StatPhys in Kigali: Book of Abstracts

Susana Alexandra Barbosa

Title: Analysis of Nonlinear Time Series of Ambient Radioactivity for Climate and Radioprotection Applications

Abstract: Ambient radioactivity refers to the background radiation that is constantly present in the environment, originating from natural sources, including cosmic radiation that continuously reaches the Earth, and terrestrial radioactive elements (such as Potassium, Uranium, and Thorium) along with their decay products, which are naturally present in the environment (air, soil, rocks, and water).

The study of ambient radioactivity has two main motivations: protecting ecosystems and human populations from the adverse effects of radiation exposure, and using it as a scientific tool to gain insights into various geoscience processes, including volcanic and seismic activity, pollution, hydrological processes, and atmospheric and climate dynamics.

Monitoring of ambient radioactivity is based on measurements of ionising radiation in various locations and environments, yielding time series relevant both for radioprotection purposes and for multidisciplinary geophysical studies. The analysis of ambient radioactivity time series typically aims to describe and quantify temporal variability across multiple time scales (hourly, diurnal, seasonal, long-term), as well as to identify and remove known co-variability—particularly with meteorological parameters—that obscures their use as geophysical proxies.

However, the analysis of ambient radioactivity time series is hindered by their heteroskedastic behavior and their inherently nonlinear and non-stationary nature, which require specific methodological approaches. This talk focuses on high-resolution time series of ambient radioactivity from the Atmospheric Radiation Measurement (ARM) Scientific User Facility Eastern North Atlantic (ENA), located on Graciosa Island (Azores archipelago, Portugal). Detailed measurements of radon and ambient gamma radiation, as well as CO2 and CH4 measurements, are being conducted at the ENA Facility as part of the NuClim project, with the aim of identifying baseline conditions representative of hemispheric background concentrations of greenhouse gases. Preliminary time series from the NuClim campaign, along with the historical ambient gamma radiation time series - measured at ENA at 1-minute intervals since 2015 - are used to illustrate the challenges and approaches involved in analyzing nonlinear time series for climate and radioprotection studies, such as recurrence analysis, matrix profile analysis, and wavelet analysis.

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Mulugeta Bekele

Title: Machine Learning Nonequilibrium Phase Transitions

Abstract: We present an investigation of a convolutional neural network (CNN) prediction that successfully recognizes the critical temperature of nonequilibrium phase transitions in 2D Ising spins on a square lattice. The model uses image snapshots of ferromagnetic 2D spin configurations as the input shape to provide the average output predictions. By considering supervised machine learning techniques, we perform Metropolis Monte Carlo (MC) simulations to generate the configurations. In the equilibrium Ising model, the Metropolis algorithm respects the detailed balance condition (DBC), whereas its nonequilibrium version violates DBC.

Analytically, we incorporate the algorithm through a parameter ϵ ($0 \leq \epsilon \leq 1$). Graphically, we find a functional solution of the critical temperature. A setup with $\epsilon = 0$ restores the usual Metropolis algorithm which helps to generate the equilibrium configurations (train_dataset). For a nonzero ϵ , the system attains nonequilibrium steady states (NESS), and the modified algorithm generates NESS configurations (test_dataset). After training the model on the train_dataset, it has been tested using the test_dataset. The result shows that CNN can determine the transition temperature for various ($\epsilon \leq \epsilon \leq 1$) which is consistent with both MC and graphical results. The discrepancy for ($0 \leq \epsilon \leq \epsilon$) is mainly due to the fact that quantum fluctuation is more pronounced at low temperature, Reference [1].

Somendra Bhattacharjee

Title: The Nature of criticality in Dynamical Quantum Phase Transitions

Abstract: When a quantum magnet is rapidly quenched from a high transverse magnetic field down to zero at absolute zero temperature, it exhibits first-order transitions or critical points during its time evolution—often resembling the behavior typically seen when varying temperature. Surprisingly, the only changing parameter in this process is time. This talk will explore the nature of these dynamical quantum phase transitions in the context of the transverse field Ising and Potts models utilizing exact renormalization group transformations in the appropriate complex plane.

