products with a long life span, while bioenergy should be derived from the use of wood residues. However, identifying the best valorisation routes requires appropriate measurement and monitoring tools to quantify the degree of cascading, which is still lacking.

Statistical entropy analysis (SEA) has been put forward as a method to quantify resource quality. This could be a powerful tool to assess cascading use. SEA measures the concentration of material along its life cycle and determines the efficiency of a system based on its ability to concentrate or dilute a substance. The concentration of material has been proposed as a proxy for quality; the higher the concentration of a material, the higher is its availability, and hence the higher would be its recoverability and recyclability. However, in the case of biological material, in particular wood, along with concentration product-size dictates the quality. Product-size is not considered in the traditional SEA methodologies, which limits its applicability to the biological material. The goal of this study is to adapt the SEA methodology to incorporate physical dimensionality. The adapted method, demonstrated by comparing different wood cascading scenarios in Flanders (Belgium), reveals valuable information about key drivers of quality loss in the value chain and identifies hotspots for improvement.



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Information Routing in Proteins: The Case of a Therapeutic Antibody

sciforum-030010

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Internal dynamics is the link between structure and biological function in proteins [1]. It has been shown that low-frequency dynamics is not only essential for a protein to function [2], but also that a correlation exists between a protein's activity and its specific dynamical properties [3]. Propagation of information between two or more distant sites on the protein network allows concerted, large-scale conformational changes to take place, triggering as a consequence biological responses. In this work, we aim at identifying patterns of information routing within the therapeutic antibody pembrolizumab [4], as communication channels that emerge from the underlying topology and drive the observed correlated motions. Specifically, we focus on the mutual information (MI) of the displacements of atomic positions, as computed from atomistic molecular dynamics simulations, both in presence and in absence of the bound antigen. MI is used to build network models of the antibody for each of the conformational clusters emerging from the simulations; these networks are then interpreted in the light of a graph-theoretical approach, to couple chemical detail and large-scale dynamics. Unveiling inter-residue communication pathways in may find application not only in biotechnological manipulation for improved therapeutic agents, but also in design of simplified, multi-resolution antibody models that, describing channels of information transfer at an appropriate high-resolution level, facilitate the dynamical investigation at a lower computational cost [5].

References

1. Berendsen, H.J.; Hayward, S. Collective protein dynamics in relation to function. *Curr. Opin. Struct. Biol.* **2000**, *10*, 165–169.
2. Yang, L.Q.; Sang, P.; Tao, Y.; Fu, Y.X.; Zhang, K.Q.; Xie, Y.H.; Liu, S.Q. Protein dynamics and motions in relation to their functions: Several case studies and the underlying mechanisms. *J. Biomol. Struct. Dyn.* **2014**, *32*, 372–393.
3. Hensen, U.; Meyer, T.; Haas, J.; Rex, R.; Vriend, G.; Grubmüller, H. Exploring protein dynamics space: the dynasome as the missing link between protein structure and function. *PLoS ONE* **2012**, *7*, e33931.
4. Scapin, G.; Yang, X.; Prosise, W.W.; McCoy, M.; Reichert, P.; Johnston, J.M.; Kashi, R.S.; Strickland, C. Structure of full-length human anti-PD1 therapeutic IgG4 antibody pembrolizumab. *Nat. Struct. Mol. Biol.* **2015**, *22*, 953–958.
5. Diggins, I.V.; P; Liu, C.; Deserno, M.; Potestio, R. Optimal coarse-grained site selection in elastic network models of biomolecules. *J. Chem. Theory Comput.* **2018**, *15*, 648–664.



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Conditional Permutation Entropy as a Measure for the Complexity of Dynamical Systems

sciforum-030142

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An important but difficult problem in the analysis of dynamical systems consists in determining the system's complexity, analytically and on the basis of given data. As a new approach to this problem, in 2002, Bandt and Pompe introduced the permutation entropy. Their method depends on the distribution of so called "ordinal patterns", which are based on the relative ordering between different values. Since this approach has many theoretical and practical advantages over alternative methods, it has been successfully applied to various real-world problems. However, it is still not completely understood on a theoretical level. In this presentation we will investigate conditional variants of the permutation entropy that were first mentioned in 2014. Two closely related types of conditional permutation entropy will be considered and compared mathematically. Additionally, we will show how this conditional permutation entropy is related to the non-conditional variant. Finally, we will demonstrate why the conditional permutation entropy can be a more efficient measure for complexity than the original permutation entropy.



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Representation and Information in Molecular Modelling

sciforum-030013

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The computational study of soft matter systems lies at the nexus among several disciplines, including material science, biophysics, statistical mechanics, and information theory. Each of them contributes objects of investigation as well as tools and perspectives unique from each field, all of these being necessary to attain a multifaceted picture of complex systems. The construction of *in silico* models of biomolecules, in particular, requires one to combine the background biological knowledge of a system with the quantitative description of the latter in those terms characteristic of mechanics and statistical physics. This is particularly true in the field of coarse-grained modelling, in which the effort to attain an ever larger accuracy of a model is replaced by the attempt to simplify it as much as possible, while at the same time retaining those essential features which make the model predictive. This talk will provide an overview of the problem of designing effective, coarse-grained models of large biomolecules. Particular attention will be posed on the issue of representability and mapping, the preservation of information content, and the extraction of biological knowledge from resolution modulation.



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Chaotic Entanglement: Entropy and Geometry

sciforum-030034

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In chaotic entanglement, pairs of interacting classically-chaotic systems are induced into a state of mutual stabilization that can be maintained without external controls and that has been shown to exhibit several properties consistent with quantum entanglement. In such a state, the chaotic behavior of each system is stabilized onto one of the system's many unstable periodic orbits (generally located densely around an associated attractor), and the ensuing periodicity of each system is sustained by the symbolic dynamics of its partner system, and vice versa. Notably, chaotic entanglement is an entropy-reversing event: the entropy of each member of an entangled pair decreases to zero during each system's collapse to the given period orbit. In this talk, we further discuss the role that entropy plays in chaotic entanglement. We also discuss the geometry that arises when pairs of entangled chaotic systems organize into coherent structures that range in complexity from simple tripartite lattices to more involved patterns. The talk will conclude with a discussion of future research directions.



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Basin Entropy: A New Method to Measure Unpredictability in Physical Systems

sciforum-030360

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In nonlinear dynamics, basins of attraction are defined as the set of points that, taken as initial conditions, lead the system to a specific attractor. This notion appears in a broad range of applications where multistability is present, which is a common situation in neuroscience, economy, astronomy, ecology, and other disciplines. Nonlinear systems often give rise to fractal boundaries in phase space, hindering predictability. When a single boundary separates three or more different basins of attraction, we call them Wada basins. Usually, Wada basins have been considered even more unpredictable than fractal basins. However, this particular unpredictability has not been fully unveiled until the introduction of the concept of basin entropy. The basin entropy provides a quantitative measure of how unpredictable a basin is. With the help of several paradigmatic dynamical systems, we illustrate how to identify the ingredients that hinder the prediction of the final state. The basin entropy together with two new tests of the Wada property have been applied to some physical systems such as experiments of chaotic scattering of cold atoms, models of shadows of binary black holes, and classical and relativistic chaotic scattering associated to the Hénon-Heiles Hamiltonian system in astrophysics.

References

1. Daza, A.; Wagemakers, A.; Sanjuán, M.A.; Yorke, J.A. Testing for basins of Wada. *Sci. Rep.* **2015**, *5*, 16579.
2. Daza, A.; Wagemakers, A.; Sanjuán, M.A. Wada property in systems with delay. *Commun. Nonlinear Sci. Numer. Simul.* **2017**, *43*, 220–226.
3. Daza, A.; Wagemakers, A.; Georgeot, B.; Guéry-Odelin, D.; Sanjuán, M.A. Basin entropy: a new tool to analyze uncertainty in dynamical systems. *Sci. Rep.* **2016**, *6*, 31416.
4. Daza, A.; Georgeot, B.; Guéry-Odelin, D.; Wagemakers, A.; Sanjuán, M.A. Chaotic dynamics and fractal structures in experiments with cold atoms. *Phys. Rev. A* **2017**, *95*, 013629.
5. Daza, A.; Wagemakers, A.; Georgeot, B.; Guéry-Odelin, D.; Sanjuán, M.A. Basin Entropy, a Measure of Final State Unpredictability and Its Application to the Chaotic Scattering of Cold Atoms. In *Chaotic, Fractional, and Complex Dynamics: New Insights and Perspectives*; Springer: Cham, Switzerland, 2018.
6. Daza, A.; Shipley, J.O.; Dolan, S.R.; Sanjuán, M.A. Wada structures in a binary black hole system. *Phys. Rev. D* **2018**, *98*, 084050.
7. Daza, A.; Wagemakers, A.; Sanjuán, M.A. Ascertaining when a basin is Wada: the merging method. *Sci. Rep.* **2018**, *8*, 9954.
8. Wagemakers, A.; Daza, A.; Sanjuán, M.A. The saddle-straddle method to test for Wada basins. *Commun. Nonlinear Sci. Numer. Simul.* **2020**, *84*, 105167.



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Thermodynamics beyond Molecules: Statistical Mechanics of Probability Distributions and Stochastic Processes

sciforum-027062

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Statistical mechanics has a universal appeal that extends beyond molecular systems, and yet, as its tools are being transplanted to fields outside physics, the fundamental questions, what is thermodynamics and how it may be applied outside the realm of physical particles, have remained unanswered. We answer these questions here: Statistical mechanics in its most general form is variational calculus applied to probability distributions and by extension to stochastic processes in general; as a mathematical theory, it is independent of physical hypotheses but provides the means to incorporate our knowledge and model assumptions about the particular problem. The fundamental ensemble is a microcanonical space of probability distributions sampled via a bias functional that establishes a probability measure on this space. The maximization of this measure expresses the most probable distribution via a set of parameters (microcanonical partition function, canonical partition function and generalized temperature) that are connected through a set of mathematical relationships that we recognize as the familiar equations of thermodynamic. Any distribution in this space maybe endowed with the status of the most probable distribution under an appropriately constructed bias functional. Entropy, Kullback-Leibler divergence and the second law have simple interpretations in this theory. We obtain statistical mechanics as a special application to molecular systems and make contact with Information Theory and Bayesian inference. We use numerical examples to demonstrate the thermodynamic treatment of generic probability distributions, present a thermodynamic algorithm (the cluster ensemble) to sample arbitrary distributions with positive argument by analogy to reacting particles and discuss the extension of statistical mechanics to stochastic processes in general.



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Entropy, Statistical Thermodynamics and Stochastic Processes

sciforum-028991

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The undeniable appeal of statistical mechanics has led to numerous attempts to extend its tools to processes and problems outside the realm of molecules and physical particles. However, no formal theory exists to guide us on the application of statistical mechanics outside physics and chemistry. In this talk I will show that *the basic elements of statistical mechanics are universal to generic stochastic processes*.

The theory views a stochastic process as a network of chemical reactions. We begin with a finite sample of the the event space at time zero and construct all possible future paths based on the transformations that are possible under the rules of the stochastic process. We define the ensemble of states that can be reached in a fixed number of steps from the initial state (feasible space), define its probability and formulate its master equation. We show that when the size of the initial sample increases indefinitely (asymptotic limit), the feasible space becomes *continuous* but its probability distribution converges to *discrete points* that represent *thermodynamic phases*. If only one phase is present the ensemble is represented by its most probable distribution. We work out the calculus of the most probable distribution in the asymptotic limit, identify the functional whose maximization produces that distribution and express the most probable distribution in terms of a partition function and its derivatives. We analyze four problems under this theory: (a) random walk, (b) binary clustering (c) binary fragmentation and (d) equilibrium exchange, and give examples of phase splitting in these systems.



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Multivariate Symmetrical Uncertainty as a Measure for Interaction in Categorical Patterned Datasets

sciforum-030017

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Interaction between three or more variables is often found in statistical models where the response variable is numeric. Techniques like regression or analysis of variance can show interaction as a composite-variable term in the model, and their algorithms include calculations to determine the size of the interaction. However, there is a lack of methods to appropriately detect and measure interactions when the variables are a mix of numerical and categorical.

In this work, we present a way of measuring interactions between n categorical variables for the case of samples with patterned records. In these datasets, of all the possible attribute value combinations only some of them are present. We explore various datasets using the Multivariate Symmetrical Uncertainty, which is a recently developed entropy-based correlation measure. MSU is unbiased for representative samples, and it detects linear and non-linear associations between any mix of categorical and discretized numerical variables.

More precisely, we explore the behavior of a number of known 3-variable record structures such as XOR, AND, OR, NAND and others, plus their extensions to more variables. Simulations using different sampling scenarios on each record structure show that every n -variable pattern possesses a characteristic minimum value M_L and a characteristic maximum value M_U for the MSU correlation.

It is observed that the M_L value, attained when the pattern occurs in a certain combination of frequencies, hints that interaction is intrinsically expressed by this minimum value. Other sampling scenarios resulting in higher MSU values carry this intrinsic interaction due to the pattern itself, plus additional correlation due to extra occurrences of some configurations.

This method of quantifying n -way categorical interactions opens up new questions on the behavior of datasets that exhibit multivariate correlation, as for example in semi-patterned and non-patterned datasets.



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Entropic Dynamics on Gibbs Statistical Manifolds

sciforum-030373

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In a modern approach to statistical physics [Jaynes: Phys. Rev. 106, 620, 1957], Gibbs distributions appear naturally as a solution to a well set optimization problem: maximizing entropy under a set of expected values constraints. Generally in physics, the space in which a canonical distribution is defined are the microstates and the set expected values define the macrostates, which can be used as coordinates in a space of such canonical distributions (statistical manifold). In the field of Information Geometry [Amari and Nagaoka: Methods of Information Geometry, American Mathematical Soc., 2007] [Ruppeiner: Rev. Mod. Phys. 68, 313, 1996] these distributions happen to have deeply interesting geometrical properties such as their metric tensor is a covariance matrix and important thermodynamical objects, such as free energy, appear naturally. This work aims to provide a systematic way to create dynamical systems in a space of canonical distributions. These dynamics are derived as an application of entropic methods of inference i.e., that is a form of entropic dynamics [Caticha: Entropy 17, 6110, 2015]. As an interesting result, the average motion in such a dynamical process reduces to the Onsager Relations [Onsager: Phys. Rev. 37, 405, 1931], derived from purely probabilistic—not intrinsically thermodynamical—arguments. This can give new insight on fields such as critical phenomena and renormalization groups as well as deal with statistical problems in which the microstate dynamics is not so well defined such as economics and ecology.



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Entropic Optimal Transport on Countable Spaces: Statistical Theory and Asymptotics

sciforum-030216

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In recent years, the theory of OT has become a fundamental tool in statistical research, e.g., the Wasserstein distance being a prominent method for inferential purposes. The large computational complexity, however, has hindered OT in becoming a routine methodology for the analysis of large scale data sets. This has encouraged the formulation of regularized OT which often turns out to be computationally more accessible. The most prominent proposal is given by entropic regularization (c.f. [1]) that serves to define an entropic OT distance (EOTD) and Sinkhorn divergence.

In the present study, we derive limit distributions for empirical EOTD (i.e., when data are sampled randomly) between probability measures supported on countable discrete spaces. In particular, we consider a general class of cost functions and state conditions on the probability measures to ensure general weak convergence for empirical EOTD. Furthermore, for bounded cost functions we show that the empirical entropic transport plan itself converges weakly in ℓ^1 -sense to a Gaussian process. The theory generalizes results derived by [2] for finite discrete spaces. Moreover, they complement recent findings by [3] for the empirical EOTD between more general probability measures on $\mathbb{R}^m$ with quadratic cost. Our approach is based on a sensitivity analysis of necessary and sufficient optimality conditions for the entropic transport plan. We demonstrate possible application for colocalization analysis of protein networks in biology.

This is joint work with Marcel Klatt and Axel Munk.

References

1. Cuturi, M. Sinkhorn Distances: Lightspeed Computation of Optimal Transport. *Adv. Neural Inf. Process. Syst.* **2013**, *26*, 2292–2300.
2. Klatt, M.; Tameling, C.; Munk, A. Empirical Regularized Optimal Transport: Statistical Theory and Applications. *arXiv* **2018**, arXiv:1810.09880.
3. Mena, G.; Weed, J. Statistical bounds for entropic optimal transport: sample complexity and the central limit theorem. *arXiv* **2019**, arXiv:1905.11882.



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Informational Harmoniums

sciforum-030289

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In this paper we introduce a type of harmoniums that uses only computations in the domain of information without resorting to probabilities. Starting from the probabilistic description of binary harmoniums—or Restricted Boltzmann Machines (RBMs)—we use the shifted Rényi information function to obtain a description of harmoniums, hence called informational harmoniums, in terms of some information semifields recently described where the harmonium architecture is concisely expressed by a matrix whose origin and range spaces of visible inputs and hidden units are semi-vector spaces.

On the one hand, inference in an informational harmonium is expressed in terms of vector-matrix operations in information semi-vector spaces. Taking the extreme values of the Rényi parameter in the information semifields we obtain the min-plus semifield and the operation of the harmoniums becomes additively-idempotent. This leads into one of four possible different forms types of Galois connections between the input and output spaces. In this extreme case, we discuss the representation spaces of the input and hidden nodes of informational harmoniums in terms of a variant of formal concept analysis.

On the other hand, learning resembles a process akin to hetero-associative morphological memory construction in a non-idempotent semifield, unless again the value of the Rényi parameter is extremized. In this situation we derive formulas where negative loglikelihood minimisation of training data are carried out algebraically without resorting to derivatives.



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New Parameters and Extensive Methodology to Describe the Three Phase Transitions in the q -States Clock Model

sciforum-029137

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In the q -state clock model the spin has q possible orientations in the plane so it can be understood as a generalization of the Ising model for which $q = 2$. The Hamiltonian is then the scalar product of the neighboring spins mediated by the ferromagnetic exchange interaction J homogeneous through the square lattice with $L/L = N$ spins. It is known that for $q \leq 4$ there is only one phase transition at a temperature T_1 , over which the ferromagnetic phase is lost. Using global order parameters it has been previously established that for $q \geq 5$ this transitions moves steadily to lower temperatures as q increases [1]. For large L the appearing of the so called Berezinskii–Kosterlitz–Thouless (BKT) phase characterized by vortex like structures is established, while a second transition to a disordered phase appears at a higher T_2 temperature. In the present paper we deeply characterize the nature of this second transition by means of new local order parameters. Surprisingly, an unexpected subtle transition appears at a temperature slightly over the second one (at T_3) requiring interpretation. This is resolved by considering pure and mixed ferromagnetic, vortex and paramagnetic phases as T increases requiring local order parameters and new methodology to better handle them. Thus, we include now information theory analysis by means of mutability and Shannon entropy characterization. Tendencies towards large N and q values are established.

