WORKSHOP

TRANSPORT PHENOMENA AND FLUCTUATIONS IN SMALL COMPLEX SYSTEMS

December 11-15, 2023. Buenos Aires, Argentina

TALKS

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LOCATIONS

Centro Cultural de la Ciencia - CABA

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NONEQUILIBRIUM VISCOELASTIC DIFFUSION MODELED BY ACTIVE FRACTIONAL LANGEVIN EQUATIONS

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Author: Jae-Hyung Jeon (Pohang University of Science and Technology)

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TRANSITION PROBABILITIES IN DENSE PARTICLE SYSTEMS AT LOCAL THERMAL EQUILIBRIUM

Name: Hoyuelos Miguel
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MOLECULAR DYNAMICS STUDY OF THE MECHANICAL PROPERTIES OF DRUG DELIVERY SYSTEMS

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Abstract:
The rational design of drug nanocarriers for specific drugs is a very active area. It could be very useful t count with theoretical tools that help in this design. Moleculardynamics simulations (MD) is a powerfull potent tool to achieve a deeper understanding of these systems. The goal of this work is use carried out extensive MD simulations to calculate different properties of copolymer based nanoparticles, and in particular we aim to calculate the pressure profiles that determine the mechanical behavior of systems considered here at the molecular level, which represents valuable information when designing and characterizing polymersomes and micelles. Due to the system size, it is possible to access a small polymersome or a flat bilayer corresponding to it copolymer bilayer using coarse-grained model retaining enough detail to correctly reproduce the cooperative phenomena that occur at the mesoscale.

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STOCHASTIC RESETTING: SUBORDINATION APPROACH

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Abstract:
Theoretical modeling of various stochastic processes in complex media, such as continuous time random walks, diffusion on constrained comb-like structures, as well as stochastic processes with multiplicative Gaussian and dichotomic noise, under resetting will be presented. The renewal equation and the subordination approach will be employed to analyse the mean squared displacement and the probability density function. The transition to the non-equilibrium steady state reached in the long time limit will be studied in terms of the large deviation function. The analytical results obtained by solving the Fokker-Planck equation will be confirmed by numerical simulations within the Langevin equation approach. Some possible applications of the considered models will be presented, as well.

Acknowledgments: The author acknowledges financial support by the German Science Foundation (DFG, Grant No. ME 1535/12-1). The author was also supported by the Alexander von Humboldt Foundation.

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GRAVITY DRIVEN TRANSPORT OF FLEXIBLE FILAMENTS IN QUIESCENT VISCOUS FLUID

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CONVERGENCE AND EQUILIBRIUM IN MOLECULAR DYNAMICS SIMULATIONS

Name: General Ignacio J.
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Authors: Franco Ormeño (Instituto de Investigaciones Biotecnológicas - Universidad Nacional de San Martín)
Ignacio J. General (ECyT, ICIFI, UNSAM-CONICET)

Abstract:
Molecular dynamics is a powerful tool that has been long used for the simulation of proteins and other biomolecules. It complements experiments, by providing detailed information about the individual atomic motions. But there is an essential and often overlooked assumption that, left unchecked, could invalidate any results from it: is the time-length of the obtained trajectory long enough, so that the system reaches thermodynamic equilibrium, and the properties to be measured from it are converged? Previous studies show mixed results in relation to this assumption, some concluding that a specific system reached convergence in dynamics and structural properties, while some others

show the contrary. Here, we present a thorough analysis of tens to a hundred microseconds long trajectories, of several system with varying size, to probe the convergence of different structural, dynamical and cumulative properties, and elaborate on the relevance of the concept of equilibrium, and its physical and biological meaning. The results show convergence of properties with the most biological interest in multi-microsecond trajectories, although other properties--like transition rates to low probability conformations--may require more time.

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BUBBLES RISING IN A HELE SHAW CELL WITH PERIODIC CONSTRICTIONS

Name: Cachile Mario
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CRITICAL DYNAMICS OF NATURAL SWARMS

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Abstract:
Experiments on insect swarms in the field have found scale-free correlations of velocity fluctuations without global velocity order, thus suggesting an interpretation of swarms as critical systems, poised at the boundary between a phase with order in the velocities, and a disordered phase. Further experiments have found signs of dynamic criticality, with time correlations obeying dynamic scaling and critical slowing down, just as described for condensed matter systems by Halperin, Hohenberg and others in the 1970s. However, the dynamic critical exponent observed for natural swarms is different from the known exponents for the classical critical dynamic models, suggesting a new universality class for active critical systems. In this talk we will summarise these experimental results as well as the theoretical efforts to account for them. In particular we will stress that, although the active field theory of Toner and Tu leads to a critical exponent different from the classical ones, and closer to the experimental result, to account for the experimental results it is essential to include inertia and consider an under-damped active field theory.