References

- 1. Amina Khatun and S. M. Bhattacharjee, Phys. Rev. Lett. 123, 160603 (2019)
- 2. S M Bhattacharjee, Phys Rev B 109, 035130 (2024)

Daniel Busiello

Title: Information propagation in multiscale systems: functional couplings and efficient nonlinear operations **Abstract:** Interconnected fluctuating processes occurring across multiple temporal scales are a hallmark of neural networks, ecological communities, biochemical architectures, and many other complex systems. These processes can interact both directly and indirectly, with interactions across timescales often exhibiting intricate internal properties. This complexity makes understanding the relationships between components of a biological or synthetic complex system a formidable challenge.

In this talk, I will explore how the distinct timescales associated with each process influence their effective couplings. By examining the probabilistic structure of a general multiscale system, I will uncover the underlying principles that govern information propagation across different timescales. In doing so, I will clarify the interplay between mutual information and causality, revealing the origin of the critical distinction between causal and functional interactions in complex stochastic systems.

The picture becomes more intricate when considering the interplay between this emerging information structure and the dynamical properties of the underlying system components. I will consider a general model where the input signal is propagated to an output unit through a processing layer via nonlinear activation functions. In particular, I will focus on two widely implemented paradigms: nonlinear summation, where signals are first processed independently and then combined; and nonlinear integration, where they are combined first and then processed. In this framework, I will demonstrate that fast-processing capabilities systematically enhance input-output mutual information and that nonlinear integration outperforms summation in large multiscale systems. On the contrary, lower-dimensional systems exhibit a nontrivial relationship between the two strategies as a function of interaction strength and heterogeneity.

Our results uncover pivotal features of information processing across temporal scales, with profound implications for both biological and artificial complex systems.

Raphael Chetrite

Title: Macroscopic fluctuations theory (MFT) for interacting particle systems with long range interactions **Abstract:** We extend the Macroscopic Fluctuations Theory (MFT) to systems in the case where the interactions are long-range, and consequently, the macroscopic effective equations are described by non-linear fractional diffusion equations.

Federico Corberi

Title: Maximal Diversity and Zipf's Law

Abstract: Zipf's law describes the empirical size distribution of the components of many systems in natural and social sciences and humanities. We show, by solving a statistical model, that Zipf's law co-occurs with the maximization of the diversity of the component sizes. The law ruling the increase of such diversity with the total dimension of the system is derived and its relation with Heaps' law is discussed. As an example, we show that our analytical results compare very well with linguistics and population datasets.

Germaine Djuidje Kenmoe

Title: How hydrodynamic effects and entropic stochastic resonance enhance transport and diffusion of particles in confined media.

Abstract: Hydrodynamic effects and entropic stochastic resonance (ESR) can play an important role in particle transport and diffusion. A space-dependent two-dimensional (2D) diffusion function, D(x,y) [1, 2], which characterizes the local geometrical constraints of the system by quantifying the inner cavity structure is considered. Using this function, the entropic stochastic resonance is computed and visualized, identifying distinct resonance peaks. These peaks correspond to optimal conditions under which the average velocity, mobility, and effective diffusion coefficients are subsequently calculated and analyzed. A notable difference between transport properties computed with and without the inclusion of the local diffusion function D(x,y) is highlighted. Thus, revealing the influence of spatial inhomogeneities in modulating particle dynamics. Furthermore, emphasize the influence of ESR peak values by evaluating mobility and diffusion for parameter regimes both above and below the resonance peak. The configurations involving simple potentials and deformable channels are compared with other works [3, 4]. That to ascertain which arrangement most efficiently facilitates transport, especially when enhanced by the combined contributions of hydrodynamic effects and entropic stochastic resonance. The findings provide insights into transport optimization in complex environments, with implications for designing efficient micro- and nanoscale devices.

References

- Xiang Yang, Chang Liu, Yunyun Li, Fabio Marchesoni, Peter Hanggi, and H. P. Zhang, National Academy of Sciences, 36, 9564 (2017).
- Zhu, Qian and Zhou, Yang and Marchesoni, Fabio and Zhang, HP, Physical Review Letters, 9, 098001 (2022).
- 3. M. Djolieu, G. Djuidje Kenmoe
- 4. N. A. Donfack Tsagni, G. Djuidje Kenmoe, Physica D, (2025)

Mohammad Reza Ejtehadi

Title: Micro-star swimmers with chemotaxis ability.