Reference

- 1 Negrete, O.A.; Vargas, P.; Peña, F.J.; Saravia, G.; Vogel, E.E. Entropy and Mutability for the q -State Clock Model in Small Systems. *Entropy* **2018**, *20*, 933.



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The Fundamental Diagram in Vehicular Traffic

sciforum-030296

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Nowadays, the study of traffic flow in highways represents a big challenge. This problem is mainly interesting when vehicular density is high enough to produce congestion. The description of such phenomena has been made through several approaches going from the phenomenological up to individual behavior of drivers. In this work we start with a generalization of the Prigogine-Herman-Boltzmann (PHB) kinetic equation to consider the vehicles' sizes, like the Enskog generalization to take into account the finite size of molecules in a moderately dense gas. Our main goal is the derivation of a fundamental diagram relating the flux with the density, in the homogeneous steady state of traffic. The conditions satisfied by the distribution function are given and their numerical solution allows the construction of the corresponding fundamental diagram. This derivation allows us to obtain some of the threshold values which separate the free and congested regimes. The model results are contrasted with recent empirical data and show excellent agreement.



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Entropy Production of Reaction-Diffusion Systems under Confinement

sciforum-030299

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Diffusion processes under confinement within a channel in which one coordinate is longer than the others have been studied by projecting the diffusion equation into one dimension. This results in the so-called Fick-Jacobs equation that introduces an effective diffusion coefficient dependent on the position. Several approaches have been used to propose position-dependent diffusion coefficients, and it has been found that it depends on the channel's width function as well as the geometric properties of the midline, such as its curvature and torsion. Within this approach we study the entropy production for a reaction-diffusion process of two species on a two dimensional channel. Recently, it has been seen that the Turing instability conditions, the range of unstable modes for patterns formation, as well as the spatial structure of the patterns themselves, can be modified through the geometric parameters of the confinement. In this contribution, the effect of the confinement on entropy production is analyzed and characterized in terms of the geometry of the corresponding channel.



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Different Scenarios Leading to Hyperchaos Development in Radiophysical Generators

sciforum-028758

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Chaos is a typical attribute of nonlinear dynamical systems in various fields of science and technology. One of the conventional indicator of chaotic dynamics is the largest Lyapunov exponent. Chaos is implemented in a situation when in the spectrum of Lyapunov exponents for a flow there is one positive, one zero and at least one negative exponents. Using full spectrum of Lyapunov exponents it is possible to classify hyperchaos, when spectrum contains two or more positive Lyapunov exponents.

In the frame of this work we describe two scenarios leading to occurrence of hyperchaos on the examples of the modified Anishchenko-Astakhov's generator and coupled generators of quasiperiodic oscillations. The first scenarios is a new scenario associated with appearance of Shilnikov's attractor, when saddle-focus with two-dimensional unstable manifold occurs via secondary Neimark-Sacker bifurcation and absorbs by chaotic attractor. For this scenario we will present cascade of secondary Neimark-Sacker bifurcations, corresponding to hierarchy of Shilnikov's attractors corresponding to hyperchaos. The second scenario was described previously, and associated with cascade of period doubling bifurcation of saddle-cycles with two-dimensional unstable manifold. Both scenarios will be presented for radiophysical generators.

The reported study was funded by RFBR according to the research project № 19-31-60030.



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Walking down over the Spatiotemporal Scales in a Particular Nonequilibrium-Thermodynamics Dissipative Phenomenon Called Friction

sciforum-029053

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It is intriguing to fully comprehend whether the simple, macroscopic scale expressing Coulomb-Amontons law, describing the static friction effect, and referring to a ratio of friction force vs. the corresponding load, preserves when looking into more fine-grained surface (or, interface) dimensional scales [1]. This question is of utmost interest when attempting to comprehend the complex friction and lubrication phenomenon, expressing its relevance in bioinspired issues, pertaining to biomimetic solutions, represented by the natural articulating devices, such as articular cartilage, examined carefully in (sub)mesoscopic scales [2–4]. In what follows, a particular nonequilibrium-thermodynamics, dissipation addressing framework has been offered to unravel explicitly the spatiotemporal, and implicitly, force-field scales. It is based upon a dissipative autonomous ordinary-differential system, equipped with fractal-like kinetics, and fully immersed in the mesoscopic scale [4]. Its nanoscopic viz microscopic extension can be introduced either by means of certain anomalous diffusion vs. (mechanical) relaxation parametric sets, or when employing thoroughly molecular dynamics computer simulations [3]. A survey of adequately formulated experimental and computer simulation based long-perspective arguments has recently been proposed in [5]. The main idea of revealing the scale peculiarities touches upon certain assumption on the structure formation in the friction interlayer. The structure formation causes the suitable microscopic response of the soft-material, i.e., diffusion-relaxation involving propensity. A certain shortage of the method proposed points unavoidably to a lack of precise information about the involved force-field magnitudes, and their consecutive characteristics. Other studies do not show up such a drawback [6] but they do not deal in full and satisfactorily with the scale problem [1–4]. Our aim is to fill in the gap by proposing a scale-sensitive formulation of the friction-lubrication problem of importance for biological systems, exemplifying by the articulating joints.

References

1. Gadomski, A. Multilevel-interaction friction procedure applicable in case of two opposing surfaces competing with one another – A gedanken experiment. *Phys. Essays* **2015**, *28*, 650–653.
2. Gadomski, A. On (sub)mesoscopic scale peculiarities of diffusion driven growth in an active matter confined space, and related (bio)material realizations. *Biosystems* **2019**, *176*, 56–58.
3. Beldowski, P.; Weber, P.; Dedinaite, A.; Claesson, P.; Gadomski, A. Physical crosslinking of hyaluronic acid in the presence of phospholipids in an aqueous nano-environment. *Soft Matter* **2018**, *14*, 8997–9004.
4. Gadomski, A.; Beldowski, P.; Rubi, J.M.; Urbaniak, W.; Augé II, W.K.; Santamaria-Holek, I.; Pawlak, Z. Some conceptual thoughts toward nanoscale oriented friction in a model of articular cartilage. *Math. Biosci.* **2013**, *244*, 188–200.

Complex Systems

Oral Presentation

5. Dédinaïté, A.; Wieland, F.; Beldowski, P.; Claesson, P.M. Biolubrication synergy: Hyaluronan–Phospholipid interactions at interfaces. *Adv. Colloid Interface Sci.* **2019**, *274*, 102050.
6. Seror, J.; Zhu, L.; Goldberg, R.; Day, A.J.; Klein, J. Supramolecular synergy in the boundary lubrication of synovial joints. *Nat. Commun.* **2015**, *6*, 6497.



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Simulation Studies of Entropy-Driven Crystallization in Athermal Chain Packings in the Bulk and under Confinement

sciforum-029273

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We present results from extensive off-lattice simulations on packings of flexible linear chains of hard spheres in the bulk and under confinement. We employ a Monte Carlo scheme, built around advanced, chain-connectivity-altering moves, for the short- and long-range equilibration even for very long and definitely entangled systems, at very high concentrations near the maximally random jammed (MRJ) state and under extreme confinement [1]. Local environment and similarity to specific crystal structures are gauged through the crystallographic element norm (CCE) metric [2] which is able to distinguish between different competing crystal structures. The established crystal morphologies range from random hexagonal close packed ones with a single or varied stacking direction(s) to pure face-centred cubic (fcc) and hexagonal close packed (hcp) crystals. We explain how the total entropy of the system increases as the local environment of the crystal phase becomes more symmetric and spherical. This entropic effect leads to the observed transition from the initial amorphous to the final crystal phase [3]. By extending the simulations to trillions of steps crystal perfection is observed in accordance to the Ostwald's rule of stages in crystal polymorphism.

In general, bond tangency of successive monomers along the chain backbone or the corresponding gaps affect profoundly the ability of chains to crystallize [4]. Based on these findings, by using simple geometric arguments, we explain the role of rigid and flexible constraints in the packing behavior (crystal nucleation and growth) of general atomic and particulate systems.

References

1. Ramos, P.M.; Karayiannis, N.C.; Laso, M. Off-lattice simulation algorithms for athermal chain molecules under extreme confinement. *J. Comput. Phys.* **2018**, *375*, 918–934.
2. Karayiannis, N.C.; Foteinopoulou, K.; Laso, M. The characteristic crystallographic element norm: A descriptor of local structure in atomistic and particulate systems. *J. Chem. Phys.* **2009**, *130*, 074704.
3. Karayiannis, N.C.; Foteinopoulou, K.; Laso, M. Entropy-driven crystallization in dense systems of athermal chain molecules. *Phys. Rev. Lett.* **2009**, *103*, 045703.
4. Karayiannis, N.C.; Foteinopoulou, K.; Laso, M. The role of bond tangency and bond gap in hard sphere crystallization of chains. *Soft Matter* **2015**, *11*, 1688–1700.



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Information Geometry & Complexity Science

sciforum-030444

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In the first part of my lecture, I will review information-geometric structures and highlight the important role of divergences. I will present a novel approach to canonical divergences which extends the classical definition and recovers, in particular, the well-known Kullback-Leibler divergence and its relation to the Fisher-Rao metric and the Amari-Chentsov tensor.

Divergences also play an important role within a geometric approach to complexity. This approach is based on the general understanding that the complexity of a system can be quantified as the extent to which it is more than the sum of its parts. In the second part of my lecture, I will motivate this approach and review corresponding work.

References

1. Ay, N.; Amari, S.I. A Novel Approach to Canonical Divergences within Information Geometry. *Entropy* **2015**, *17*, 8111–8129, doi:10.3390/e17127866.
2. Ay, N.; Jost, J.; Le, H.V.; Schwachhöfer, L. *Information Geometry*; Ergebnisse der Mathematik und Ihrer Grenzgebiete/A Series of Modern Surveys in Mathematics; Springer: Cham, Switzerland, 2017.
3. Ay, N. Information Geometry on Complexity and Stochastic Interaction. *Entropy* **2015**, *17*, 2432–2458, doi:10.3390/e17042432.



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Shannon Entropy and Hydrothermal Processes

sciforum-030201

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Hydrothermal processes modify the chemical and mineralogical composition of a rock. These modifications can be regarded as a form of information imposed on the rock and may potentially be quantifiable. However, there are no existing single measures to quantify these effects, nor do we have a good notion of what parameters should be measured. In this presentation, concepts from information theory are used to provide new insights into the effect of hydrothermal processes on rock, which enable measurement and quantification.

We used the Shannon entropy to quantify the differences in chemical compositions, and the shortwave infrared spectral response between altered and unaltered rocks. The results showed that the Shannon entropy can capture these differences in compositions, where hydrothermally altered rocks have lower entropies compared to their precursors. A relationship was found between the heat of a magma source and Shannon entropy, where the heat of a cooling sub-volcanic intrusion drove fluid circulation in the hydrothermal system causing intense alteration of rock and a decrease in Shannon entropy. We show that the Shannon entropy has the potential to be used as a proxy for parts of the thermodynamic entropy of hydrothermally altered environments. The insights from this study enable new directions of research on the relationships between hydrothermal processes, entropies, information and the effects on mineralized and early life environments.



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Entropy Measure for Planning, Prediction and Online Estimation in Biotechnological Processes

sciforum-030231

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Recently, a generic bioprocess gray box modeling approach [1] used entropy measure to plan the feeding solution profile. Multiple industrial experiments showed that such modeling is useful in cultivations with limited substrate feeding. The feeding profile served as a scaled approximation of the cumulative biomass profile. The cumulative glucose volume served as uncertainty to find the gray box model parameters in the feedback control scenarios. The numeric convex approach passed an analysis of its sensitivity to different initial computational conditions. The validation showed that the numeric routines were independent of the selected initial conditions. Such simplicity makes it useful for practical industrial applications. Maximization of entropy presented online estimation of biomass concentration in fed-batch cultures of four types of recombinant *E.coli* strains and *Saccharomyces cerevisiae* cells [2]. Practical experience disclosed that entropy is a relevant measure for both limited substrate feeding and dosed substrate feeding biotechnological processes. Moreover, the approach showed neither numeric nor structural model dependence on the strain type. Research progress revealed that entropy measure by the use of fundamental knowledge could make the general model (Luedeking-Piret) more common for technological use when estimating target protein, compared to a sophisticated artificial neural network (ANN) [3]. In fact, it replaces the ANN approach without compromising estimation accuracy.

Funding: This project has received funding from European Regional Development Fund (project No 01.2.2-LMT-K-718-03-0039) under grant agreement with the Research Council of Lithuania (LMTLT).

References

1. Urniežius, R.; Galvanauskas, V.; Survyla, A.; Simutis, R.; Levisauskas, D. From Physics to Bioengineering: Microbial Cultivation Process Design and Feeding Rate Control Based on Relative Entropy Using Nuisance Time. *Entropy* **2018**, *20*, 779.
2. Urniežius, R.; Survyla, A.; Paulauskas, D.; Bumelis, V.A.; Galvanauskas, V. Generic estimator of biomass concentration for *Escherichia coli* and *Saccharomyces cerevisiae* fed-batch cultures based on cumulative oxygen consumption rate. *Microb. Cell Fact.* **2019**, *18*, 190.
3. Urniežius, R.; Survyla, A. Identification of Functional Bioprocess Model for Recombinant *E. Coli* Cultivation Process. *Entropy* **2019**, *21*, 1221.



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Approximate Entropies of Resting State Continuous Neurocardiovascular Physiological Signals Are Associated with Physical Frailty in Older Adults

sciforum-030250

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Frailty in older adults is characterised by dysregulation in multiple physiological systems. The frailty phenotype is defined on the basis of exhaustion, unexplained weight loss, weakness, slowness and low physical activity (one or two: pre-frail; 3 or more: frail). Our aim was to explore if increasing frailty is associated with the complexity of resting state physiological signals in a large cohort of community-dwelling older adults, enrolled as part of The Irish Longitudinal Study on Ageing (TILDA).

Systolic/diastolic blood pressure (SBP/DBP), mean arterial pressure (MAP), and heart rate (HR) were measured in 3154 participants (66.2% non-frail; 31.3% pre-frail; 2.5% frail) using a *Finometer*[®] device at 200 Hz; and frontal lobe oxygenation (tissue saturation index (TSI)) in 2749 individuals (66.3% non-frail; 31.3% pre-frail; 2.4% frail) at 50Hz using an *Artinis Portalite*[®] near infrared spectroscopy system. Data were acquired continuously during five minutes of supine rest and the last minute (downsampled to 5 Hz) was utilised in these analyses. The complexity of signals was quantified using approximate entropy (ApEn) with $m = 2$ and an optimal r derived via multiple iterations, implemented in Matlab (*R2019a*). Statistical analysis was performed using multivariate linear regression models in STATA (*v14.1*), controlling for age, sex, education, antihypertensive medication, diabetes, number of cardiovascular conditions, smoking, alcohol, and depression.

Mean age for both groups was 64.3 ± 8.1 years and 53% were female. The pre-frail group was associated with significantly increased ApEn for all measures investigated (sBP: $\beta = 0.014$, $p \leq 0.001$; dBP: $\beta = 0.009$, $p = 0.002$; MAP: $\beta = 0.012$, $p \leq 0.001$; HR: $\beta = 0.011$, $p = 0.003$; TSI: $\beta = 0.009$, $p = 0.002$). Likewise, the frail group was associated with further increased ApEn for all measures investigated (sBP: $\beta = 0.031$, $p = 0.002$; dBP: $\beta = 0.028$, $p = 0.003$; MAP: $\beta = 0.038$, $p \leq 0.001$; HR: $\beta = 0.034$, $p = 0.001$; TSI: $\beta = 0.018$, $p = 0.029$).

Approximate entropy seems to be a sensitive method to capture increasing signal complexity in multiple physiological systems associated with the frailty phenotype during resting state.



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On the Implementation of Downsampling Permutation Entropy Variants in the Detection of Bearing Faults in Rotatory Machines

sciforum-030267

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Background: The Multiscale Permutation Entropy (MPE) is a powerful tool in the differentiation of physiological electrical activity. In particular, the literature has found a clear link between the presence of faults in rotatory machines signals (Zheng 2018), and a reduction in Entropy within them. Therefore, any improvement in the precision of the MPE estimation enhances the chances of detecting increasingly nuanced changes in fault detection.

Objectives: In the present work, we first provide an alternative Permutation Entropy approach: the Refined Composite Downsampling Multiscale Permutation Entropy (rcDPE), which further reduces the variance over Refined Composite Multiscale Permutation Entropy (rcMPE) [Humeau-Heutier, 2015], by applying an alternative to the widely used coarse-graining procedure for multiscaling.

Methodology: Using the Bechhoffer bearing fault dataset (2013), we performed a 3-way ANOVA test with the following factors: Type of signal (presence of faults), Method, and Dimension. We also found the optimal parameters in this dataset in order to increase the entropy difference between faulty and non-faulty components.

Results: From the ANOVA test, we found all factors and interactions to be statistically significant ($p < 0.001$). Furthermore we found that, albeit rcDPE greatly reduces the variance in PE measurements, the difference between Type of signal is reduced due to aliasing effects. The best performance is achieved with the use of an anti-aliasing filter in conjunction with rcDPE. For this particular dataset, classification between Types is reduced with increased Dimension, where only the filtered rcDPE remains significant. Therefore, rcDPE presents an important alternative in the exploration of Complexity-based classification techniques, capable of discerning more subtle changes between fatigued and non-fatigued muscle contractions.



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Aspects of Gravity's Rainbow in Black Hole Entropy

sciforum-030339

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Quantum Field Theory is plagued by divergences in the attempt to calculate physical quantities. Standard techniques of regularization and renormalization are used to keep under control such a problem. Gravity's Rainbow seems to offer a different scheme which is able to remove infinities when Black Hole Entropy is computed in contrast to what happens in conventional approaches. In particular, we apply the Gravity's Rainbow regularization scheme to the computation of the entropy of a Schwarzschild black hole from one side. In a second step, we will consider the effects of rotations on the calculation of some thermodynamical quantities like the free energy, internal energy and entropy. Even in this case, in ordinary gravity, when we evaluate the density of states of a scalar field close to a black hole horizon, we obtain a divergent result which can be kept under control with the help of some standard regularization and renormalization processes. Once again we will show that when we use the Gravity's Rainbow approach such regularization/renormalization processes can be avoided. A comparison between the calculation done in an inertial frame and in a comoving frame is presented.