TUESDAY

HETEROGENEOUS INTRACELLULAR DYNAMICS MODELED AS SWITCHING FRACTIONAL BROWNIAN MOTION

Name: Krapf Diego
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Author: Diego Krapf (Colorado State University, Fort Collins)

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ENSEMBLE SELF-REINFORCEMENT FOR THE ANOMALOUS TRANSPORT OF HETEROGENEOUS POPULATIONS

Name: Fedotov Sergei
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Author: Sergei Fedotov (The University of Manchester)

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A STUDY OF CALCIUM TRANSPORT IN CELLS REVEALS THE COMPLEXITY OF THE INTRACELLULAR MEDIUM

Name: Ponce Dawson Silvina
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TRANSPORT PHENOMENA AND MECHANICS IN 3D TISSUE MODEL APPLICATIONS

Name: Heinrich Doris
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Author: Doris Heinrich (Technische Universität Ilmenau, Germany - Institut für Bioprozess – und Analysenmesstechnik e.V. (iba), Heilbad Heiligenstadt, Germany)

Abstract:
3D tissue models have become an integral part of biomedical research. They adequately depict processes of cell orientation, cell differentiation and adaptation to stimuli. Using mathematical simulations, predictions can be made, for example, how tissue reacts to stimuli, how fluid microenvironments can be optimized and how digital twins can be used to optimize clinical therapies.
Using application-oriented research examples, studies of surface-triggered interaction between cells and surface structures in quasi 3D spaces, the use of 3D environments as a niche for tissue engineering with stem cells and their integration into microfluidic systems are presented, Further simulations e.g. of flow processes in medical and ecological applications, but also the use of AI are discussed.

WEDNESDAY

CRYO-COOL RIBOSOMES

Name: Grubmueller Helmut
Institution: Max-Plack Institute for Multidisciplinary Sciences, Department of Theoretical and Computational Biophysics, Göttingen

Authors: Lars V. Bock (Max-Plack Institute for Multidisciplinary Sciences, Department of Theoretical and Computational Biophysics, Göttingen)
Helmut Grubmuller (Max-Plack Institute for Multidisciplinary Sciences, Department of Theoretical and Computational Biophysics, Göttingen)

Abstract:
The recent resolution revolution in cryo-electron microscopy (cryo-EM) has revealed an unparalleled amount of new information about the structure as well as the structural heterogeneity and dynamics of many biomolecules and biomolecular complexes. How much of the ambient temperature ensemble of biomolecules is preserved during shock freezing prior to image acquisition is, however, an unsolved question. In shock cooling atomistic simulations of fully solvated ribosomes at realistic time scales we observed, depending on cooling rates, a marked decrease of structural heterogeneity. Small barriers between the states (<10 kJ/mol) are overcome during cooling and do not contribute to the heterogeneity of the structural ensemble obtained by cryo-EM, whereas conformational states separated by barriers above 10 kJ/mol are expected to be trapped during plunge-freezing. Our results will allow one to quantify the heterogeneity of biologically relevant room-temperature ensembles from cryo-EM structures.

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TRANSPORT AND FLUCTUATIONS IN A COMPOSITE BIOHYBRID SYSTEM – HOW AMOEBOID CELLS MOVE PASSIVE MICRO-CARGO

Name: Beta Carsten
Institution: Universität Potsdam

Author: Carsten Beta (Universität Potsdam)

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NON-EQUILIBRIUM STATISTICAL MECHANICS OF LASER-COOLED ATOMS

Name: Akimoto Takuma
Institution: Tokyo University of Science

Author: Takuma Akimoto (Tokyo University of Science)

Abstract:
Equilibrium statistical mechanics describes the velocity distribution of atoms confined by a heat bath with a constant temperature, i.e., Maxwell-Boltzmann distribution. In this talk, I will present the velocity distribution when atoms are cooled by a laser. In a subrecoil laser cooling, there is no steady state distribution in the velocity distribution. However, there exists an infinite invariant density in the velocity distribution for a stochastic model of subrecoil laser cooling. I will show that the infinite invariant density plays an important role in determining a transition of ergodic properties, where a new type of distributional limit theorem in infinite ergodic theory emerges.