Abstract: Here, we present a three-dimensional microswimmer model designed to operate in low-Reynolds number environments. The swimmer consists of five spherical beads arranged in a tetrahedral arrangement. The swimmer's movement patterns show that regular arm activity sequences generate spiral trajectories. Beyond normal swimming, we investigate the effects of stochastic perturbations in arm activity sequences and demonstrate diffusion behavior that strongly depends on the chemical concentrations in the environment. Most notably, our model exhibits robust chemotactic behavior, with the swimmer exhibiting directed motion along chemical gradients. This work provides insights for the development of artificial 3D microswimmers for applications in targeted drug delivery and environmental sensing.

Rosemary Harris

Title: Insights from non-Markovian random walks (and applications to decision modelling) **Abstract:** TBA

Rhoda Hawkins

Title: TBA Abstract: TBA

Doris Heinrich

Title: Controlling Dynamical Cellular Processes and Emergence of Patterns in 3D Organ Systems Abstract: 3D tissue models have become an indispensable component of modern biomedical research. They offer a realistic representation of biological processes and provide valuable insights into cellular behavior under various conditions. In particular, they allow for the detailed investigation of processes such as cell orientation, differentiation, and the response and adaptation of cells to external stimuli. These models enable researchers to make informed predictions, for example, about how tissues respond to specific stimuli. Moreover, fluidic microenvironments can be precisely tailored and optimized to elicit desired biological effects. Another promising application is the development of so-called digital twins—virtual representations of biological systems—that are increasingly being used to personalize and improve clinical therapies and treatment strategies. Using application-oriented research examples, a range of innovative approaches is presented. These include studies of surface- triggered interactions between cells and structured surfaces within (quasi-) 3D environments, as well as the use of three-dimensional niches for tissue engineering based on stem cells. Such environments are often integrated into microfluidic systems, allowing for the construction of complex and controllable experimental platforms. Additionally, the use of simulation techniques is discussed, such as the modeling of flow processes relevant to both medical and environmental applications. The integration of AI is also gaining momentum, particularly for the analysis of large datasets and for enhancing the modeling and prediction of complex biological systems.

Jean Francois Joanny

Title: Self-organized patterns of microtubules and molecular motors

Authors: JF Joanny, S. Pattanayak, A. Sciortino, L. Blanchoin and M. Théry

Abstract: The internal organization of cells is largely determined by the architecture and orientation of the microtubule network. Microtubules serve as polar tracks for the selective transport of specific molecular motors toward either their plus or minus ends.

We present experiments on reconstituted systems and theory to study the interaction of microtubules with both plus-and minus-end directed motors bound to a fluid membrane. Depending on motor concentrations, the system leads either to the constant transport of microtubules or to their alignment, stacking, and immobilization in regular bands that separate motors into domains of opposite polarities.

In bands, microtubules all share the same polarity and segregate the two opposing motors. The regular patterns result from the balance of forces produced by the two motors as they walk in opposite directions along each microtubule.

The microtubule patterns result from active microphase separation where the microtubules can be considered as active surfactants pumping the motors on on each side depending on their polarity. We present a model for the steady state patterns in one and two dimensions and an active Cahn Hilliard theory, wich describes the kinetics of the phase separation.

Stephane Kenmoe

Title: TBA Abstract: TBA

Timoleon Crepin Kofane

Title: TBA Abstract: TBA

Tanniemola B. Liverpool

Title: The statistical physics of wound healing

Abstract: I will discuss some recent work looking quantitatively at the process of wound healing using ideas from thermodynamics, continuum and statistical mechanics. Wound healing is a highly conserved process required for survival of an animal after tissue damage. The wound repair process is not only of great interest in its own right but is also a laboratory to study complex tissue dynamics and regeneration.

Many wounds involve damage to an epithelial (barrier) tissue (like skin) that separates different regions of the body of a living organism. I will describe some recent work on studying wound healing in two dimensional epithelial tissues of a fruit fly pupal wing. This epithelium was chosen because it is transparent and accessible to sophisticated imaging techniques. We use live confocal time-lapse microscopy to follow the behaviour of cells in a tissue before and after wounding.

I will focus on three cell-behaviours that are generally accepted to contribute to wound re-epithelialisation: cell shape deformation, cell division, and cell migration.