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Complexity as Causal Information Integration

sciforum-030208

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Complexity measures in the context of the Integrated Information Theory of consciousness, developed mainly by Tononi [1], try to assess the strength of the causal connections between different neurons. This is done by minimizing the Kullback-Leibler-Divergence between a full system and one without causal connections. Various measures have been proposed in this setting and compared in, for example, [2–6]. Oizumi et al. develop in [7] a unified framework for these measures and postulate properties that they should fulfill. Furthermore, they introduce an important candidate of these measures, denoted by Φ , based on conditional independence statements. Unfortunately it cannot be computed analytically in general and the KL-Divergence has to be optimized numerically.

We propose an alternative approach using a latent variable which models a common exterior influence. This leads to a measure, causal information integration, that satisfies all of the required conditions provided the state space of the latent variable is large enough and it can serve as an upper bound for Φ . Our measure can be calculated using an iterative information geometric algorithm, the em-algorithm. Therefore we are able to compare its behavior to existing integrated information measures.

References

1. Tononi, G. An information integration theory of consciousness. *BMC Neurosci.* **2004**, *5*, 42.
2. Amari, S.I.; Tsuchiya, N.; Oizumi, M. Geometry of information integration. In *Information Geometry and Its Applications IV*; Springer: Cham, Switzerland, 2016; pp. 3–17.
3. Ay, N. Information geometry on complexity and stochastic interaction. *Entropy* **2015**, *17*, 2432–2458.
4. Kanwal, M.S.; Grochow, J.A.; Ay, N. Comparing information-theoretic measures of complexity in Boltzmann machines. *Entropy* **2017**, *19*, 310.
5. Langer, C. Theoretical Approaches to Integrated Information and Complexity. Master's Thesis, 2019.
6. Mediano, P.A.; Seth, A.K.; Barrett, A.B. Measuring integrated information: Comparison of candidate measures in theory and simulation. *Entropy* **2019**, *21*, 17.
7. Oizumi, M.; Tsuchiya, N.; Amari, S.I. Unified framework for information integration based on information geometry. *Proc. Natl. Acad. Sci. USA* **2016**, *113*, 14817–14822.



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An Information Geometry Approach for Unifying Mean Field Theories of Asymmetric Kinetic Ising Systems

sciforum-030266

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Many physical and biological dynamical systems operate away from thermodynamic equilibrium, driven by their own activity as well as their interaction with the environment. The kinetic Ising model is a prototypical model for studying such non-equilibrium dynamics. Since its behaviour is generally intractable for large sizes due to combinatorial explosion, mean field theories are often employed to approximate network dynamics. However, mean field methods are often unable to capture systems displaying long-range correlations such as those operating near critical phase transitions. To tackle this problem, different variants of mean field approximations have been proposed for kinetic Ising models, each making unique assumptions about the correlation structure of the system. This disparity complicates the challenge of systematically advancing beyond previous contributions. Here, using information geometry, we propose that existing methods can be described and extended in a unified framework. Our method is defined as a family of expansions (called Plefka expansions) of an intractable marginal probability distribution around a specific point of a simplified model, defined in an information geometric space. These points are obtained by an orthogonal projection to a sub-manifold of probability distributions displaying a simplified correlation structure. This approach not only unifies previous methods but allows us to define novel methods that make unusual assumptions for mean field methods, like models preserving specific correlations of the system. By comparing analytic approximations and exact numerical simulations in a kinetic Sherrington Kirkpatrick model, we show that the new approximations found by our method provide more accurate estimates of the dynamics of the systems than classical equations, even near critical phase transitions presenting large fluctuations. In sum, our framework unifies and extends existing mean field methods in the kinetic Ising model from an information theoretic view, constituting a powerful tool for studying the dynamics of complex systems.



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Entropy in Software Architecture

sciforum-030281

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In building software architectures, the relations between elements in different diagrams are often overlooked. When constructing software architecture, IT architects more or less consciously however introduce elements that represent the same object instance on different diagrams with similar names. These connections are called consistency rules and are usually not saved in any way in the modeling tool. It was mathematically proved that the application of consistency rules increases the information content of software architecture. The feelings about increasing readability and ordering of software architecture by means of consistency rules have their mathematical rationale. In this article it was carried out a proof of decreasing information entropy while applying consistency rules in the construction of software architecture of IT systems. Therefore, it has been shown that marking selected elements in different diagrams with similar names is therefore an implicit way to increase the information content of software architecture while simultaneously improving its orderliness and readability.



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On the Search of Minimum Information Loss in Coarse-Grained Modelling of Biomolecules

sciforum-030011

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The computational resources required by atomistic simulations of biomolecular systems still limit their applicability to relatively short time and length scales, at odds with those typically characterising biological processes. By integrating out most of the microscopic degrees of freedom in favor of a description in terms of few sites interacting through effective potentials, coarse-grained (CG) models constitute a powerful instrument for broadening the class of accessible phenomena, at the same time providing accurate results [1]. Also an exact CG procedure, however, inherently comes at a price: a loss of information, quantified by an increase in entropy, arising when a system is observed through “CG glasses” [2]. Interestingly, this loss only depends on the mapping, i.e., the sites one employs to represent the system at the CG level, which are often a priori selected only based on physical intuition [3].

Several questions follow: how wide and diverse is the space of possible CG mappings of a biomolecule? Within this space, are there representations that minimise the information loss, and do these “privileged” mappings give hints on the underlying biological processes? In this work, we address these topics by first characterising the space of CG representations of a system through the definition of a distance between mappings. Subsequently, we develop a workflow enabling to estimate the increase in entropy of a protein arising from CG’ing. Finally, we show that minimising this quantity over the space of possible CG representations suggests a connection between the biological relevance of a chemical fragment composing the biomolecule and the amount of information it contains [4].

References

1. Menichetti, R.; Pelissetto, A.; Randisi, F. Thermodynamics of star polymer solutions: A coarse-grained study. *J. Chem. Phys.* **2017**, *146*, 244908.
2. Rudzinski, J.F.; Noid, W.G. Coarse-graining entropy, forces, and structures. *J. Chem. Phys.* **2011**, *135*, 214101.
3. Diggins, I.V.; P; Liu, C.; Deserno, M.; Potestio, R. Optimal coarse-grained site selection in elastic network models of biomolecules. *J. Chem. Theory Comput.* **2018**, *15*, 648–664.
4. Giuliani, M.; Menichetti, R.; Shell, M.S.; Potestio, R. An Information-Theory-Based Approach for Optimal Model Reduction of Biomolecules. *J. Chem. Theory Comput.* **2020**, *16*, 6795–6813.



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The Mathematical State of Equations of State

sciforum-030191

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The van der Waals equation of state was a breakthrough of a genius. However, while it was a masterpiece from a conceptual point of view, it is not quantitatively accurate. Many equations of state have been proposed to date, the accuracy of which has been improved by introducing temperature-dependence of coefficients, and various ways to treat the volume of the molecules themselves. Long time ago, the author analyzed the mathematical aspects of equations of state and proved that the general form must be $P = A(V)T - B(V)$, where P is the pressure, T is the absolute temperature, V is the volume, and A and B are functions of V only. Thus, the corrections to the van der Waals equation should depend on the volume only and not on the temperature. Practical implications of this conclusion are demonstrated.

Another major problem is the construction of equations of state of mixtures. The prevalent approach is to define mixing rules for the parameters of the equation of state, by which the mixture is treated as if it is a single component with some averaged parameters of the individual components. However, this approach leads to discontinuities in the isotherms. A new approach that avoids this problem is suggested and demonstrated.



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Conformational and Translational-Rotational Entropy from Molecular Ensembles

sciforum-030234

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Entropy calculation is an important step in the postprocessing of molecular dynamics trajectories or predictive models. In recent years the nearest neighbor method proposed by Demchuk and coworkers [1] has emerged as a powerful method to deal in a flexible way with the dimensionality of the problem. Applications to most important biomolecular processes have been presented [2,3] and a specific development has concerned the computation of rotational-translational entropy which required in turn the definition of a metric in rotation-translation space [4]. Two programs have been developed to compute conformational and rotational-translational entropies from biomolecular ensembles [5]. Possible extensions of the method will be presented.

References

1. Singh, H.; Misra, N.; Hnizdo, V.; Fedorowicz, A.; Demchuk, E. Nearest neighbor estimates of entropy. *Am. J. Math. Manag. Sci.* **2003**, *23*, 301–321.
2. Fogolari, F.; Corazza, A.; Esposito, G. Free energy, enthalpy and entropy from implicit solvent end-point simulations. *Front. Mol. Biosci.* **2018**, *5*, 11.
3. Fogolari, F.; Corazza, A.; Fortuna, S.; Soler, M.A.; VanSchouwen, B.; Brancolini, G.; Corni, S.; Melacini, G.; Esposito, G. Distance-based configurational entropy of proteins from molecular dynamics simulations. *PLoS ONE* **2015**, *10*, e0132356.
4. Fogolari, F.; Fomthum, C.J.D.; Fortuna, S.; Soler, M.A.; Corazza, A.; Esposito, G. Accurate Estimation of the Entropy of Rotation-Translation Probability Distributions. *J. Chem. Theory Comput.* **2016**, *12*, 1–8.
5. Fogolari, F.; Maloku, O.; Fomthum, C.J.D.; Corazza, A.; Esposito, G. PDB2ENTROPY and PDB2TRENT: Conformational and Translational-Rotational Entropy from Molecular Ensembles. *J. Chem. Inf. Model.* **2018**, *58*, 1319–1324.



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Analysis of the Nonlinear Maxwell-Cattaneo-Vernotte Equation

sciforum-029082

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It is well-known that the Fourier equation for heat conduction is not satisfactory in many cases, such as low-temperature situations. It motivated the researchers to find possible extensions. There are numerous approaches in the literature, here we apply non-equilibrium thermodynamics with internal variables.

The first, and successfully applied generalized constitutive equation is called Maxwell-Cattaneo-Vernotte (MCV) equation. It is quite straightforward to derive using the internal variable theory. However, when nonlinear attributes come into the picture, there are some significant consequences that must be investigated further.

In the present paper [1], we are considering temperature-dependent material parameters, e.g., the thermal conductivity and the relaxation time both depend on the temperature. A consistent analysis shows that in some cases, the temperature dependence of mass density follows immediately. It cannot be avoided; thus, the mechanical field has to be introduced to obtain a physically admissible solution.

On the other hand, we investigated the numerical solutions of such a nonlinear MCV equation. We found that the nonlinear numerical stability analysis can be substituted with the linear one by estimating the maximum of the temperature field apriori. Here, we present the effects of temperature dependence and demonstrating the usage of the developed numerical code.

Reference

1. Kovács, R.; Rogolino, P. Numerical treatment of nonlinear Fourier and Maxwell-Cattaneo-Vernotte heat transport equations. *Int. J. Heat Mass Transf.* **2020**, *150*, 119281.



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Stability under limited control in weakly dissipation cyclic heat engines

sciforum-029423

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In this work we study the effect of natural stability mechanisms in stochastic trajectories produced by deviations of the operation regime due to fluctuations on the heat exchanges between the heat device and the thermal reservoirs. Perturbations on the operation regime from external sources produce stochastic trajectories along one cycle and the energetic consequences of the restitution forces are then analyzed. The main energetic functions such as power output, efficiency and entropy production, as well as compromise based functions are analyzed and the role of the stability basin, the so-called nullcline (which determine the restitution strength) and the endoreversible and irreversible limits (linked to a thermodynamic optimization) are put together to establish a connection between stability and a self-optimization feature.

The return maps of the dynamics allow us to understand the biggest contribution of the stability in the energetic evolution of the system. Additionally, fluctuations of the thermodynamic functions allow us to deepen into the susceptibility of each energetic function.



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The Entropy of Supermassive Black Holes during Its Evaporation Time

sciforum-030028

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Is it possible to quantify in General Relativity, RG, the entropy generated by supermassive black holes, BHs, during its evaporation time, since the intrinsic Hawking radiation in the infinity that, although insignificant, is important in the effects on the thermal quantum atmosphere?

The purpose was to develop a formula that allows us to measure the entropy generated during the evaporation time of different types of BHs of: i. remnant BH of the binary black holes' merger, BBH: GW150914, GW151226 and LTV151012 detected by the Laser Interferometer Gravitational-Wave Observatory (LIGO), and ii. Schwarzschild, Reissner-Nordström, Kerr and Kerr-Newman, and thus quantify in GR the "insignificant" quantum effects involved, in order to contribute to the validity of the generalized second law (GSL) that directly links the laws of black hole mechanics to the ordinary laws of thermodynamics, as a starting point for unifying quantum effects with GR. This formula could have some relationship with the detection of the shadow's image of the event horizon of a BH.

This formula was developed in dimensional analysis, using the constants of nature and the possible evaporation time of a black hole taking into account its distance to the Earth, to quantify the entropy generated during that time. The energy-stress tensor was calculated with the 4 metrics to obtain the material content and apply the proposed formula.

The entropy of the evaporation time of BHs proved to be insignificant, its temperature is barely above absolute zero, however, the calculation of this type of entropy allows us to argue about the importance of the quantum effects of Hawking radiation mentioned by authors who have studied the quantum effects with arguments that are fundamentally based on the presence of the surrounding thermal atmosphere of the black hole.



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The Fourth Law of Thermodynamics: Every Nonequilibrium State Is Characterized by a Metric in State Space with Respect to Which Its Spontaneous Attraction towards Stable Equilibrium Is along the Path of Steepest Entropy Ascent

sciforum-044256

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When thermodynamics is understood as the science (or art) of constructing effective models of natural phenomena by choosing a minimal level of description capable of capturing the essential features of the physical reality of interest, the scientific community has identified a set of general rules that the model must incorporate if it aspires to be consistent with the body of known experimental evidence. Some of these rules are believed to be so general that we think of them as laws of Nature, such as the great conservation principles, whose ‘greatness’ derives from their generality, as masterfully explained by Feynman in one of his legendary lectures. The first law and second law are universally contemplated among the great laws of Nature. In the logical development of thermodynamic theory they support the definitions of the energy and the entropy of every state of the modelled system, respectively. The recent paper <https://dx.doi.org/10.1098/rsta.2019.0168> shows that in the past four decades, an enormous body of scientific research devoted to modeling the essential features of nonequilibrium natural phenomena has converged from many different directions and frameworks towards the general recognition (albeit still expressed in different but equivalent forms and language) that another rule is also indispensable and reveals another great law of Nature. We call it the ‘fourth law of thermodynamics’ and state it as follows: every non-equilibrium state of a system or local subsystem for which entropy is well defined, must be equipped with a metric in state space with respect to which the irreversible component of its time evolution is in the direction of steepest entropy ascent compatible with the conservation constraints. A powerful feature of the fourth law is that it provides (nonlinear) extensions of Onsager reciprocity and fluctuation-dissipation relations to the far-non-equilibrium realm.



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Entropy Measurements with Infrared Sensors

sciforum-044176

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Infrared sensors (IRS) have been used for long to measure non-contact body temperatures, as in thermal cameras. These sensors are based on thermopiles that measure heat flows, which are converted to temperature through sensor's calibration curve. In this contribution we aim to combine the physical heat measurements with the inferred temperature measurements of the emitter to characterize the emitter radiated entropy reaching the sensor. We implemented a data acquisition system based on Arduino UNO microcontroller. Several IRS sensors, which had both thermopile and thermistor for independent environment temperature were tested. As thermal emitters, we used resistors whose power dissipation could be selected by controlling their current and voltage. We investigated the emitter transferred entropy reaching the IRS sensor as a function of emitter-sensor distance and the emitter dissipated power. Thus, the measurement system manages the emitter temperature and power dissipation, the heat reaching the sensor and the temperature of the sensor. From this data, we were able to monitor non-contact radiated entropy. This setup was used to characterize resistor ageing as resistor ageing is related to its entropy production. Degradation accelerated tests were carried out. Emitter resistors were submitted to dissipation powers well beyond their nominal power rate to speed up its degradation mechanisms. We were, thus, able to monitor resistor degradation with a non-contact sensor by evaluating the entropy reaching the sensor.



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Quantal Response Statistical Equilibrium: A New Class of Maximum Entropy Distributions

sciforum-028811

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The principle of maximum entropy has been applied fruitfully to many economic and social situations. One limitation of such applications, however, is the tendency neglect of the joint determination of social outcomes and the actions that shape them in the formal modeling despite the fact that both dimensions of the problem are typically articulated in the theoretical exposition. The fact that closed-form marginal distributions are good model candidates for many economic variables in statistical equilibrium based on fit has the unfortunate consequence of leading to economic rationalization based on mathematical necessity of the constraints. From the Principle of Maximum Entropy perspective the use of closed-form distributions is premature. While there may be good reasons to rely on such distributions for modeling statistical equilibrium in some situations, in general this limits inference to an arbitrary subset of models.

This research explores an alternative approach to modeling economic outcomes based on the Principle of Maximum Entropy called the quantal response statistical equilibrium (QRSE) model of social interactions. The QRSE model provides a behavioral foundation for the formation of aggregate economic outcomes in social systems characterized by negative feedbacks. It can approximate a wide range of commonly encountered theoretical distributions that have been identified as economic statistical equilibrium and displays qualitatively similar behavior to the Subbotin and Asymmetric Subbotin distributions that range from the Laplace to the Normal distribution in the limit. Asymmetry in the frequency distributions of economic outcomes arises from the unfulfilled expectations of entropy-constrained decision makers and asymmetric impacts of actions. The logic of the model is demonstrated in an application to US stock market data, firm profit rate data, and the distribution of income from a classical perspective.



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Developing an Information Theory of Quantitative Genetics

sciforum-029297

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Quantitative genetics has evolved dramatically in the century since its foundation, and the modern proliferation of genetic data both in quantity and in type now enables new kinds of analysis beyond the scope of its theoretical foundations. We have begun laying the foundations of an alternative formulation of quantitative genetics based on information theory since it can provide sensitive and unbiased measures of statistical dependencies among variables, as well as a natural mathematical language for an alternative description of quantitative genetics. After all, genetics is fundamentally the science of information transfer between generations. Earlier work has applied information theory to descriptions of evolution and some aspects of population genetics. In our previous work we examined the information content of discrete functions, which are useful in describing genetic relations and applied this formalism to the analysis of genetic data. We describe a set of relationships that both unifies the information measures for these discrete functions and uses them to express key genetic relationships in genotype and phenotype data. We present information-based measures of the genetic quantities of penetrance, heritability and degrees of statistical epistasis. We analyze two- and three-variable dependencies for independently segregating variants, which captures a range of phenomena including genetic interactions, and two phenotype pleiotropy. Note however that this formalism applies naturally to multi-variable interactions and higher-order complex dependencies as well, and can be extended to account for population structure, genetic linkage and non-randomly segregating markers. We discuss our progress towards laying the groundwork for a full formulation of quantitative genetics based in information theory.