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FIRST PASSAGE PROCESSES IN TIME-DEPENDENT ENVIRONMENTS

Name: Falcke Martin
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FLOCKING OF TWO UNFRIENDLY SPECIES: THE TWO-SPECIES VICSEK MODEL

Name: Rieger Heiko
Institution: Saarland University

Author: Heiko Rieger (Saarland University)

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INFLUENCE OF WATER TRANSPORT MECHANISMS ON THE SOLUBLE SOLIDS DISTRIBUTIONS AT PORE–SCALE DURING NON-ISOTHERMAL DRYING OF PDMS MICROMODELS

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Marco Guzmán-Meza (Food Engineering Department, Universidad del Bío-Bío, Chillán, Chile)
João Laurindo (Chemical and Food Engineering Department, Universidad Federal de Santa Catarina, Florianópolis, SC, Brasil)
Marcela Jarpa-Parra (Universidad Adventista de Chile, Chillán, Chile)
Diego Vasco (Mechanical Engineering Department, Universidad de Santiago de Chile, Estación Central, Santiago, Chile)

Abstract:
The non-isothermal drying of an aqueous sucrose solution in a polydimethylsiloxane (PDMS) micromodel that simulate plant-based food tissue was studied experimentally. The aim of this study was to determine influence of water transport mechanisms on the soluble solids distributions at pore–level during non-isothermal drying. PDMS micromodels were built through a modified photolithographic technique. The built micromodels were impregnated with aqueous sucrose-pyranine solutions, and were placed over an analytical balance illuminated with ultraviolet light. The temperature, velocity and relative humidity of the drying air were 60 °C, 4.5 ms-1, and 10%, respectively. The morphology of drying fronts displayed a hierarchical behavior and the largest diameter throats dried first. Two kind of soluble solids distributions at pore-level were observed, external and internal distributions. The liquid water transport mechanism dragged soluble solids towards the open side of porous medium, producing the external deposition. Then, when the hydraulic conductivity of the porous medium was interrupted, the evaporation allowed the internal deposition of soluble solids. PDMS micromodels could be applied to study several processes that involve both the mass and heat transfer in plant-based food tissue.

Key words: drying, PDMS micromodels, pore-scale approach, vegetable microstructure.

Acknowledgements: The authors would like to acknowledge the Fondecyt 1201520 project of the National Research and Development Agency of Chile (ANID).

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DIFFUSIVE TRANSPORT ON THE NANOSCALE

Name: Smith Ana-Suncana
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HEAT FLOW THROUGH A LIQUID-VAPOR INTERFACE IN A NANO-CHANNEL: THE EFFECT OF END-GRAFTING POLYMERS ON A WALL

Name: Pastorino Claudio
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NEAR-FIELD HEAT TRANSFER BETWEEN POLAR MATERIALS CLOSE TO THE CONTACT AND IN NON RECIPROCAL MANY-BODY SYSTEMS

Name: Ben-Abdallah Philippe
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SIMULATION OF REACTIVE MULTIPHASE FLOWS IN CONFINEMENT

Name: Harting Jens
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ANALYSIS OF ENTROPY GENERATION FOR OPTIMIZING MICROCHANNEL HEAT SINKS

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Abstract:
In the present work, the optimal height of mini-channels and microchannels is determined by minimizing the entropy generation by performing CFD numerical simulations. The laminar flow of water and 0.1 wt% silver-decorated reduced graphene oxide nanofluids (rGO-Ag) has been studied using rectangular channels of eight heights with two different heat fluxes at the bottom wall (10,000 W/m2 and 50,000 W/m2). The numerical results allowed determining that there is no optimum height since it depends on the heat flux to be dissipated, with the channels of lower height the most effective for higher heat fluxes, while those of intermediate height become more efficient by dissipating a lower heat flux. In addition, the thermal and frictional entropy generation results of the channels are compared using an rGO-Ag nanofluid and water as working fluids. The numerical results are validated experimentally, analyzing the optimal channels fabricated by 3D printing. With the experimental work, it is possible to validate the numerical results presented for two microchannels (MCH-2 and MCH-3) and one minichannel (MNC-1), obtaining percentage differences of less than 20%.