I will describe how we are beginning to use a combination of mathematics, physics and biology to disentangle some of the organising principles behind the complex orchestrated dynamics that lead to wound healing.

Emanuele Locatelli

Title: Adsorption properties of polymeric brushes in and out of equilibrium

Abstract: We consider polymer brushes able to adsorb colloidal-like solutes and we study, using computer simulations and scaling theory, their conformational and adsorption properties in and out of equilibrium. In equilibrium, Langevin Dynamics simulations show, with increasing the amount of solute, the collapse of the brush followed by a successive re-swelling. We rationalize this phenomenology through a scaling theory, following Alexander and de Gennes, where adsorption is seen as a progressive worsening of the solvent conditions[1]. Going towards practical applications, we study adsorption out-of-equilibrium introducing fluid flow and hydrodynamic interactions. We find that increasing colloid flux, either by an increase in applied pressure or colloid density, unexpectedly promotes adsorption[2].

References

- C. F., Vorsmann, S. Del Galdo, B. Capone, and E. Locatelli, Colloidal adsorption in planar polymeric brushes, Nanoscale Advances, 6 (2024) 816-825.
- 2. C. F., Vorsmann, E. Orlandini, and E. Locatelli, Colloidal adsorption in functionalized nano-channels, In preparation (2025)

Hildegard Meyer-Ortmanns

Title:Heteroclinic units acting as pacemakers for entrained dynamics of cognitive processes

Abstract: Heteroclinic dynamics is a suitable framework for describing transient and reproducible dynamics such as cognitive processes in the brain. We demonstrate how heteroclinic units can act as pacemakers to entrain larger sets of units from a resting state to hierarchical heteroclinic motion such as given by fast oscillations modulated by slow oscillations. The entrainment range depends on the type of coupling, the spatial location of the pacemaker and the individual bifurcation parameters of the pacemaker and the driven units. Noise as well as a small back-coupling to the pacemaker considerably facilitate synchronization. Units can be synchronously entrained to different temporal patterns, depending on the selected path in the hierarchical heteroclinic network. Such patterns are believed to code information in brain dynamics.

Depending on the number and the location of pacemakers on a two-dimensional grid, synchronization can be maintained in the presence of many resting state units and mediated via target waves when the pacemakers are concentrated to a small area of such a grid. In view of brain dynamics, our results indicate a possibly ample repertoire for coding information in temporal patterns, produced by sets of synchronized units, without finetuning of the parameters, and distributed in space. We also discuss relaxation times in heteroclinic dynamics. As it turns out, the relaxation is underdamped and depends on the nesting of the attractor space, the size of the attractor's basin of attraction, the depth of the quench, and the level of noise. In the case of coupled heteroclinic units, it depends on the coupling strength, the coupling type, and synchronization between different units. Depending on how these factors are combined, finite relaxation times may support or impede a fast switching to new external input. Our results also shed some light on the discussion of how the stability of a system changes with its complexity.

Cesare Nardini

Title: TBA Abstract: TBA

Jean-Pierre Nguenang

Title: On the Non-Hermitian phase transitions and mobility edges in connected incommensurate optical lattices with PT symmetry

Abstract: We investigate the electronic mobility features of the non-Hermitian incommensurate quantum lattices in the framework of tight-binding for which, the on-site energies are distributed following the Aubry-André quasi-periodic potential, while displaying a Parity-Time (PT) symmetry.

By decoupling a two strands quantum ladder network into two effective one dimensional chains, we get two tunable delocalization-localization distinct transition points that correspond to those of the PT symmetric breaking counterpart. In addition to the conducting and the insulating phases found from each of the single chains, we also highlight the existence of a selectively tunable intermediate phase region for the ladder system. We have unveiled the simultaneous mixture of both extended and localized states as well as the simultaneous mixture of the real and imaginary parts of the eigenenergies. These mixtures subsequently leads to the critical energy which is also named the mobility edge (MEs). Furthermore, to make the current study self-consistent, we have also probed the electronic's localization phase transition for a generalized case with several chains. This theoretical analysis can be helpful to describe the control mechanisms and the switching behavior of electronic localization in various types of such set of connected Hermitian and non-Hermitian quasi-crystals systems.