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The Atrial Resting Potential Distribution within a Fibrotic Zone and Its Effects on the Conduction on Non-Fibrotic Zones: A Simulation Study

sciforum-029338

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Atrial fibrillation (AF) is a heart condition commonly diagnosed within the clinical praxis. During an AF episode, rapid and irregular heartbeats are present and they underly a complex electrical activity. It is known that the atrial structural alterations play a role in establishing the fibrillatory propagation patterns. However, the specific mechanisms are not fully understood. Fibrosis is a hallmark of AF and it represents structural abnormalities that disturbs the atrial electrical conduction. In this work, the behavior of the cardiomyocytes resting action potential in a fibrotic tissue, under distinct textures, is studied. A computational model of atrial electrophysiology is implemented. For the fibrosis model, spatial complex-order derivatives are used. Several values for the derivative order are tested in order to generate different degrees of structural complexity. The fibrosis model also includes cellular heterogeneity through the presence of fibroblasts coupled to cardiomyocytes. Diffuse, interstitial and compact fibrosis textures are implemented in a 2D domain and the amount of fibrosis is varied. The distribution of the resting potential is assessed using the Shannon entropy and the tissue is stimulated in order to evaluate the conduction velocity. The results indicate that, the distinct fibrosis structural conditions generate a wide range of resting potential distributions: from normal to heavy-tailed. The entropy values indicate the changes in the resting potential distribution when the structural complexity varies. Such analysis evinced that the amount of fibrosis generates specific entropy curves respect the derivative order. Moreover, the conduction velocity outside the fibrotic area is affected by the fibrotic configuration, which evinces the long-range effect of the fractional derivative operator and agrees with experimental observations. These results suggest that the proposed complex-order model can be useful for modeling fibrosis during atrial fibrillation and the entropy approach allows characterizing the wide range of fibrillatory scenarios under distinct fibrosis configurations.



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Cracking the Code of Metabolic Regulation in Biology Using Maximum Entropy/Caliber and Reinforcement Learning

sciforum-030015

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Experimental measurement or computational inference/prediction of the enzyme regulation needed in a metabolic pathway is hard problem. Consequently, regulation is known only for well-studied reactions of central metabolism in a few organisms. In this study, we use statistical thermodynamics and metabolic control theory as a theoretical framework to determine the enzyme activities that are needed to control metabolite concentrations such that they are consistent with experimentally measured values. A reinforcement learning approach is utilized to learn optimal regulation policies that match physiological levels of metabolites while maximizing the entropy production rate and minimizing the work to maintain a steady state. The learning takes a minimal amount of time, and efficient regulation schemes were learned that agree surprisingly well with known regulation. The learning is facilitated by a new approach in which steady state solutions are obtained by convex optimization based on maximum entropy rather than ODE solvers, making the time to solution seconds rather than days. The optimization is based on the Marcelin-De Donder formulation of mass action kinetics, from which rate constants are inferred. Consequently, a full ODE-based, mass action simulation with rate parameters and post-translational regulation is obtained. We demonstrate the process on three pathways in the central metabolism *E. coli* (gluconeogenesis, glycolysis-TCA, Pentose Phosphate-TCA) that each require different regulation schemes.



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Definition of Frame-Invariant Soret Coefficients for Ternary Mixtures

sciforum-030502

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Definition of frame-invariant Soret coefficients for ternary mixtures.

The definition of the Soret coefficient of a binary mixture includes a concentration prefactor, $x(1 - x)$ when mol fraction x is used, or $w(1 - w)$ when mass fraction w is used. In this presentation the physical reasons behind this choice are reviewed, emphasizing that the use of these prefactors makes the Soret coefficient invariant upon change in the reference frame, either mass or molar. Then, it will be shown how this invariance property can be extended to ternary mixtures by using an appropriate concentration prefactor in matrix form. The presentation will be completed with some considerations of general non-isothermal diffusion fluxes, binary limits of the concentration triangle, selection of the dependent concentration in a ternary mixture, and, finally, extension to multi-component mixtures.

Reference

1. Ortiz de Zárate, J.M. Definition of frame-invariant thermodiffusion and Soret coefficients for ternary mixtures. *Eur. Phys. J. E* **2019**, *42*, 43.



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Abstracts

Posters

A Model-Based Reinforcement Learning Approach for a Rare Disease Diagnostic Task

sciforum-029156

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In this work, we study the problem of inferring a discrete probability distribution using both expert knowledge and empirical data.

This is an important issue for many applications where the scarcity of data prevents a purely empirical approach. In this context, it is common to rely first on an a priori from initial domain knowledge before proceeding to an online data acquisition. We are particularly interested in the intermediate regime, where we do not have enough data to do without the initial a priori of the experts, but enough to correct it if necessary.

We formalize expert knowledge as a set of priors, e.g., on the marginals or on the support of distribution. The expert distribution is defined as the distribution of the maximum entropy that satisfies the constraints set by the experts. In turn, empirical data is used to construct the empirical distribution.

We present a new method for objectively choosing the weight to be given to the experts in relation to the data. We define our estimator as the projection of the experts on the confidence interval centered on the empirical distribution. This is the closest distribution from the experts which is consistent with the observed data. The confidence level is the unique parameter of this method.

We show, both empirically and theoretically, that our proposed estimator is always more efficient than the best of the two models (expert or data alone) within a constant.

Our estimator allows a bad a priori to be abandoned relatively quickly when the inconsistency of the data collected with the initial a priori is observed. At the same time, this same mixture makes it possible to keep the initial a priori if it is good. We prove empirically that our method outperforms a parametric Bayesian approach in such a task.



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On Conditional Tsallis Entropy

sciforum-029276

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Tsallis entropy, a generalisation of Shannon entropy that depends on a parameter alpha, provides an alternative way of dealing with several characteristics of nonextensive physical systems given that the information about the intrinsic fluctuations in the physical system can be characterized by the nonextensivity parameter alpha. It is known that as the parameter alpha approaches 1, the Tsallis entropy corresponds to the Shannon entropy. Unlike for Shannon entropy, but similarly to Rényi entropy (yet another generalisation of Shannon entropy that also depends on a parameter alpha and converges to Shannon entropy when alpha approaches 1), there is no commonly accepted definition for the conditional Tsallis entropy. In this work, we revisit the notion of conditional Tsallis entropy by studying some natural and desirable properties in the existing proposals: when alpha tends to 1, the usual conditional Shannon entropy should be recovered; the conditional Tsallis entropy should not exceed the unconditional Tsallis entropy; and the conditional Tsallis entropy should have values between 0 and the maximum value of the unconditional version. We also introduce a new proposal for conditional Tsallis entropy and compare it with the existing ones.



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Predicting Human Responses to Syllogism Tasks Following the Principle of Maximum Entropy

sciforum-030038

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Syllogistic reasoning is one of the major research domains in cognitive science. Syllogisms are quantified semi-logical statements that consist of two premises, each relating two terms by one quantifier out of “All”, “No”, “Some”, and “Some not”. While one of the terms is mentioned in both premises, one is interested in what conclusion can be drawn about the relationship between the other two terms. For example, a well-formed syllogism task is “If all A are B and no B is a C, what, if anything, follows about the relationship between A and C?” While some syllogism tasks have a logically valid conclusion (in the example above, “No A is a C.” is logically valid), some have not, like “If all A are B and some B are C, what follows about A and C?” In cognitive science, human responses to syllogism tasks are studied in order to better understand the human understanding of quantification and uncertainty in reasoning.

In order to predict human responses to syllogism tasks, we develop a probabilistic model of syllogisms based on the principle of maximum entropy. For this, we translate the premises of syllogisms into probabilistic conditional statements and derive the probability distribution that satisfies the conditional probabilities while having maximal entropy. Then, we calculate the probabilities of all possible conclusions and compare them with the respective quantifier. As a prediction, we basically choose the option with the best matching. Based on empirical data, we show that our maximum entropy model predicts human responses better than established cognitive models.



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The Entropy Universe

sciforum-030222

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About 160 years ago, the concept of entropy was introduced in thermodynamics by Rudolf Clausius. Since then, it has been continually extended, interpreted, and applied by researchers in many scientific fields, such as general physics information theory, chaos theory, data mining, and mathematical linguistics. Based on the original concept of entropy, many variants have been proposed. This paper presents a universe of entropies, which aims to review the entropies that had been applied to time series. The purpose is to answer important open research questions such as: How did each entropy emerge? What is the mathematical definition of each variant of entropy? How are entropies related to each other? What are the most applied scientific fields for each entropy? Answering these questions, we describe in-depth the relationship between the most applied entropies in time series for different scientific fields establishing bases for researchers to properly choose the variant of entropy most suitable for their data.

The number of citations over the past fifteen years of each paper proposing a new entropy, was accessed. The Shannon/differential, the Tsallis, the sample, the permutation, and the approximate entropy were the most cited entropies. Based on the ten categories with the most significant number of records obtained in the Scopus categories, the areas in which the entropies are more applied are computer science, physics, mathematics, and engineering. From the top ten, the application area with less citations of papers proposing new entropies is the medical category.



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Information Geometry of Estimating Functions in Parametric Statistical Models

sciforum-030229

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In information geometry, a parametric statistical model (a family of probability density functions) is treated as a differentiable manifold, where the Riemannian metric called Fisher metric and the pair of two torsion-free dual affine connections called the exponential and mixture connections play essential roles for statistical inference. For example, the maximum likelihood estimation in an exponential family can be interpreted as the orthogonal projection of the geodesic defined by the mixture connection. This comes from the fact that an exponential family is a dually flat space, where the curvature and the torsion tensors of the two dual affine connections are all equal to zero. Recently, it has been found by the authors that a general estimating function naturally induces a similar geometric structure on a statistical model, that is, a Riemannian metric and a pair of dual affine connections, through the concept called pre-contrast function. In this case, however, one of the affine connections is not necessarily torsion-free, especially when the estimating function is not integrable with respect to the parameter of the statistical model. In this presentation, we explain the construction and some properties of this geometric structure with related concepts in information geometry. In addition, some of its statistical implications are discussed using an example of non-integrable estimating functions which induces a partially flat space, where only one of the induced affine connections is flat (curvature-free and torsion-free).



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Gauge Freedom of Entropies on q -Gaussian Distributions

sciforum-030271

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This is a joint work with Asuka Takatsu at Tokyo Metropolitan University.

A q -Gaussian distribution is a generalization of an ordinary Gaussian distribution. The set of all q -Gaussian distributions admits information geometric structures such as an entropy, a divergence and a Fisher metric via escort expectations. The ordinary expectation of a random variable is the integral of the random variable with respect to its probability distribution. Escort expectations admit us to replace the law to any other distributions. A choice of escort expectations on the set of all q -Gaussian distributions determines an entropy and a divergence. The q -escort expectation is one of most important expectations since this determines the Tsallis entropy and the alpha-divergence.

The phenomenon gauge freedom of entropies is that different escort expectations determine the same entropy, but different divergences.

In this talk, we first introduce a refinement of the q -logarithmic function. Then we demonstrate the phenomenon on an open set of all q -Gaussian distributions by using the refined q -logarithmic functions. We write down the corresponding Riemannian metric.



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A Kolmogorov Complexity for Multidisciplinary Domains

sciforum-030295

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Kolmogorov complexity, or algorithmic information theory, measures information in an individual object as its smallest possible representation. These metrics have been applied in Computer Science and in several other scientific disciplines. It is known that this measure is not computable, however, we can approach it from above using standard compressors.

In the scope of statistical or clustering methods, it is important to measure the absolute information distance between individual objects. The Normalized Information Distance (NID) measures the minimal amount of information needed to translate between two objects, however, it is uncomputable. There is a set of metrics used to approximate the NID, such as Normalized Compression Distance (NCD), Compression-Based Dissimilarity Measure (CDM) and Lempel–Ziv Jaccard Distance (LZJD). These methods, unlike other approaches, do not require any specific background knowledge of the dataset, that is, the user of this method only needs to have some knowledge about data mining techniques or data visualization.

It is utmost important to improve current implementations in order to create a central, simply usable repository that supports multiple metrics, ensuring that a researcher can use some of the most important past work techniques to extract the most accurate information with the approach of NID. Current implementations are poorly document and lake the support to some enhancements already presented in past work literature. An example is the need to replace the compressed size with the percentage of compression in each of the files to achieve comparison with different file sizes.



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Entropy Analysis of n-Grams and Estimation of the Number of Meaningful Language Texts

sciforum-043535

Anastasia Malashina

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When solving a number of information security problems, one of the problems is to estimate the number of possible meaningful texts of fixed length. To estimate this value, various approaches can be used, in each of which the key parameter is the information entropy. To estimate the number of short plaintexts, the entropy of n-grams is used. For long ones, in turn, we use the entropy of the language (specific entropy). N-grams, in this case, are n consecutive characters of meaningful text. The well-known information-theoretic approach allows us to obtain an asymptotic estimate of the meaningful text number based on the second Shannon theorem. In practice, to implement this approach, the text under study is presented in the form of a Markov source.

We consider a different approach to estimating the number of meaningful language texts, using the combinatorial method, the origins of which go back to the ideas of Kolmogorov. Representing a text as a set of independent n-grams, we experimentally estimate the number of semantic n-grams in a language by compiling dictionaries based on a large text corpus. In order to evaluate the I type errors of taking a meaningful n-gram for a random one, which inevitably occur during experimental evaluation, we developed a methodology for evaluating the coverage of the dictionary. We use this amount of coverage to refine and recalculate the original volume of the dictionary. Based on the number of meaningful n-grams of the language, we determine the entropy of short texts of various lengths. This sequence of estimates allows us to mathematically model the further change in the entropy function, extrapolate for long segments, and find the specific value of the entropy of the language.



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A Dual Measure of Uncertainty: The Deng Extropy

sciforum-043584

Francesco Buono

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Lad, Sanfilippo and Agrò (2015) introduced the extropy as the dual concept of entropy. This measure of uncertainty has attracted the interest of researchers, and several versions of the extropy have been studied in the literature. Moreover, in the context of the Dempster–Shafer theory of evidence, Deng studied a new measure of discrimination, named the Deng entropy. In this talk, we define the Deng extropy and study its relation with Deng entropy, and examples are proposed in order to compare them. The behaviour of Deng extropy is studied under changes of focal elements. A characterization result is given for the maximum Deng extropy and, finally, a numerical example in pattern recognition is discussed in order to highlight the relevance of the new measure.

References

1. Buono, F.; Longobardi, M. A Dual Measure of Uncertainty: The Deng Extropy. *Entropy* **2020**, *22*, 582.
2. Deng, Y. Deng entropy. *Chaos Solitons Fractals* **2016**, *91*, 549–553.
3. Lad, F.; Sanfilippo, G.; Agrò, G. Extropy: Complementary dual of entropy. *Stat. Sci.* **2015**, *30*, 40–58.



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Generalized Inference for the Efficient Reconstruction of Weighted Networks

sciforum-044156

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Introduction. Network reconstruction is an active field of research. Among the methods proposed so far, some assume that the binary and weighted constraints jointly determine the reconstruction output; others consider the weights estimation step as completely unrelated to the binary one. Amidst the former ones, a special mention is deserved by the Enhanced Configuration Model; the algorithms of the second group, instead, are those iteratively adjusting the link weights on top of some previously-determined topology.

Methods and Results. Here we develop a theoretical framework that provides an analytical, unbiased procedure to estimate the weighted structure of a network, once its topology has been determined, thus extending the Exponential Random Graph (ERG) recipe. Our approach treats the information about the topological structure as a priori; together with the proper weighted constraints, it represents the input of our generalized reconstruction procedure. The probability distribution describing link weights is, then, determined by maximizing the key quantity of our algorithm, i.e., the conditional entropy under a properly-defined set of constraints. This algorithm returns a conditional probability distribution depending on a vector of unknown parameters; in alignment with previous results, their estimation is carried out by considering a generalized likelihood function. In our work, we compare two possible specifications of this framework.

Conclusions. The knowledge of the structure of a financial network gives valuable information for estimating the systemic risk. However, since financial data are typically subject to confidentiality, network reconstruction techniques become necessary to infer both the presence of connections and their intensity. Recently, several “horse races” have been conducted to compare the performance of these methods. Here, we establish a generalised likelihood approach to rigorously define and compare methods for reconstructing weighted networks: the best one is obtained by “dressing” the best-performing, available binary method with an exponential distribution of weights.



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Constraint Choice and Model Selection in the Generalized Maximum Entropy Principle

sciforum-044173

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The maximum entropy principle (MEP) is a powerful statistical inference tool that provides a rigorous way to guess the probability distribution of the states of a system which is known only through partial information.

Generalizing the Shore and Johnson's axioms, Jos Uffink (1995) proved that the functionals which are suitable to be used in the MEP belong to a one-parameter family, which the Shannon entropy is a member of. The resulting probability distributions are generalized exponentials, of which Boltzmann distribution is a special case. It has been discussed (P. Jizba and J. Korbel, 2019) that this generalized approach is suitable to study systems which do not respect standard hypothesis such as ergodicity, short-range interactions or exponential growth of the sample space: the resulting probability distributions take into account correlations that may not have been observed.

In this presentation, the maximum likelihood method to evaluate the parameters of such distributions and to perform model selection starting from empirical data will be discussed.

In particular, it will be shown that the maximum likelihood approach to estimate the Lagrange multipliers leads to an equation that justifies the use of the q-generalized momenta as constraints in the entropy maximization. Moreover, it will be shown that the likelihood function spontaneously emerges from the maximization of entropy: in particular, it will be proved that the log-likelihood is equal to minus the entropy once the Lagrange multipliers are fixed to satisfy the maximum likelihood condition.

Lastly, simple examples based on synthetic data will be presented to show that this approach provides accurate estimations of the parameters.



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Fisher Information of Landau States and Relative Information against the Lowest Level

sciforum-028896

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An electron in a constant magnetic field has the energy levels known as the Landau levels. One can obtain the corresponding radial wave function in cylindrical polar coordinates (e.g., textbook of Landau & Lifshitz). This system is not explored so far in terms of information-theoretical point of view. We here focus on Fisher information associated with these Landau states specified by the two quantum numbers. Fisher information provides a useful measure of the electronic structure in quantum systems such as hydrogen-like atoms [1,2] and molecules under Morse potentials [3]. We numerically evaluate the generalized Laguerre polynomials contained in the radial wave functions. We report that Fisher information increases linearly with the quantum number n that specifies energy levels, but decreases monotonically with the quantum number m (i.e., the index of the generalized Laguerre polynomial).

Also, we present relative Fisher information of the Landau states by setting the lowest Landau state as a reference density. The analytical form is just $4n$, which does not depend on the other quantum number m .

References

1. Yamano, T. Relative Fisher information of hydrogen-like atoms. *Chem. Phys. Lett.* **2018**, *691*, 196–198.
2. Yamano, T. Fisher information of radial wavefunctions for relativistic hydrogenic atoms. *Chem. Phys. Lett.* **2019**, *731*, 136618.
3. Yamano, T. Relative Fisher information for Morse potential and isotropic quantum oscillators. *J. Phys. Commun.* **2018**, *2*, 085018.



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ECG and EDA Information Transfer on Emotion Evaluation

sciforum-030218

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Emotions are behind decision-making, perception and learning. Studying emotions and their responses allow us to understand people's preferences and their strategies to adapt across contexts. Both peripheral and central nervous systems are activated by emotions, which are translated on behavioural and physiological alterations. Usually, the ecological validity of emotion induction studies is truly compromised due to the multiple electrodes used in the experiment, affecting the usual participants' daily routine. The major idea of this study is to compare signals in emotion quantification, to select the optimal data collection setup. In this work, we targeted two physiological signals: electrocardiogram (ECG), and electrodermal activity (EDA) in the happy condition.

Data from 4 participants were collected in healthy volunteers, which came to the lab three times. Each session intended to induce one emotion between happy, fear, neutral. At the beginning, participants rested for 4 minutes to collect baseline data. Afterwards, they watched intense movies associated with each condition for 25 minutes.

In this work, it is intended to study the information transfer between ECG and EDA, for the baseline and happy condition. The information dynamics based on the linear Gaussian approximation was computed to characterize information storage and transfer between ECG and EDA signals.

Considering the self-entropy of each signal, EDA presented slightly greater values than ECG. It was observed that in all participants, the ECG transfers information to the EDA, indicating that the ECG information may pertain in the system. Hence, the exploratory results achieved in this study may indicate that the ECG is a stronger signal when we want to evaluate emotions in real contexts. Future studies should address the study of information transfer between these and other physiological signals, and also different emotional conditions.



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Hellinger Entropy Concept: Multidisciplinary Applications

sciforum-032537

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The use of a metric to assess distance between probability densities is an important practical problem used in artificial intelligence or recommendation systems. The generalized α -formalisms introduced by Rényi and Tsallis are the basis of well-known entropies and divergence models. A particular α -divergence that, was presented in a previous work from the co-authors. This particular α -divergence, in our perspective, was already essentially defined by Hellinger. The concept of Hellinger entropy makes it possible, through a maximum-entropy syllogism, to state a bound for the Hellinger metric. The square root divergence is a metric, and its nonparametric estimator has information-theoretic bounds, that can be directly computed from the data. Information-theoretic bounds for Hellinger distance are developed in this work. The asymptotic behavior allows to use this metric, in a competitive scenario with three or more densities, like clustering. The bound can be directly computed from the data making this method suitable for streaming data.



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Statistical Entropy Opens a New Way to Assess the Recyclability of Products

sciforum-043475

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Statistical entropy is applied to assess various treatment technologies in waste management. It measures the effect of a treatment on waste flows, and thus the mixing/concentrating of materials and substances. The stronger the mixing, the higher is the produced statistical entropy (which is in accordance to the law of thermodynamics), and vice versa. For example, recyclers aim to generate outputs of concentrated target materials out of a mixed waste input, which corresponds to a statistical entropy decrease. The recycling effectiveness increases, the lower the statistical entropy is. Besides assessment of processes, statistical entropy can also be used to assess individual products and their material distribution respectively. Thus, complex products that consist of manifold materials show an increased material distribution/mixing, which again translates into high statistical entropy. As recycling efforts increase, the more complex products are, it seems feasible to assess the product inherent recyclability by statistical entropy. The lower the statistical entropy of the product, the higher is the recyclability. Because material concentrations can vary substantially within the different product components, information on the product structure needs to be considered too. Thus, the developed statistical entropy approach bases on material concentrations and information on the product assembly. To demonstrate the new application of statistical entropy, a case study is presented in which the recyclability of a typical smartphone is evaluated. The results show that statistical entropy is an appropriate metric to describe the recyclability of products and enables important insights in the design of products. It could act as a planning tool for product designers and manufacturers to promote products of higher recyclability. Further, the new statistical entropy approach could be of relevance for the implementation of the European Union's Circular Economy Package.



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Detection of Internal Defects in Concrete and Evaluation of a Healthy Part of Concrete by Non-Contact Acoustic Inspection Using Normalized Spectral Entropy

sciforum-044112

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In recent years, deterioration of concrete structures has become a social problem, and there is a demand for a non-contact, non-destructive method for inspecting internal defects in concrete structures. In our noncontact acoustic inspection, a target surface of concrete is vibrated with strong aerial sound waves, the vibration velocity distribution is measured two-dimensionally using a scanning laser Doppler vibrometer. Then, after time-frequency gate process, acoustic features quantities (vibrational energy ratio and spectral entropy) are calculated. By analysis using them, it has become possible to detect and visualize internal defects from a long distance (5–30 m). Traditional spectral entropy has no problem in evaluating the fluctuation of spectral entropy value within the same measurement condition or a measurement plane. However, it was not possible to directly compare and evaluate the spectral entropy values because the meaning of the upper and lower limit of spectral entropy values are ambiguous between different measurement conditions and different objects. To solve this, we introduce normalized spectral entropy. It will become possible to compare the values in different measurement conditions and different objects on the same scale, and it becomes possible to statistically evaluate a healthy part of concrete as well as detect defects.



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Design of High-C Cr-Co-Ni medium Entropy Alloy for Tribological Applications

sciforum-044153

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Medium and high entropy alloys (MEAs/HEAs), which typically have three or more main elements, were initially designed to have high configurational entropy (S_{conf}) stabilizing a simple, single-phase solid solution (SS) over multi-phase alloys. Having multiple main elements will indeed increase the S_{conf} of simple SSs, but it may decrease the enthalpy also increase, in a lower degree, S_{conf} of other complex phases, leading to multi-phase microstructures. Therefore, although the initial idea behind MEAs/HEAs was refuted, the interest remains, the focus shifted to exploring its vast compositional field, which includes an almost infinite number of alloys. Some of them with potentially better properties than those existing today. The Cantor alloy (equiatomic CrMnFeCoNi) and the equiatomic CrCoNi alloy, both single-phase with face-centered cubic (FCC) structure, are among the toughest materials ever reported. In this work, computational thermodynamic calculations (CALPHAD method) predicted that C additions in the Cr₄₀Co₄₀Ni₂₀ MEA favor the formation of a promising multi-phase microstructure for wear applications. A large amount of C was incorporated into the alloy by melting in a graphite crucible, this process allowed C saturation in the melt, which as will be shown, can be well controlled by carefully selecting the casting temperature, in this case we achieved 24 at% C by melting at 1600 °C. A Cr_{30.4}Co_{30.4}Ni_{15.2}C₂₄ MEA was produced, characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM) equipped with energy-dispersive spectroscopy (EDS). Experimental results revealed a microstructure composed of: graphite flakes, hard primary Cr-rich carbides, and a tough eutectic matrix of FCC phase and carbides; in good agreement with thermodynamic calculations. These findings highlight the great flexibility and potential in MEAs/HEAs design, making it possible to obtain microstructures and sets of properties that are beneficial for a given application.



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Near Zero Energy Buildings Entropy Performance

sciforum-044174

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Buildings are one of the main areas of energy consumption in Europe. At European level, last agreements and guidelines are focused to optimize energy efficiency. New architecture paradigm evolves towards nearly Zero Energy Building (nZEB). The aim of this contribution is to evaluate building energy performance in terms of entropy production and entropy flows. We projected an nZEB at La Roca del Vallès, close to Barcelona (Spain). Special attention was given to thermal envelope adapted to the location's climate, highly efficient radiant floor with aerothermal equipment both for heating and cooling, high energy-efficient appliances and illumination while keeping comfort conditions. Energy balance was investigated with Cypetherm software for all energy sources and flows with the environment. From this energy balance and taking into account the temperature of the building and environment, we investigated the entropy balance of the building in terms of the Gouy-Stodola theorem, both considering entropy generation due to thermal exchanges, electrical consumption and occupancy along with thermal flows through the envelope. We simulated the nZEB entropy performance under different efficiency designs and irradiance in order to establish guidelines between the entropy production and the energy efficiency in buildings. As expected, the energy and entropy balance for a whole year are zero. However, entropy generation is strongly affected by the efficiency of the building along with sun irradiance. Moreover, the standard models used in architecture for building energy characterization are found to be insufficient to describe internal entropy changes, and thus, building aging. These results would help to relate energy efficiency to building life cycle analysis.



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Battery Charge and Discharge Strategies in Terms of Entropy Production

sciforum-044177

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At present, batteries are the bottle neck of electric mobility, both for their cost and management. In this contribution, we aim to evaluate optimal battery charge in terms of entropy production and relate it to charging time and cost, with the aim to take advantage of vehicle-to-grid configuration. Li-ion batteries are usually charged using a constant current constant voltage strategy (CC-CV). The shift between CC and CV occurs when the battery reaches the maximum charging voltage. In terms of energy efficiency, this is not the most efficient approach. We develop Matlab® software scripts to simulate the performance of a real cell during charging by shifting from constant current to constant voltage at different battery state of charge b . We carried out a variational analysis of the charging/discharging processes in order to obtain its entropy performance so that it could be related to optimal energy efficiency in terms of b and in terms of cost/benefit according to the present Spanish electric market prices. Finally, these magnitudes studied at different charge rates and at different battery aging levels. We find that entropy is a valuable magnitude to characterize battery charge/discharge processes and find the optimal strategy in terms of cost, time and energy.



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Sample Entropy Approach to the Examination of Cardio-Respiratory Coupling in Response to Cardiac Resynchronization Therapy

sciforum-044181

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Cardiac resynchronization therapy (CRT) is a well-established therapy for symptomatic patients with heart failure and reduced left ventricular ejection fraction. It is known that patients with heart failure have altered cardio-respiratory interactions, but it has not been examined whether resynchronization therapy leads to changes in coupling of cardiac and respiratory rhythm, and whether the success of this therapy leads to restoring of cardio-respiratory interactions. In these patients, in addition to sinus rhythm, different types of arrhythmias usually appear, which limits the application of linear methods in analysis of interbeat interval time series. Therefore they should be analyzed with non-linear techniques and we applied the sample entropy approach.

Twenty minutes of ECG (RR intervals) and respiratory signal were recorded simultaneously in 47 patients with heart failure and CRT indication. The interbeat interval time series in patients with sinus rhythm, sinus rhythm with ventricular extrasystoles and with atrial fibrillation were analyzed. Sample entropy values were calculated from RR interval time series (SampEnRR) and respiratory signal time series (SampEnResp) to assess their complexity/regularity as well as cross sample entropy (CrossSampEn) to estimate their asynchrony. Measurements were performed before (baseline) and approximately 9 months after CRT implantation (follow-up). After follow-up, patients were divided into two groups, responders and non-responders, in relation to the response to CRT, which was assessed according to changes in certain clinical parameters.

In both groups, there was no difference in SampEnRR between baseline and follow-up. However, in the non-responders group, a significant increase was obtained in SampEnResp and CrossSampEn ($p < 0.05$). Responders to CRT showed significant decrease in heart rate and breathing frequency, while non-responders showed only a significant decrease in heart rate. Our results indicate that in non-responders to CRT, respiratory rhythm is not adapting to changes in cardiac dynamics, which resulted in loss of their synchrony.



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On the Estimation the Probability of Cardiovascular and Cerebrovascular Events in Hypertensive Patients Using Nonlinear Analysis, Time and Frequency Domain Methods

sciforum-044191

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Applications of entropy-based parameters to the time series generated by physiological systems of the human body are revealing hidden information of interest, which is allowing to improve diagnosis and treatment of several diseases [1]. In this context, a widely analysed physiological time series is the heart rate variability, obtained from the Surface electrocardiograma (ECG) [2]. For example, its entropy-based analysis has allowed to detect abnormalities associated with letal and non-letal cardiac arrhythmias. In addition to provide information about the instantaneous heart rhythm, it is today accepted that this time series reflects the behavior of the autonomic nervous system.

In this study, the heart rate variability is analyse to anticipate the risk of occurence of an adverse cardiovascular event in hypertensive patients (i.e., myocardial infarction, stroke, syncopal event, etc.), which is the pathology with the most prevalence amongst the developed countries [3]. Briefly, several entropy-based measures haven been applied to the heart rate time series derived from 24 h-length ECG signals acquired from 139 patients, who were followed during 1 year. These parameters consist of sample entropies, Fuzzy-based entropies, symbolic entropies, etc.

Entropy measures based on different approaches, such irregularity, symbolization, ordinal pattern quantification, etc. were analyzed these indices were only able to discern between hypertensive and non-hypertensive patients who suffered an event within the follow up time, with a 70% accuracy, their combination with other common time and frequency domain parameters estimated from heart rate variability improved diagnostic accuracy to about 80% [4].

As a conclusion, nonlinear analysis of the heart rate variability provided by entropy-based measures provides complementary information to other linear indexes, at high-risk of developing future cardiovascular events, which can lead them to imminent death.

References

1. Goldberger, A.L. Non-linear dynamics for clinicians: Chaos theory, fractals, and complexity at the bedside. *Lancet* **1996**, *347*, 1312–1314.
2. Goldberger, A.L.; Peng, C.K.; Lipsitz, L.A. What is physiologic complexity and how does it change with aging and disease? *Neurobiol. Aging* **2002**, *23*, 23–26.

Statistical Physics

Poster

3. Spasic, S.Z.; Kesic, S. Nonlinearity in living systems: Theoretical and practical perspectives on metrics of physiological signal complexity. *Front. Physiol.* **2019**, *10*, 298.
4. Solaro, N.; Malacarne, M.; Pagani, M.; Lucini, D. Cardiac baroreflex, HRV, and statistic: An interdisciplinary approach in hypertension. *Front. Physiol.* **2019**, *10*, 478.



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Epoch-Based Entropy: A Statistical EEG Marker for Alzheimer's Disease Detection

sciforum-044198

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The utility of electroencephalography (EEG) in Alzheimer's disease (AD) research has been demonstrated over several decades in numerous studies. EEG markers have been employed successfully to investigate AD-related alterations, by comparing EEG recordings of AD patients to those of healthy subjects.

It is widely admitted that AD leads to a reduction in the complexity of EEG signals and changes in EEG synchrony. These modifications in EEG recordings have been used as discriminative features for AD diagnosis using several complexity, especially entropy-based measures, and synchrony measures. Usually, these measures are applied with two main drawbacks: first, they are computed on the whole EEG sequences without addressing the problem of EEG non-stationarity; secondly such measures do not consider the EEG signal as a multidimensional time series: the prevailing paradigms extract information from EEG signals by averaging them over channels.

We expose a new EEG marker based on an entropy measure, termed epoch-based entropy. This measure quantifies the information content or the disorder of EEG signals both at the time level and spatial level, using local density estimation by a Hidden Markov Model on inter-channel stationary epochs.

We investigated the classification performance of this EEG marker, its robustness to noise, and its sensitivity to sampling frequency and to variations of hyper-parameters. We showed that this measure is efficient for AD detection since the statistical modelling of the multidimensional EEG signal allows characterizing the information content induced by the coupling of neural activity in EEG signals recorded at different locations.

Reference

1. Houmani, N.; Vialatte, F.; Gallego-Jutglà, E.; Dreyfus, G.; Nguyen-Michel, V.H.; Mariani, J.; Kinugawa, K. Diagnosis of Alzheimer's disease with Electroencephalography in a differential framework. *PLoS ONE* **2018**, *13*, e0193607.



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From Network Reconstruction to Network Econometrics: Unbiased Estimation of Average Effects

sciforum-044208

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The International Trade Network (ITN) can be thought of as a set of countries (nodes) that are linked among each other by trade relationships (links). Such a network can be described at the topological level, discerning the partners of each country, and at the weighted level, where our interest shifts to the trade volume among partners.

In Economics, the focus has traditionally been on the estimation of trade volumes and marginal effects, at times forgetting the importance of the network structure. A correct estimation of such a structure increases the precision of the estimation of the parameters and hence of trade volumes. Even if the Econometric models can reproduce the expected number of zeros, they cannot reproduce ITN topological statistics.

An alternative way of studying the ITN structure has been advanced by the Network Science community and consists in a constrained maximization of the Graph Entropy. A recent development is the so-called Enhanced Gravity Model (EGM) where the Lagrange Multipliers are expressed in terms of the rescaled GDPs. The EGM has been proven to accurately predict both topological and weighted statistics. Here we rephrase the EGM into an Econometric model at different degrees of topological detail. Such a model can be used for unbiased estimation of covariate effects on trade volumes taking into account the possible bias given by the underlying topological structure.

Our results confirm that Network Econometric Models replicate the principal network statistics and are associated with the smallest AIC and BIC scores with respect to Econometric models commonly used in International Trade such as Poisson, Negative Binomial and Zero-Inflated.

Our contribution sheds light on how International Trade Econometrics can be updated and completed with Network Regression Models derived from a constrained Maximum Entropy principle.



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Analysing Discursive Communities and Semantic Networks on Twitter: An Entropy-Based Approach

sciforum-044214

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At the intersection between social sciences and network theory, the aim of this presentation is that of illustrating an entropy-based, data-driven approach to infer communities of Twitter users and looking at their interactions within a specific discussion. Amongst the various kind of interactions, the retweets have been chosen as a particularly insightful relational mechanism featured by Twitter. Our approach is based on a Shannon entropy maximization under certain constraints which guarantees that the procedure is unbiased and suitable for being applied to any properly-defined Twitter discussions.

One of the main results of our analysis is the operational definition of “discursive communities” as groups of users who share significantly-similar retweeting patterns. Comparing the observed bipartite network of users retweeting activities with the outcome of a properly-defined benchmark model, i.e., the Bipartite Configuration Model (BiCM), our inference method validate the similarity in the online activity of Twitter users who share the same contents, published by the accounts of public figures, to infer the presence of users communities with supposedly common features. The discursive communities recovered by our method display a coherent picture of its users behavior, in terms of retweeting and mentioning activities; besides, these communities are consistent with the political coalitions and sensitive to the dynamics characterizing the relationship within and between these coalitions as well.

A second core result of our analysis concerns the study of the mechanisms that shape the Twitter discussions characterizing the aforementioned discursive communities. By monitoring, on a daily and a monthly basis, the structural evolution of the community-generated semantic networks, the users in each community are observed to be characterized by a significantly different online behavior, thus inducing semantic networks with diverse topological structures.