Innocent Nkurikiyimfura

Title: TBA Abstract: TBA

Kingsley Obodo

Title: TBA Abstract: TBA

Silvina Ponce Dawson

Title: The frequency codification of environmental changes equip cells with a scale invariant discriminating power

Abstract: Cells continuously sense their surroundings to detect modifications and generate responses. Very

often these modifications correspond to changes in the concentration of extracellular effectors that, upon binding to plasma membrane receptors, induce intra-cellular changes that generate the end response. The result of this signaling cascade not only depends on the presence/absence of the extracellular ligand but also on its concentration. How well cells can discriminate extracellular concentrations depends on how these concentrations are encoded in the intermediaries of the pathway. Cells use two main codification schemes: amplitude and frequency encoding in which increasing ligand concentrations yield increasing intermediary concentrations or induce a pulsatile behavior of increasing frequency, respectively. Intracellular Ca2+ signals are an example of the latter. Experiments showed that intracellular Ca2+ pulses are stochastic with a mean interpulse frequency that scales exponentially with the extracellular ligand concentration, a behavior that was also observed in the nuclear localization of transcription factors. In this talk I will show how this scaling arises in noise-driven excitable systems and how it endows cells with a scale invariant discrimination power in which extracellular concentrations can be distinguished equally well across different concentration ranges. Using the pheromone response pathway in yeast as example, I will discuss the limits to the scale invariance that the subsequent steps of the pathway impose and how the combination of frequency and (the qualitatively different) amplitude encodings can expand the range over which pheromone concentrations can be discriminated.

Edgar Roldan

Title: Martingale theory for stochastic thermodynamics **Abstract:** TBA

Daniel Madulu Shadrack

Title: Breaking Barriers in Drug Discovery: The Fusion of Atomistic Simulation and Machine Learning in Computational Biophysics

Abstract: In recent years, the field of drug design has undergone a remarkable transformation due to advancements in computer hardware and algorithms. This talk will explore how computational biophysics tools are driving this revolution, ultimately accelerating therapeutic discovery. The presentation will commence with an introduction to various computational biophysics tools utilized in drug design, providing attendees with a comprehensive understanding of the technological landscape shaping the field. Following this, specific examples will be presented to illustrate the profound impact of techniques such as molecular dynamics and enhanced sampling coupled with machine learning in drug design. These examples will highlight the unprecedented insights and efficiencies gained through the integration of computational methods into the drug discovery process. Drawing from my research group experiences, the talk will delve into the entire drug design pipeline, spanning from target identification to lead optimization and clinical trials. Research findings will be shared, elucidating key insights and successes achieved through the application of computational techniques. Lastly, the presentation will conclude with a discussion on the broader societal implications of employing these innovative approaches. By leveraging computational biophysics tools, we have the potential to address pressing societal challenges and advance the development of novel therapeutics, ultimately improving human health and well-being.

Yusuf Shaidu

Title: Advancing Neural Network Potentials for the Temperature-Dependent Dynamics of Complex Energy Materials

Abstract: The accurate prediction of temperature-dependent properties in energy materials is critical for the design and optimization of next-generation technologies in energy storage, conversion, and harvesting. However, the state-of-the-art atomistic simulation methods, such as those based on density functional theory (DFT), are computationally prohibitive in predicting these properties at relevant length and time scales due to poor scaling with system size. Artificial neural networks can efficiently approximate the complex potential energy surfaces of these materials, thanks to their expressiveness and computational efficiency, making them the preferred method for accurately simulating temperature-dependent properties at relevant scales. In this talk, I will present recent advances in the development of neural network potentials (NNPs) for capturing temperature-dependent properties in complex energy materials. I will highlight our development of NNPs using accurate DFT data and their application to systems such as elemental carbon, carbon capture in amine-appended metal-organic frameworks (MOFs), and moiré superlattices of stacked transition metal dichalcogenide (TMD) monolayers. Additionally, I will discuss strategies to incorporate electrostatic interactions into NNPs, which are essential for accurately modeling charged systems and interfaces. These advances can significantly enhance the scalability and accuracy of atomistic simulations, enabling deeper insights into the temperature-dependent properties of energy materials across a wide range of applications.