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Assessing Transfer Entropy in Cardiovascular and Respiratory Time Series: A VARFI Approach

sciforum-044218

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In the study of complex biomedical systems represented by multivariate stochastic processes, such as the cardiovascular and respiratory systems, an issue of great relevance is the description of the system dynamics spanning multiple temporal scales. Recently, the quantification of multiscale complexity based on linear parametric models, incorporating autoregressive coefficients and fractional integration, encompassing short term dynamics and long-range correlations, was extended to multivariate time series. Within this Vector AutoRegressive Fractionally Integrated (VARFI) framework formalized for Gaussian processes, in this work we propose to estimate the Transfer Entropy, or equivalently Granger Causality, in the cardiovascular and respiratory systems. This allows to quantify the information flow and assess directed interactions accounting for the simultaneous presence of short-term dynamics and long-range correlations. The proposed approach is first tested on simulations of benchmark VARFI processes where the transfer entropy could be computed from the known model parameters. Then, it is applied to experimental data consisting of heart period, systolic arterial pressure and respiration time series measured in healthy subjects monitored at rest and during mental and postural stress. Both simulations and real data analysis revealed that the proposed method highlights the dependence of the information transfer on the balance between short-term and long-range correlations in coupled dynamical systems.



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Maximum Entropy Method Applied to Time-Series Data in Real-Time Time-Dependent Density Functional Theory

sciforum-044245

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Density functional theory (TDDFT) in real-time, which is expected to be a key technique to calculate optical spectra. We solve the time-dependent equation, keeping track of the dipole moment as time-series data. In the traditional optical analysis, the oscillator strength distribution is related to the imaginary part of the polarizability, which is usually calculated by the Fourier transform (FT) of the dipole moment. Theoretically, it works only if the time-series data is quite large.

To obtain spectra of fairly high resolution with a relatively small number of time-series data, we have recognized that, from our analysis, even simple MEM provides the oscillator strength distribution at high resolution even with a half of the evolution time of a simple FT. In the practical optical analysis, we are much interested in the lower energy region near the band gap to obtain photo absorption and emission spectra. However, long enough time-evolution is still required in the calculation.

We propose that, as a further improved MEM analysis, we use the concatenated data set made from the several-times repeated raw data. In this process, we also introduce an appropriate phase for the target peak frequency to reduce the side effect of the artificial periodicity. In this procedure, we can effectively take into account the information from large lags of autocorrelation, which represent the interesting signal in the lower energy region.

We have compared the result of our improved MEM and that of FT for the analysis applied to the time-series data in the spectrum analysis of small-to-medium size molecules. As a result, we can observe the clear spectrum of MEM. Our new technique provides higher resolution in fewer time steps, compared to that of FT.



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Work Sharing as a Metric and Productivity Indicator for Administrative Workflows

sciforum-028983

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A mathematical method was developed to generate an indicator on the productivity of administrative complex workflows. The indicator can roughly and steadily reveal the definition of productivity as a state of endosectoral (among internal sector agents) and exosectoral (among external sector agents) administrative services sharing. The indicator can be used by public and private managers to measure human resource efficiency in proportion to work requests/inputs of all administrative services occurring in a given workflow.

Defining administrative workflow events as a nonlinear dynamics that assume a random ordered or disordered growth rate of information processing, a method has been proposed for large-scale administrative systems defined as structures of hybrid system variables (continuous or discrete), iterated and composed of fixed-point attracted events at which for all possible metric spaces solutions, the modeling of variables from Lyapunov exponential stability point of view allows the projection of system performance to be oriented, that is in other words, the relationship between the number of agents and the number of administrative services within an administrative workflow environment.

This definition differs from traditional or differentiated key performance indicators (KPI), such as working hours, medical certificate, per capita productivity, among others and the proposed methodology is only suitable for large-scale administrative activities that have a wide range of activities as well as the number of agents that perform them.

For system management purposes, it is possible to view the possibility of administrating system discretization, computerization and monitoring in order to be able to predict and validate the exponential function as a valid indicator of nonlinear systems where the results were defined by the amount of work sharing effect.



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A Kinetic Model for Pedestrian Evacuation in a Corridor with an Aggressive Sparse Countercurrent

sciforum-030294

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The modeling of pedestrian flow is a relevant topic which can lead to valuable information for urban planning as well as for improving evacuation strategies. Most works in this field include a heavy numerical component while theoretical predictions are scarce. In the present work we propose a simple yet rich model for bidirectional pedestrian flow in a one dimensional evacuation scenario where a dense crowd of passive walkers exit the building while a sparse group of aggressive individuals attempt to re-enter. The model is based on a kinetic theory treatment with Boltzmann-like equations considering a two moment approach for the transport equations. The corresponding system is linearly analyzed in order to identify stability regions where the flow towards the exit is uninterrupted provided the countercurrent is aggressive enough. The criterion for the onset of a congestion, and thus the relevant parameters in order to avoid it, are obtained in a purely analytical fashion based on statistical physics.



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On the Relation of Eckart and Landau-Lifshitz Reference Frames for Higher Orders in the Dissipative Fluxes Couplings

sciforum-030300

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In the kinetic description of a relativistic gas, macroscopic quantities are usually studied either in the reference frame that moves with the fluid (the so-called Eckart frame) or in the frame where there is no energy dissipation flux (Landau Lifshitz frame). In a closer and detailed view, the Landau Lifshitz reference frame requires several approximations to relate it with the Eckart's or particle frame. For the energy-momentum tensor not contain energy fluxes is necessary to neglect couplings among dissipative flows. It is well known that at first order particle 4-flux contains a dissipative term related to the heat flux and also defines a Lorentz reference frame through a timelike vector. In this work, we relate these reference frames up to higher orders in dissipative fluxes couplings and compare the properties of the corresponding systems of transport equations in both frames emphasizing the entropy balance and its consistency with the second law.



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Nonlinear Dynamical Screening Effects and strong Local Fluctuations of Drag Forces in Collective Scattering of Particle Streams on Impurity Ensembles

sciforum-043622

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We study the effects of nonequilibrium correlations and interactions between constituent particles of a bunch or pulsed beam, arising in course of its motion through a medium, or under the scattering of particle stream on a cluster or finite cloud of impurities [1]. Formally, these correlations are determined by the effect of dynamical screening. Such induced correlations and dynamical friction forces on impurities are manifested most pronouncedly in the case of collective dynamical screening effect and are enhanced in the case of a nonlinear medium when strong local fluctuations of scattered field begin to act as additional scattering elements along with impurities. In addition, collective scattering effects depend on the degree of impurity cluster disorder [2]. We focus on effects provoked by the collective scattering on randomly inhomogeneous structures and by the presence of local fluctuations. The presence of strong fluctuations of the scattered field is shown to give rise to strong local fluctuations of nonequilibrium forces acting on certain particles within the impurity cluster that can be a precursor of dynamical instability of the cluster, which is manifested in the peculiar behavior of the tails of probability distribution function for the drag force [3]. The description of the impurity cluster in terms of effective parameters breaks down due to the presence of such fluctuations.

Acknowledgments: This work was partially supported by a grant for research groups of young scientists from the National Academy of Science of Ukraine (Project No. 0120U100155).

References

1. Kliushnichenko, O.V.; Lukyanets, S.P. Effects of gas interparticle interaction on dissipative wake-mediated forces. *Phys. Rev. E* **2017**, *95*, 012150.
2. Kliushnichenko, O.V.; Lukyanets, S.P. Effects of collectively induced scattering of gas stream by impurity ensembles: Shock-wave enhancement and disorder-stimulated nonlinear screening. *Phys. Rev. E* **2018**, *98*, 020101.
3. Kliushnichenko, O.V.; Lukyanets, S.P. Collective wake-mediated interactions in lattice fluids: Effects of strong local force fluctuations stimulated by impurity disorder. *arXiv* **2020**, arXiv:2012.09266.



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Breaking of Ensemble Equivalence in Networks

sciforum-044158

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It is generally believed that, for physical systems in the thermodynamic limit, the microcanonical description as a function of energy coincides with the canonical description as a function of temperature, the original argument being that in the canonical ensemble at fixed temperature the energy fluctuations are negligible with respect to the average energy. Today, most textbooks in statistical physics still convey the message that the equivalence of ensembles holds universally for every physical system; however, various examples have been identified for which the microcanonical and canonical ensembles are not equivalent (e.g., for certain many-body systems encountered in models of fluid turbulence, quantum phase separation, etc.).

Here we show that ensemble nonequivalence can manifest itself also in discrete enumeration problems. We argue that, for any enumeration problem where we need to count microcanonical configurations compatible with a given constraint, there exists a dual problem involving canonical configurations induced by the same constraint. We then prove a general result showing that, for discrete systems, ensemble equivalence reduces to equivalence of the large deviation properties of microcanonical and canonical probabilities of a single microstate. As specific examples, we consider ensembles of networks with topological constraints. We find that, while graphs with a given number of links are ensemble-equivalent, graphs with a given degree sequence (including random regular graphs, sparse scale-free networks, and core-periphery networks) are not. We also find that, as the heterogeneity of the degree distribution increases, the violation of non-equivalence gets more severe.

Our proof of the breakdown of ensemble equivalence in graphs with given degree sequence provides a theoretical explanation for some recent observations, namely the fact that the canonical and microcanonical entropies of random regular graphs are different even in the thermodynamic limit and the non-vanishing of canonical fluctuations in the configuration model.



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Adsorption of Long Straight Rigid Rods on Two-Dimensional Lattices: Study of Orientational Surface Phase Transitions from Entropic Considerations [†]

sciforum-029138

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The orientational phase transitions occurring in a system of long straight rigid rods of length k (k -mers) on square lattices are studied by combining Monte Carlo simulations and theoretical analysis. The phenomenology of this model was examined in Refs. [1–5]. A nematic (N) phase, characterized by a big domain of parallel k -mers, is separated from a disordered-isotropic (D) state, by a continuous transition occurring at intermediate density. A second phase transition, from an N order to an ordered-isotropic (O) state, occurs near saturation density values. In the present work, the process is analyzed by following the number of accessible adsorption states along the vertical[horizontal] direction as a function of the surface coverage $W_v(q)[W_h(q)]$, which allows us to define a vertical[horizontal] configurational entropy. These quantities show strong variations with coverage (eventually leading to ergodicity breakdown), allowing to identify the different phases (N, D and O) characterizing the critical behavior of the system. Comparisons between Monte Carlo simulations and analytical calculations were performed in order to evaluate the reaches and limitations of the theoretical model.

References

1. Ghosh, A.; Dhar, D. On the orientational ordering of long rods on a lattice. *EPL (Europhys. Lett.)* **2007**, *78*, 20003.
2. Matoz-Fernandez, D.A.; Linares, D.H.; Ramirez-Pastor, A.J. Determination of the critical exponents for the isotropic-nematic phase transition in a system of long rods on two-dimensional lattices: Universality of the transition. *EPL (Europhys. Lett.)* **2008**, *82*, 50007.
3. Kundu, J.; Rajesh, R.; Dhar, D.; Stilck, J.F. Nematic-disordered phase transition in systems of long rigid rods on two-dimensional lattices. *Phys. Rev. E* **2013**, *87*, 032103.
4. Vogel, E.E.; Saravia, G.; Ramirez-Pastor, A.J. Phase transitions in a system of long rods on two-dimensional lattices by means of information theory. *Phys. Rev. E* **2017**, *96*, 062133.
5. Vogel, E.E.; Saravia, G.; Ramirez-Pastor, A.J.; Pasinetti, M. Alternative characterization of the nematic transition in deposition of rods on two-dimensional lattices. *Phys. Rev. E* **2020**, *101*, 022104.



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General Entropy-Based Framework for a Robust and Fail-Safe Multi-Sensor Data Fusion

sciforum-032529

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The 21st century will be the one that will undoubtedly mark the advent of data as a new digital gold. Intelligence is found everywhere in ever-smaller sensors that we no longer perceive. In this study, we are interested in the autonomous vehicle application, vehicles become intelligent, communicating together and with infrastructures. Data is there, everywhere, and constitutes an immaterial source that allows us to increase or even to delegate our decision-making power.

But for certain critical applications from a safety point of view, such as autonomous driving, a decision-based on intentional or non-intentional false, partial or incoherent knowledge could induce dangerous actions having negative effects on goods or people. The delegation of decision-making power to such safety-relevant applications makes regulatory authorities reluctant. It is for these types of applications that the concept of Fault-Tolerant Fusion (FTF) is developed. Being able to detect inconsistencies, while implementing a mitigation strategy (discard or compensation) makes it possible to almost continuously ensure state estimation, and therefore makes at each instant appropriate decisions/action, with a high level of integrity.

In this study, we present a general entropy-based framework for the development of a robust and fail-safe multi-sensor data fusion. From the informational form of the robust used stochastic filter, the MCCUIF (Maximum Correntropy Criterion Unscented Information Filter), to the adaptive diagnostic (FDI: Fault Detection and Isolation) layer based on α -Rényi divergence, passing through optimized thresholding (making it possible to maximize the availability of the system while ensuring the high required level of safety), this framework is an efficient and powerful tested example of FTF. It has been tested in real-time and with real data for the high-integrity ego-localization of a vehicle using GNSS and odometer measurements.



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Entropy and Entropic Forces to Model Biological Fluids

sciforum-029275

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Biological systems tend to exhibit common organizational patterns despite their diversity and different spatial and temporal scales. Living cells are complex systems that may be characterized by fluids crowded by hundreds of different elements in particular by a high density of polymers; they are an excellent and challenging laboratory to study exotic emerging physical phenomena where entropic forces emerge from organization processes of many-body interactions. There may be many entropic forces emerging in a biological fluid but most of them are consequences or can be reduced to the crowding and exclusion volume effects. Since entropic forces are emergent phenomena resulting from the tendency of a thermodynamic system to maximize its entropy, the macroscopic variables describing the system tend to evolve from one state to another state that is statistically more probable. If an external force exerted on the system points in the direction of decreasing its entropy while the entropic forces generated by the system point in the direction of increasing its entropy, when the system reaches its maximum entropy, the entropic force becomes zero. Therefore, the competition between entropic and physical forces may generate complex behaviors like phase transitions that living cells may use to accomplish their functions. In the era of the big data, when biological information abounds but general principles and precise understanding of the microscopic interactions are scarce, the entropy methods may offer significant information including statements of the physical interactions between the diversity of constituent elements, inferred only from experimental data. In this work we develop a model of a biological fluid involving the competition of entropic and physical forces that living cells seem to use to accomplish their functions as has been recently started to be understood. The target audience for this article are interdisciplinary researchers in complex systems, particularly in biophysics modeling.



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Confined Polymers as Self-Avoiding Random Walks on Restricted Lattices

sciforum-029325

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Through extensive Monte Carlo simulations [1] we study the crystallization of freely-jointed chains of tangent hard spheres under conditions of extreme confinement. The latter is realized through the presence of flat, parallel and impenetrable walls in one or more dimensions [2]. Extreme confinement corresponds to the state where the inter-wall distance, in at least one dimension, approaches the monomer size. Results are presented for quasi-1D (tube-like) and quasi-2D (plate-like) polymer templates. In both cases we observe the entropy-driven formation of highly ordered regions of close-packed, slightly defective crystals of different orientations. In a second stage we map the confined polymer chains onto the self-avoiding random walk (SAW) model on restricted lattices [3]. We enumerate all possible chain configurations (or SAWs) on a specific regular lattice subject to spatial restrictions arising from confinement. Through this we can determine the conformational component of entropy and eventually predict the thermodynamic stability of each distinct polymer crystal. In parallel, we obtain approximate expression for the SAW behavior as a function of chain length, type of lattice, and level of confinement. We present a simple geometric argument to explain, to first order, the dependence of the number of restricted SAWs on the type of SAW origin. Restricted lattices correspond to the cubic (simple, body center and face center) crystal system and results are compared against the ones of the bulk (unrestricted) case.

References

1. Ramos, P.M.; Karayiannis, N.C.; Laso, M. Off-lattice simulation algorithms for athermal chain molecules under extreme confinement. *J. Comput. Phys.* **2018**, *375*, 918–934.
2. Foteinopoulou, K.; Karayiannis, N.C.; Laso, M. Monte Carlo simulations of densely-packed athermal polymers in the bulk and under confinement. *Chem. Eng. Sci.* **2015**, *121*, 118–132.
3. Benito, J.; Karayiannis, N.C.; Laso, M. Confined polymers as self-avoiding random walks on restricted lattices. *Polymers* **2018**, *10*, 1934.



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Investigating the Structure-Dynamics-Function Relationship in Antibodies

sciforum-030055

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The paradigm that connects sequence, structure and function in proteins has been revisited in recent years, opening new perspectives on the importance of dynamics [1]. In this work we tackle this issue through the analysis of all-atom molecular dynamics (MD) simulations, with the final objective of correlating motions and structural features. We first characterize the dynamics of an antibody, through 2 μ s of all-atom molecular dynamics simulations, to investigate the correlation between structural features and the flexibility of the molecule. Subsequently we perform 2 μ s of all-atom MD simulations of the same antibody bound to its antigen, to investigate the changes in dynamics [2].

We analyzed the simulations through various different techniques among which we highlight the power of those based on the calculation of the information transfer between different amino acids [3]. These types of measurements allow us to identify significant correlations among protein regions, providing clues on the mechanism of protein function. The investigations carried out in this work also serve as a guide in the identification of those structural patterns whose preservation is necessary in the construction of coarse-grained models. Overall this study is meant as a starting point for the application of a multi-scale method to biologically relevant macromolecules.

References

1. Hensen, U.; Meyer, T.; Haas, J.; Rex, R.; Vriend, G.; Grubmüller, H. Exploring protein dynamics space: the dynasome as the missing link between protein structure and function. *PLoS ONE*, **2012**, 7, e33931.
2. Scapin, G.; Yang, X.; Prosise, W.W.; McCoy, M.; Reichert, P.; Johnston, J.M.; Kashi, R.S.; Strickland, C. Structure of full-length human anti-PD1 therapeutic IgG4 antibody pembrolizumab. *Nat. Struct. Mol. Biol.* **2015**, 22, 953–958.
3. Bowerman, S.; Wereszczynski, J. Detecting Allosteric Networks Using Molecular Dynamics Simulation. *Methods Enzymol.* **2016**, 578, 429–447.



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Measurement and Minimisation of the Mapping Entropy of a Coarse-Grained Biomolecular System

sciforum-030064

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All-atom Molecular Dynamics (MD) is the standard approach to perform in silico simulations of biomolecular systems. Despite its central role in modern computational biophysics, MD cannot span the time scales where the majority of relevant biological processes take place. An alternative is represented by coarse-grained (CG) modelling [1], that is, those lower-resolution representations of the system which aim at effectively reducing the number of degrees of freedom of a biomolecule in order to reach previously inaccessible time scales. Among the several statistical mechanics-based CG'ing techniques, we focused on those that measure the difference in information content between the coarse-grained and the all-atom system. We developed a protocol [2] able to compute the Mapping Entropy, which quantifies the amount of information retained upon the process of CG'ing due only to the choice of the Mapping. Our approach can therefore provide the user with the subset of sites which are maximally informative about the original, fully atomistic system. Tests conducted over a set of well-known proteins showed that regions retained with high probability are often related to the biological function of the molecule.

References

1. Noid, W.G. Perspective: Coarse-grained models for biomolecular systems. *J. Chem. Phys.* **2013**, *139*, 09B201_1.
2. Giulini, M.; Menichetti, R.; Shell, M.S.; Potestio, R. An Information-Theory-Based Approach for Optimal Model Reduction of Biomolecules. *J. Chem. Theory Comput.* **2020**, *16*, 6795–6813.



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Complexity Inside and Outside the Brain: How to Manage Internal (Interoceptive) and External (Domotics) Environment during Adaptive Inter-Actions

sciforum-030110

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Previous studies supported the notion that brain activity is slightly sub-critical in normal waking consciousness (Priesemann et al., 2013), and in this way, it can exert better control over the rest of the world, most of which is critical. This control may take the form of managing endogenous processes within the brain or interacting with the environment in order to functionally shape it (Carhart-Harris et al., 2014). The relationship between complex systems, i.e., human-to-environment relation, from an adaptive perspective is mediated by the sensory system with the main goal of maintaining a balance, aiming for harmony and avoiding ruptures. Through the description of two pilot studies, the advantages of adopting neuroscientific tools for exploring neurophysiological brain-and-body activity during complex inter-actions will be elucidated. This research has been conducted in two different fields of application: the first one investigated how the person answer to a complex domotic environment; the second one regards the deepening of interoceptive awareness as a possible factor influencing functional empathic response to external challenge. In the first study, some distinguishing effects of domotics on users' cognitive and emotional behavior are highlighted by using the neuroscientific approach. In order to define effects of Smart Home System (SHS) on UX, a neuroscientific wireless multi-methodology was adopted with the purpose of recording and confronting the neural activity (Electroencephalography, EEG) and autonomic system responses (with Biofeedback) of 19 individuals during a resting state (RS) baseline and the exploration of 5 different tech-interaction areas in a domotic environment. In the second study, a BIO-EEG-fNIRS (functional Near Infrared Spectroscopy) co-registration approach was adopted while 20 healthy participants performed a new paradigm for investigating the effects of interoceptive ability on empathy. Overall, the advantages and limitations of the applications of neuroscientific paradigms and tools for analyzing human interaction with complex systems will be discussed.



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Complexity as Cardiorespiratory Coupling Measure in Neonates with Different Gestational Ages

sciforum-030251

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After the transition from fetal to neonatal life, the cardio-respiratory system needs to adapt to the extrauterine condition. Both the cardiac and respiratory systems display complex dynamics. This study aimed to investigate the relationship between cardiorespiratory coupling, heart rate variability (HRV), and respiration of neonatal with gestational age (GA). Several complexity measures have been developed to quantify the complexity of physiological signals. In this study, we applied sample entropy (SampEn) and the bzip2 compressor to the time series. The mutual information (MI) and the normalized compression distance (NCD) were used to quantify the complexity of the cardiorespiratory coupling.

We analyzed a dataset composed of 30-minutes traces of RR intervals and respiration signals, acquired in the first two days of life, for 33 neonates with GA between 27 and 41 weeks. Of these 33 neonates, 22 babies were premature (<37 weeks), and 4 babies were considered extremely premature (<28 weeks). The Pearson correlation was computed to assess the association between complexity measures and GA.

Results obtained show that for the respiratory signals, SampEn increases as GA increases ($r=0.46$, $p=0.008$). However, the SampEn for RR intervals and MI gave non-significant correlations. When we applied the bzip2 compressor to the RR signals, we obtained a positive correlation with GA ($r=0.69$, $p<0.001$), but there is no significant correlation between bzip2 of respiratory signals and GA. For the complexity of cardiorespiratory coupling with NCD, we obtained a negative correlation with GA ($r=-0.74$, $p<0.001$).

We infer that SampEn presents better results for respiratory signals. However, bzip2 is better when using RR signals. While the complexity of the time series increases with GA, the complexity of the coupling decreases. This finding might emerge from the fact that the heart rate is highly modulated by respiration in premature babies. Future studies should investigate the complementary of these complexity measures.



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Entropy-Driven Phase Transition of Semiflexible Hard-Sphere Polymer Packings in Two and Three Dimensions

sciforum-044171

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We study, at the atomic level, the behaviour of athermal, linear semiflexible polymers of tangent spheres in thin films of one-layer thickness (2-D systems) and bulk 3-D systems. We employ extensive Monte Carlo simulations [1] at progressively increased concentrations adopting the hard-sphere model to represent interactions between monomers. Extreme, plate-like confinement for thin films is realized through the presence of flat, parallel walls in one dimension with the inter-wall distance being equal to the diameter of the spherical monomers. Chain stiffness is controlled by a tuneable potential for the bending angles whose intensity dictates the rigidity of the polymer backbone. At very high values of bending intensity, the polymer model approaches that of freely-rotated chains and bending angles sample the whole range from acute to obtuse angles, reaching the limit of rod-like polymers. We study how packing density, chain length and stiffness affect the entropy-driven phase transition from initially disordered (random) to ordered (crystal) local and global structures in dense polymer packings in 2-D and 3-D systems and compare against fully flexible chains and monomeric counterparts [2]. To gauge local order, we employ the characteristic crystallographic element (CCE) norm, a descriptor, which can detect and quantify, with high precision, similarity to reference crystals in general atomic and particulate systems [3,4]. In all cases, we identify the critical volume fraction for the phase transition and gauge the established crystal morphologies.

References

1. Ramos, P.M.; Karayiannis, N.C.; Laso, M. Off-lattice simulation algorithms for athermal chain molecules under extreme confinement. *J. Comput. Phys.* **2018**, *375*, 918–934.
2. Karayiannis, N.C.; Foteinopoulou, K.; Laso, M. Spontaneous crystallization in athermal polymer packings. *Int. J. Mol. Sci.* **2013**, *14*, 332–358.
3. Karayiannis, N.C.; Foteinopoulou, K.; Laso, M. The characteristic crystallographic element norm: A descriptor of local structure in atomistic and particulate systems. *J. Chem. Phys.* **2009**, *130*, 074704.
4. Ramos, P.M.; Herranz, M.; Foteinopoulou, K.; Karayiannis, N.C.; Laso, M. Identification of Local Structure in 2-D and 3-D Atomic Systems through Crystallographic Analysis. *Crystals* **2020**, *10*, 1008.



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Chaotic and Thermodynamic Interplay in Nanocavities

sciforum-044201

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Molecular confinement in nanocavity networks implies interplay between thermodynamic and chaotic response leading to surface entropic variations. Molecules, especially water molecules near surfaces are successively trapped and escape from nanocavities [1]. The time scale of physical interactions inside the nanocavities is governed by the molecular mean escape time from the nanocavities, pointing to a non-thermal equilibrium state inside the cavity. On the contrary, the external water vapour domain is in a thermal equilibrium state and the time scale is specified by the mean trapping time—the time a molecules travels in the outside domain before being trapped. Random walk simulations inside and outside different size nanocavities reveal the differentiation of time scales inside and outside nanocavities, pointing to an interplay between the thermodynamic state (vapor domain) and the chaotic state (nanocavity domain), leading to a variation of the number of available microstates [2]. Increment of microstates is responsible for entropy deviation during molecular water confinement, experimentally measured in complex nanocavity networks, crafted on polymeric matrixes by 157 nm vacuum ultraviolet laser light. The methodology is used for quantifying entropic variations caused by confined water or other molecules on surfaces.

References

1. Ruggeri, F.; Krishnan, M. Entropic Trapping of a Singly Charged Molecule in Solution. *Nano Lett.* **2018**, *18*, 3773–3779, doi:10.1021/acs.nanolett.8b01011.
2. Gavriil, V.; Chatzichristidi, M.; Christofilos, D.; Kourouklis, G.A.; Kollia, Z.; Bakalis, E.; Cefalas, A.-C.C.; Sarantopoulou, E. Entropy and Random Walk Trails Water Confinement and Non-Thermal Equilibrium in Photon-Induced Nanocavities. *Nanomaterials* **2020**, *10*, 1101, doi:10.3390/nano10061101.



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Computing Variations of Entropy and Redundancy under Nonlinear Mappings Not Preserving the Signal Dimension: Quantifying the Efficiency of V1 Cortex

sciforum-029112

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In computational neuroscience, the Efficient Coding Hypothesis argues that the neural organization comes from the optimization of information-theoretic goals [Barlow Proc.Nat.Phys.Lab.59]. A way to confirm this requires the analysis of the statistical performance of biological systems that have not been statistically optimized [Renart et al. Science10, Malo&Laparra Neur.Comp.10, Foster JOSA18, Gomez-Villa&Malo J.Neurophysiol.19].

However, when analyzing the information-theoretic performance, cortical magnification in the retina-cortex pathway poses a theoretical problem. Cortical magnification stands for the increase the signal dimensionality [Covey&Rolls Exp. Brain Res.74]. Conventional models based on redundant wavelets increase the dimension of the signal by 1 order of magnitude [Watson CVGIP87, Schwartz&Simoncelli Nat.Neurosci.01]. Such increase implies a problem to quantify the efficiency of the transforms. In fact, previous accounts of the information flow along physiological networks had to do some sort of approximation to deal with magnification, e.g., (1) using orthonormal wavelets or preserving dimension [Bethge JOSA06, Malo&Laparra Neur.Comp.10], or (2) using a reference for the relations introduced by the redundant transform [Laparra&Malo JMLR10, Gomez-Villa&Malo J.Neurophysiol.19].

In this work, we address the information theoretic analysis of such nonlinear systems that do not preserve dimension using no approximation. On the one hand we derive the theory to compute variations of entropy and total correlation under such transforms, which involves the knowledge of the Jacobian of the system wrt the input. To that end, we use the analytical results in [Martinez&Malo PLOS18]. On the other hand, we compare such predictions with a recently proposed non-parametric estimator of information-theory measures: the Rotation-Based Iterative Gaussianization [Laparra&Malo IEEE Trans.Neur.Nets11, Johnson, Laparra&Malo ICML19]. Consistency between the results validate the theory and provide new insights into the visual neural function.



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Bi-Dimensional Colored Fuzzy Entropy Applied to Melanoma Dermoscopic Images

sciforum-029203

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Recently, a bi-dimensional fuzzy entropy measure has been proposed for image texture evaluation. Herein, a new bi-dimensional fuzzy entropy is proposed to process colored images. Our algorithm, FuzEnc_{2D}, in opposition to dos Santos et al. (2018) definition, evaluates each color channel individually with consideration of global and local characteristics. We propose to apply it for the characterization of melanoma's dermoscopic images. In this work, FuzEnc_{2D} is tested by evaluating its sensitivity to change of parameters, rotation sensitivity, ability to determine irregularity through shuffling pixels, and consistency according to different image sizes. For those purposes, white noise and colored Brodatz textures are used. The algorithm is also applied to dermoscopic images of the public PH2 dataset to evaluate its performance in distinguishing common nevi, atypical nevi, and melanoma lesions. The results reveal a relative decrease of, at most, 29.97% for FuzEnc_{2D}-values when considering different parameters values. On the other hand, the consistency and low rotation sensitivity of the algorithm are revealed by analyzing the same texture with different sizes (maximum relative difference of 4.34%) and when comparing the entropy of an image upon rotation (maximum relative difference of 0.36%). Besides, after shuffling the pixels of an image, FuzEnc_{2D}-values of shuffled images increases up to 8.9 times of the original values. Moreover, using the red channel's entropy, a common nevi lesion is statistically different from an atypical one ($p = 0.004$ with the *Kruskal-Wallis* test). Regarding the green channel, a statistical difference ($p = 0.034$) is observed between atypical nevi lesions and melanoma. Also, differentiating a common nevi lesion from lesions diagnosed as melanoma is possible regardless the RGB channels. Finally, the FuzEnc_{2D} algorithm appears as a promising algorithm to analyze, through an entropy-based measure, the texture of colored images.



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Estimation of Relative Entropy Measures Based on Quantile Regression

sciforum-029249

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The estimation of relative entropy measures such as mutual information, conditional and joint entropy, or transfer entropy requires the estimation of conditional and joint densities. When the data are continuous, a multi-variate kernel density estimation or a discretization scheme is usually applied. The problem with this discretization approach is that for mutual information as well as transfer entropy the resulting measure does not converge monotonically to the true value when the number of discrete bins is increased. In the absence of a distribution theory, hypothesis testing is only possible by means of bootstrapping. We propose to estimate the necessary joint and conditional frequencies by means of quantile regression. This allows us to avoid arbitrary binning and all associated problems. Moreover, due to the semi-parametric nature of this approach, the computational burden is decisively reduced compared to multi-variate kernel density estimation. Instead, we show that we can flexibly use quantile regressions to estimate densities in order to calculate joint, conditional and transfer entropy as well as mutual information. Furthermore, by casting our into a Generalized Method of Moments framework, we develop the asymptotic theory to conduct inference on relative entropy measures for multiple variables.



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Preliminary Study of Entropy-Based Indicators to Discriminate Cancer-Related Characteristics

sciforum-029286

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Select entropy-based indicators (such as Kolmogorov Complexity, Shannon Information Entropy and the Index of Regularity) have been used in this preliminary study to classify genes with acceptable results. This need for classification is driven by the interest of the scientific community in determining whether a given gene possesses or lacks cancer-related characteristics. A subset of genes was chosen, based on previous studies and on random selection. These genes have been represented by their DNA sub-sequence and have been divided into two groups: those that have a relation to cancer (that is, they either cause cancer, as in oncogenes, or are tumor suppressors) and those that are not related to cancer issues (i.e., normal genes). Initially, eleven classifiers were used and compared, some of which reflected an accuracy rate of over 70%. This accuracy rate represents the percentage of correct predictions (cancer-related or not) within a test set of genes. These results shed some light on the fact that, in effect, oncogenes and normal genes have different patterns and structures and can potentially be used as a predictor for novel genes and features. This exploratory study also analyzes non-classic classifiers and evaluates the prospects of clustering and advanced machine-learning algorithms to determine significant patterns within DNA sequences.



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A Stepwise Assessment of Parsimony and Entropy in Species Distribution Modelling

sciforum-029311

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Entropy is an intrinsic characteristic of the geographical distribution of a biological species. A species distribution with higher entropy involves more uncertainty, i.e., is more gradually constrained by the environment. Species distribution modelling tries to yield models with low uncertainty, but normally has to produce them by increasing their complexity, which is detrimental for another desirable property of the models, parsimony. By modelling the distribution of 18 vertebrate species in mainland Spain, we show that entropy may be computed along the forward-backward stepwise selection of variables in Generalized Linear Models to check whether uncertainty is reduced at each step. This allows selecting the model that best combines the complementary characteristics of certainty and parsimony. This also allows to disentangle the entropy due to the intrinsic uncertainty of the species distribution from that due to failure in the model specification. A reduction of entropy was produced asymptotically in each step of the model, with some exceptions. This asymptote could be used to distinguish the entropy attributable to the species distribution from that attributable to model misspecification. We discussed the differential suitability of Shannon and fuzzy entropy for this end. The use of Shannon entropy in distribution modelling has not biogeographical sense, because it computes probability of presence as if the species were only present in one cell of the study area. Fuzzy entropy has not such restriction and always has values between zero and one, which produces results that are commensurable between species and study areas. Fuzzy entropy is also more correlated with AUC values. Using a stepwise approach and fuzzy entropy may be helpful to counterbalance the uncertainty and the complexity of the models. The model yielded at the step with the lowest entropy combines reduction of uncertainty with parsimony, which results in high efficiency.



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Superresolved Light Microscopy Information on the Structure of the Stained Dental Tissue Section Obtained by Point Divergence Gain Analysis

sciforum-029348

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Light microscopy is an unavoidable tool in understanding of the internal structure and chemical composition of materials. It has its limits of resolution [1] which have been analysed mostly from the point of view of the ability of a user of the microscopic instrument to distinguish two objects unambiguously.

We have developed a new variable, point divergence gain (PDG), which enables us to find centroids of the imaging function in any expectable context. In the standard terminology of the light microscopy, irrespectively of the nature of the light-matter interactions, we may create a 3D superresolved map of the interior of a dense semi-transparent material. We have demonstrated this ability on the structure of a living cell [2]. Now we show the ability of PDG-based superlocalisation on a histological sample stained by methods dating back to 1770.

The localization of the elementary centroid of the absorbing object was achieved with the precision of $78 \times 78 \times 5 \text{ nm}^3$. The comparison of subsequent images shows that these localisations are unique, i.e., do not repeat in consequent images. This indicates that the elementary coloured objects are of macromolecular size. The coloured objects are grouped into structures which may be identified as histologically relevant elements but, in this case, we understand their internal structure.

Besides technical description of the results, we compare the PDG-based results with the standard terms of light microscopy such as resolution and depth of focus and demonstrate their proper definitions based on the theory of information.

References

1. de Villiers, G.; Roy Pike, E. *The Limits of Resolution*; CRC Press: New York, NY, USA, 2016.
2. Rychtáriková, R.; Náhlík, T.; Shi, K.; Malakhova, D.; Macháček, P.; Smaha, R.; Urban, J.; Štys, D. Super-resolved 3-D imaging of live cells' organelles from bright-field photon transmission micrographs. *Ultramicroscopy* **2017**, *179*, 1–14.



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Case Studies of Statistical Entropy Analysis in Recycling Processes: A Tool in Support of a Circular Economy

sciforum-029521

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Statistical entropy (SE), has been used alongside material flow analysis (MFA) to aid studies of resource efficiency and waste management. Given that statistical entropy operates based on principles of information theory, it can be used to describe quantitatively systems with mixed materials flow, including their overall distribution of components throughout transformational stages, e.g., mechanical pre-treatment stages in recycling processes. In the present work, we present two cases where our research group has used statistical entropy analysis as an analytical tool for recycling process, with the aim of supporting a transition towards a circular economy.