Ana-Suncana Smith

Title: Building a smart material inspired by living tissue **Abstract**:

Hulda Swai

Title: TBA Abstract: TBA

Conrad Bertrand Tabi

Title: TBA Abstract: TBA

Tatek Yergou

Title: Transport dynamics of comb-like polymers in confined environments driven by external forces: A simulation study

Abstract: We examine the translocation dynamics of comb-like polymers through confined environments under an externally applied force using computational simulations. Two distinct simulation approaches and systems are employed: (1) Monte Carlo (MC) simulations to study polymer translocation through a simplified pore under an imposed electric field, and (2) Langevin dynamics (LD) simulations to investigate polymer transport through a nanochannel subjected to a pulling force applied on a terminal monomer of the backbone. The study systematically explores a broad range of system parameters, including chain size, backbone length, side-chain length, grafting density, and applied force/field magnitude. For electric fielddriven translocation, the mean translocation time exhibits a non-monotonic dependence on the field strength, with a critical threshold marking the transition between smooth and chaotic translocation regimes. In the case of nanochannel confinement under a pulling force, the mean exit time similarly displays a non-monotonic relationship with grafting density, peaking at an optimal grafting density that maximizes translocation time. In both scenarios, the mean translocation time scales linearly with backbone and side-chain lengths.

Hugo Touchette

Title: Testing nonequilibrium currents with the stochastic area

Abstract: Determining whether a system is in an equilibrium or nonequilibrium state from simulations or experiments is a fundamental problem in statistical physics. In this talk I will discuss how this problem is normally approached by measuring the probability current in space and how it can be made more precise by defining statistical tests involving projections of the current. I will illustrate this point by considering a specific linear projection of the current for diffusion systems, related to the stochastic area, first studied by Paul Lévy in the 1940s for Brownian motion. This area is a good observable for testing the nonequilibrium

or nonreversible nature of diffusions as it is a scalar and its statistics can be studied in a precise way using large deviation theory.

Antonio Trovato

Title: Calorimetric cooperativity revisited and generalized: the role of intermediate states

Abstract: The calorimetric criterion is one of the experimental approaches used in the last decades, in particular in the context of protein folding, for assessing the cooperativity of many biophysical processes, modelled as transitions between a high temperature to a low temperature state. In a maximally cooperative two-state transition, no intermediate states are present at equilibrium, implying that the effective two-state van't Hoff enthalpy change equals the experimentally measured enthalpy change. The ratio of the former quantities is then defined as the calorimetric cooperativity index, which is typically evaluated at the transition temperature. Here we prove a quantitative connection, valid at all temperatures, between the deviation of the cooperativity index from unity and the properties of the ensemble of intermediate states. This result appears to be surprisingly absent in the literature so far, and it allows us to show how deviations from two-state behaviour do not simply depend on how much intermediate states are populated, but rather on the distribution of their energy values. Moreover, it shows that the calorimetric criterion is in principle a necessary and sufficient condition for a two-state process, contrary to previous claims. We discuss how the latter ones are due to a non correct characterization of the high temperature state, highlighting how the definition of the low temperature and high temperature states as "macroscopic" ensembles of microscopic states is taken into account within our result. In fact, experimental data provide "per se" only a little knowledge about the two ensembles, with the arbitrariness of ensemble definition leading to a corresponding arbitrariness in the value of the cooperativity index. Finally, we discuss the above ideas, and how the generalized cooperativity index can be used to characterize dynamical transitions, from cooperative to noncooperative behaviour, within a simple exactly solvable model of sequential folding.

Etienne Wamba

Title:Using a thin grey soliton to learn and impact the nonlinear dynamics of quantum systems **Abstract:** Grey solitons, which are a type of localized excitation characterized by a dip in a continuous wave, play an important role in nonlinear systems, particularly in optics, low- temperature physics and fluid dynamics. Despite the reduction in intensity, grey solitons maintain their shape and speed as they propagate, due to a delicate balance between nonlinear effects and dispersion. Such a speed is a measure of the grayness of the soliton, yielding dark solitons as a special case with zero speed. In this poster, using two examples, we show that a thin grey soliton can be used to change or learn about the dynamics of nonlinear systems. In the first example, taking the case of an ultracold quantum gas, we show that a grey soliton can allow us to track the breakdown of adiabaticity at different scales in a system that undergoes a strong ramp of interparticle interaction. The second example is devoted to an atomic cloud that is continuously bombarded by a well controlled electron beam.