In the first place, a comparison between two lithium-ion battery recycling processes was carried out by the combination of material flow analysis and statistical entropy. In this manner, an efficiency weight at a systemic level is given to the mechanical processing stages, which is reflected by the entropic values at final stages. In other words, while both systems obtained recycled materials with similar characteristics, the system that presented a more efficient pre-processing stage (i.e., lower statistical entropy value) presented a lower entropy value of the substances at final stage. Secondly, statistical entropy and material flow analysis was used as to aid in the design of mechanical processing stages for thermoelectric devices (TEDs). A total of 106 thermoelectric devices were mechanically processed by different comminution methods, physical and chemical characterization were carried out and the entropy values evaluated in each stage. The statistical entropy results were used to design a process which presented a fast and efficient entropy reduction in all the throughput, such, entailed a total of 5 stages and obtained fractions of high purity and treatability.



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Entropy-Based ECG Biometric Identification

sciforum-029885

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There is a great interest nowadays in using ECG for biometric identification, due to some of its intrinsic properties. There are different proposals in the literature to solve this task. Most of them based on feature extraction and machine learning methods applied on those features and, recently, others based on deep learning algorithms applied directly on the signals—providing better results, but requiring a much higher computational cost. In this study we aim to show how an approach based on compression methods can be used to perform this task. Our approach uses the notion of relative compression to provide a measure of similarity from a new signal to the different participants present on the database. This is an approach which relies heavily on the entropy of the data sources, as the compressors used to perform the relative compression are based on finite-context models (similar to Markov models). We aim to show that it is possible to perform biometric identification using ECG signals using this methods, even without applying any kind of fiducial point detection on the ECG, making the method, in theory, more general than for this specific task or type of signal. Our results show that this approach is feasible in practical terms and provide competitive results, achieving an accuracy of around 89.3% using an publicly available database with 25 participants.



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Entropy of Vostok Ice Core Data and Kalman Filter Harmonic Bank Climate Predictor

sciforum-030175

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Entropy of Vostok ice core data together with our notion of Kalman Filter Harmonic Bank (KFHB) Climate Prediction Engine (CPE) are introduced in this paper. In particular we examine CO₂ Cycle 1 data (the most recent data cycle), and analyze so called Spectral Entropy of CO₂ harmonics obtained by standard Fast Fourier Transform (FFT) analysis. We also introduce treatment of Vostok Data as a sample from a corresponding non stationary stochastic process for which, instead of FFT, we can use Karhunen-Loeve Expansion (KLE) for a set of discrete data values and the corresponding autocorrelation matrix, defining Representation Entropy as a broader concept compared to Spectral Entropy for FFT. Initial results for Spectral Entropy are presented as a measure of amplitude and energy analysis informational effectiveness which determines a set of signal harmonics implemented in a form of KFHB whereas each harmonic is generated by a two state Kalman Filter. The total signal is then represented as a sum of a set of amplitude or energy significant harmonics (hence the name Kalman Filter Harmonic Bank). Spectral Entropy calculations point to a suitable number of FFT generated harmonics to be used for signal synthesis by harmonic truncation. We also analyze using amplitude vs. energy (amplitude squared) as a base for entropic calculations. Similarly in the case of KLE, Representation Entropy would play the same role. Ultimately we are working to implement this approach into an effective Machine Learning short and long term CPE. It is critical to perform very detailed time and frequency data analysis as a solid base for the CPE methodology for modelling variations in climate.



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Measuring Functional Connectivity of Human Intra-Cortex Regions with Total Correlation

sciforum-032526

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The economy of brain organization makes the primate brain consume less energy but efficiency. The neurons densely wired each other dependent on both anatomy structure connectivity and functional connectivity. Here, I only describe functional connectivity with Functional Magnetic Resonance Imaging (fMRI) data. Most importantly, how to quantitative measure information share or separate among functional brain regions, what's worse, fMRI data exist large dimensional problems or "curse dimensionality" [1]. However, the multivariate total correlation method can perfectly address the above problems. In this paper, two things measured with the information-theoretic technique—total correlation [2–4]. First and foremost, quantitative measures intra-cortex regions dependent or independent from others from the information-theoretic view. Second, quantitative measures of intra-cortex functional connectivity play a crucial role in the mental clinical diagnosis.

The brain's sensitivity to the perceptual environment then adapts and responds to the outside world. The information integrated and separated happens in the brain and consumes less energy [5,6]. In other words, the brain can be treated as an energy, entropy, physical complex system, or it's a naturally perfect stochastic complex system. Mathematically, the brain function can be denoted as: $R = S(X)$, X represents stimuli from the outside world, S refers to unknown nonlinear functions which describe brain information processes, and R denotes response. In this paper, we use functional brain atlases to extract time series, then information estimated with total correlation, it can capture non-linear or even non-monotonic relationships in the high-dimensional data compared to other approaches, e.g., Spearman- ρ [7] and the Kendall- τ [8] et al.

In summary, this paper shows the estimated intra-cortex brain region's functional connectivity and also addresses non-linear relationships in the brain signal through total correlation.

Reference

1. Hastie, T.; Tibshirani, R.; Friedman, J. *The Elements of Statistical Learning*. Springer: Berlin, Germany, 2009.
2. Kullback, S.; Leibler, R.A. On information and sufficiency. *Ann. Math. Stat.* **1951**, *22*, 79–86.
3. McGill, W.J. Multivariate information transmission. *Psychometrika* **1954**, *19*, 97–116.
4. Han, T.S. Nonnegative entropy measures of multivariate symmetric correlations. *Inf. Control* **1978**, *36*, 133–156.
5. Anderson, N. Unified Psychology Based on Three Laws of Information Integration. *Rev. Gen. Psychol.* **2013**, *17*, 125.
6. Toker, D.; Sommer, F. Information integration in large brain networks. *PLOS Comput. Biol.* **2019**, *15*, E1006807.
7. Spearman, C. The proof and measurement of association between two things. *Am. J. Psychol.* **1904**, *15*, 72–101.
8. Kendall, M.G. A new measure of rank correlation. *Biometrika* **1938**, 81–93.



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Evaluation of the Performance of Permutation Entropy Variants for Classifying Auditory Evoked Potentials

sciforum-044132

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The aim of the present work was to investigate the performance of entropic tools to classify, subjects with normal hearing and those with pathologies in the auditory pathway, using short-latency records of auditory evoked potentials. To accomplish with this objective, traditional permutation entropy, weighted permutation entropy and a modified version of the original permutation entropy, correcting the count of the missing or forbidden patterns.

The database used consisted of two age groups, one of minors aged from a few months to four years and the other of older aged over 18 years.

For both minor and older subjects, thirty samples were randomly selected from both normal and hearing-impaired subjects.

Once the different varieties of entropy had been calculated, the difference in mean values was analyzed using statistical tests to check whether the difference between them was significant or not. The differences between means of the groups with and without pathology were found to be significantly different at a level of 99.9%.

Finally, the choice of the most appropriate entropy was made based on the calculation of the specificity, selectivity, precision and area under the operation reception curve. The results obtained showed that for the differentiation of healthy and pathological records in the case of minors, the weighted permutation entropy was more appropriate and the modified version of the permutation in the case of older adults.



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Design and Characterization of $\text{Cr}_{29.7}\text{Co}_{29.7}\text{Ni}_{35.4}\text{Al}_{4.0}\text{Ti}_{1.2}$ Precipitation Hardened High Entropy Alloy

sciforum-044154

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In 2004 a new class of metallic alloys, called high entropy alloys (HEA), was introduced in the literature. The main concept behind these alloys is that they have multiple main elements instead of only one or two. Therefore, they can exist under a vast compositional landscape, most of which is yet to be explored. In the early studies on HEAs, a great effort was made on searching for single-phase alloys with optimized properties, mainly those with a face-centered cubic structure (FCC). Recently, in the so-called “second generation” of HEAs, research focus has been broadened to multi-phase alloys. In particular, those alloys with FCC matrix plus L_{12} precipitates or BCC matrix with B2 precipitates to compete with traditional superalloys. In the present work, CALPHAD method (via Pandat® software) was used to aid the design of a new precipitation hardened, namely $\text{Cr}_{29.7}\text{Co}_{29.7}\text{Ni}_{35.4}\text{Al}_{4.0}\text{Ti}_{1.2}$ (a.t %), with a FCC matrix and L_{12} precipitates. The alloy was produced, solution-treated, cold-rolled and annealed, the alloy was then cut into different pieces and aged at 850 °C for different times. The microstructure was composed of spherical precipitates distributed uniformly in the FCC matrix. The characterization of the microstructure showed that thermodynamic calculation was accurate. The improvement in mechanical properties caused by introducing the ordered precipitates, analyzed through microhardness test, showed a promising mechanical behavior of the new designed alloy.



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Entropy: From Thermodynamics to Information Theory

sciforum-044185

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Entropy is a concept that remote to the 19th century. It was associated with the heat used by a thermal machine to realize work in the context of the Industrial Revolution. The 20th century saw an unprecedented scientific revolution, and one of the essential innovations from this time was Information Theory, which also has a concept of entropy. A natural question arises: ‘what is the difference, if any, between the entropies used in each field?’ The concept is misused misconceptions about the theme. There have been attempts to conciliate the entropy of thermodynamics with that of information theory. The most common use is defining entropy as “disorder”, however, it is not a good analogy since “order” is a subjective human concept, and “disorder” is not the measurement that can always be obtained with entropy. Another way is relating complexity to entropy. Computer science and statistics have boarded the problem of complexity utilizing Kolmogorov Complexity. Again, the abstraction level of the concept can make researchers from other areas, such as biologists and chemists (in which the study of complexity plays an essential role in misunderstood concepts). In this paper, the historical background for the evolution of “entropy” is presented, and mathematical proofs and logical arguments for the concept’s interconnection in various science areas.



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New Explanation for the Mpemba Effect

sciforum-028919

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The purpose of this study is to check out the involvement of entropy in Mpemba effect. Provided that preheating of the water the cooling duration is reduced, we theoretically show that water gains more entropy when warmed and re-cooled to the original temperature. Water molecules are oriented dipoles joined by hydrogen bonds. When water is heated, this structure collapses (i.e., the entropy increases). When water is re-cooled to a lower temperature, the previous structure is not re-formed immediately. Sometimes, when the re-cooling is performed within a freezer, there is not enough time for the structure to re-form because of the high cooling rate. The entropy reduction curve as a function of the temperature, $S = f(T)$, shows retardation (a lag) relative to the entropy growth curve. Water that has been heated and re-cooled to the initial temperature shows greater entropy than that before it was heated. This means that, while its molecules now have the same kinetic energy, their thermal motion after heating is less oriented with respect to the structure mentioned above. After re-cooling, random collisions are more likely, owing to this the temperature decreases more quickly.



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Quasistatic and Quantum-Adiabatic Otto Engine for a Two-Dimensional Material: The Case of a Graphene Quantum Dot

sciforum-029657

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The concept of quantum heat engines (QHEs) was introduced by Scovil and Schultz-Dubois in Ref. [1], in which they demonstrate that a three-level energy maser can be described as a heat engine operating under a Carnot cycle. This important research gave way to the study of quantum systems implemented as the working substances of heat machines with the goal of realizing efficient nanoscale devices. These devices are characterized by the structure of their working substance, the thermodynamic cycle of operation, and the dynamics that govern the cycle [2,3]. In this study, we analyze the performance of a quasi-static and quantum-adiabatic magnetic Otto cycle for a two-dimensional material: the case of a graphene quantum dot [4]. For graphene quantum dots [5,6], the low-energy approach using the Dirac equation with boundary conditions is an excellent approximation. Modulating an external/perpendicular magnetic field, in the quasistatic approach, we found behaviors in the total work extracted that are not present in the quantum-adiabatic formulation. Additionally, we find that, in the quasi-static approach, the engine yielded a higher performance in terms of total work extracted and efficiency as compared with its quantum-adiabatic counterpart. In the quasi-static case, this is due to the working substance being in thermal equilibrium at each point of the cycle, maximizing the energy extracted in the adiabatic strokes.

References

1. Scovil, H.E.; Schulz-DuBois, E.O. Three-level masers as heat engines. *Phys. Rev. Lett.* **1959**, *2*, 262.
2. Bender, C.M.; Brody, D.C.; Meister, B.K. Entropy and temperature of a quantum Carnot engine. *Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci.* **2002**, *458*, 1519–1526.
3. Feldmann, T.; Geva, E.; Kosloff, R.; Salamon, P. Heat engines in finite time governed by master equations. *Am. J. Phys.* **1996**, *64*, 485–492.
4. Peña, F.J.; Zambrano, D.; Negrete, O.; De Chiara, G.; Orellana, P.A.; Vargas, P. Quasistatic and quantum-adiabatic Otto engine for a two-dimensional material: The case of a graphene quantum dot. *Phys. Rev. E* **2020**, *101*, 012116.
5. Grujić, M.; Zarenia, M.; Chaves, A.; Tadić, M.; Farias, G.A.; Peeters, F.M. Electronic and optical properties of a circular graphene quantum dot in a magnetic field: influence of the boundary conditions. *Phys. Rev. B* **2011**, *84*, 205441.
6. Thomsen, M.R.; Pedersen, T.G. Analytical Dirac model of graphene rings, dots, and antidots in magnetic fields. *Phys. Rev. B* **2017**, *95*, 235427.



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Dissipative Extension of Electrodynamics

sciforum-030309

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In nonequilibrium thermodynamics, electrodynamic interaction and electrodynamic forces appear as non-dissipative, external phenomena. Irreversibility is due to Ohm's law and polarisation. However, the theoretical approaches of polarisation and thermal couplings do not apply to Lorentz force and electromagnetic stresses. The choice of state variables is also problematic. Thermodynamic stability cannot be valid for para- and diamagnetic materials at the same time, choosing either magnetisation or the magnetic field strength, or the corresponding four quantities in a special relativistic framework, as a state variable. Moreover, any particular choice leads to shape-dependent homogeneous thermodynamic bodies, and therefore the extensivity condition of thermodynamic state variables cannot be introduced without any further ado. In the presentation, I survey the problems of thermodynamic compatibility of electrodynamics and suggest some explanations. The main ideas are originated in a novel approach to gravity in the framework of nonequilibrium thermodynamics, where the gravitational potential is a thermodynamic state variable, and the balances of mass, momentum and energy are constraints for the entropy inequality. Naturally, for electrodynamics, special relativity is a necessary background.



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The Minimum Entropy Production Principle and Heat Transport in Solids with Internal Structure

sciforum-044169

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Variational principles have a long story in the study of the time evolution of dissipative systems. There is a wide variety of formulations of such principles, some of which are ad hoc techniques like doubling of the dynamic variables, restricted variations, etc. There also exist some principles which have a fundamental character like the minimum entropy production principle, MEPP, which refers to the stationary state eventually reached by a system after it has been taken out of equilibrium. Much has been discussed whether the MEPP has general application or whether it is of rather limited validity. In particular, it has been concluded that for systems with constant phenomenological Onsager coefficients the entropy production can only decrease in time until a minimum is reached when the system is in the stationary state, it yet being on debate. In this work heat transport in non-homogeneous solids is considered. We study the case of solids with internal structure within the framework of a two temperature description. The internal structure is introduced in the model through the dependence of the thermal conductivity on position. The time evolution equations are obtained through the usual methods of irreversible thermodynamics and from the MEPP. We find that in our approach both sets of evolution equations coincide and that, without imposing any restriction on the phenomenological coefficients other than those coming from the internal structuring of the solid, the appropriate temperature profiles are obtained. We exemplify this finding with the case of pure Aluminum subjected to a heat pulse.



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Comparative Performance Analysis of a Brownian Carnot Cycle from the Perspective of a Stochastic Model against the Linear Irreversible Thermodynamics Theory

sciforum-044184

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In this work we present a Brownian Carnot Cycle, which has already been studied by Schmiel et al. (2007) as well as Izumida and Okuda (2010); but now considering two different working regimes, namely the Maximum Ecological Function (MEF) and the Maximum Efficient Power (MEP). For the MEF and MEP working regimes, the thermodynamic properties of the cycle are obtained, in particular, it showed that the maximum efficiency now depends on two parameters α and β , instead of only one parameter obtained previously by Schmiel et al. In maximum power regime. It is worthwhile to notice that for characteristic values of α and β the original results obtained by Schmiel are recovered.

From the previous observations, the authors consider that the results obtained represent a more general case that includes other working regimes. An important remark is that one of the most astonishing results obtained, is that those thermal engine models show some universality regarding the behavior of the efficiency when it works at the maximum power regime [1], although the analyzed models were different in nature and scale.

Reference

1. Norma Sanchez-Salas, L López-Palacios, S Velasco, A Calvo Hernández, Optimization criteria, bounds, and efficiencies of heat engines. *Phys. Rev. E* **2010**, 82, 051101.



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Efficiency of an Arrangement in Series of Irreversible Thermal Engines Working at Maximum Power

sciforum-044190

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Within the context of finite-time thermodynamics several regimes of performance have been used to study the well known Curzon-Ahlborn (CA) heat engine model [1–5]. Also the optimal performance and the effects on environment are studied to find the best approximation with real heat engines.

In this work we present a model of an arrangement in series of irreversible Carnot heat engines, which consist of k reservoirs connected in series, this heat engine model is working under three different regime of performance: maximum power output, maximum ecological function [6] and maximum efficient power [7]. At first we used three reservoirs, and we calculated its efficiency. For the case of maximum power output we calculated the efficiency for the case of the generalizing of k reservoirs, and we get an efficiency expression similar to the one of Curzon-Ahlborn, the irreversibilities are taken into account by irreversibility parameter R . Finally we present the comparison of the efficiencies obtained under three different regimes of performance.

References

1. Carnot, S. *Reflexions sur la Puissance Motrice du Feu, et sur les Machines Propres Developper cette Puissance*; Bachelier: Paris, France, 1824.
2. De Vos, A. *Endoreversible Thermodynamics of Solar Energy Conversion*; Clarendon Press: Oxford University, Oxford, UK, 1992.
3. Wu, C. *Recent Advances in Finite-time Thermodynamics*; Nova Science: New York, NY, USA, 1999.
4. Curzon, F.; Ahlborn, B. Efficiency of a Carnot Engine at Maximum Power Output. *Am. J. Phys.* **1975**, *43*, 22.
5. Novikov, I.I. The efficiency of atomic power stations (a review). *J. Nucl. Energy* **1954**, *7*, 125-128.
6. Angulo-Brown, F. An ecological optimization criterion for finite-time heat engines. *J. Appl. Phys.* **1991**, *69*, 7465-7469.
7. Yilmaz, T. A new performance criterion for heat engine: efficient power. *J. Energy Inst.* **2006**, *79*, 38-41.



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