Acknowledgment: The authors would like to express their gratitude for the financial support of the project USACH Dicyt Asociativo 052216VC_DAS.

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MECHANICAL PROPERTIES OF MITOCHONDRIA IN LIVING CELLS

Name: Bruno Luciana
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FROM EXPERIMENTS TO MODEL AND BACK: ACTIVITY FLOW IN THE APOPTOTIC NETWORK

Name: Grecco Hernán E.
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Abstract:
Apoptosis, a form of programmed cell death central to all multicellular organisms, plays a key role during organism development and is often misregulated in cancer. Devising a single model applicable to distinct stimuli and conditions has been limited by lack of robust observables. Indeed, previous numerical models have been tailored to fit experimental datasets in restricted scenarios, failing to predict response to different stimuli. Using an anisotropy based FRET sensor array, we obtained a comprehensive dataset in which the activity of three caspases simultaneously upon intrinsic or extrinsic stimulation. We modeled the time between maximum activity of intrinsic, extrinsic and effector caspases, a robust observable of network dynamics, to create the first integrated Apoptotic Reaction Model (ARM). Observing how effector caspases reach maximum activity first irrespective of stimuli used, led us to identify and incorporate a missing feedback into a successful model for extrinsic stimulation. By simulating different recently performed experiments, we corroborated that ARM adequately describes them. This integrated model provides further insight into the indispensable feedback from effector caspase to initiator caspases.

FRIDAY

CROWDING RELIEVES BI-DIRECTIONAL CLOGGING IN NUCLEAR PORE COMPLEX TRANSPOT

Name: Zilman Anton
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MODELING OF THE NON-DEBYE RELAXATION PROCESSES IN SYSTEMS OF POLAR MOLECULES

Name: Petreska Irina
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Author: Irina Petreska (Ss. Cyril and Methodius University in Skopje, Faculty of Natural Sciences and Mathematics - Institute of Physics, Skopje, Macedonia)

Abstract:
The focus of the talk will be on modeling of the non-Debye relaxation in a medium composed of polar molecules. Being motivated by our previous studies of the torsional stochastic switching at a single molecule level, we will discuss the possibilities to employ the rotational diffusion equation with a generalised memory kernel in the context of dielectric relaxation processes in a bulk molecular system. We will show that depending on the choice of the memory kernel, Debye and non-Debye relaxation can be comprised in one model. The autocorrelation function and the complex susceptibility, obtained via the probability density function will be analysed in detail. A special attention will be paid to a three-parameter memory kernel, which simultaneously incorporates the interplay between Debye and Cole–Cole relaxation processes. In real-life examples, especially where rotational degrees of freedom of organic molecules are of interest, it is most likely that the complexity of the system is manifested in its response to external stimuli through the presence of clusters with different inherent properties. Therefore, the combined three-parameter memory kernel enables to account for both distinct types of dielectric relaxation, Debye and Cole–Cole, at the same time. In the summary of the talk, we will comment on the interplay between the intramolecular torsional degrees of freedom as one of the sources of the thermally induced fluctuations and the dielectric relaxation of a bulk system of rigid rotators.

Acknowledgement: This work was supported by the German Science Foundation (DFG, Grant number ME 1535/12-1).

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THERMAL RELAXATION ASYMMETRY IN REVERSIBLE AND DRIVEN SYSTEMS

Name: Godec Aljaz
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IS BEING HETEROGENEOUS ADVANTAGEOUS OR DISADVANTAGEOUS?

Name: Baldovin Fulvio
Institution: Università di Padova

Author: Fulvio Baldovin (Università di Padova)

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ACTIVE OSCILLATORS

Name: Frydel Derek
Institution: Federico Santa Maria Technical University

Author: Derek Frydel (Federico Santa Maria Technical University)

Abstract:
An ideal gas of active particles in a harmonic potential is a non-trivial mathematical problem. The talk will explore different ways of obtaining analytical expressions for this system. A general method is then developed based on the transformation of the Fokker-Planck equation into a recurrence relation for generating moments of a stationary distribution. The stationary distributions are then recovered from those moments. The suggested approach is valid for all canonical models of active particles and for any system dimension.

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ENTROPY PRODUCTION IN SYSTEMS DRIVEN BY NEAR-FIELD THERMAL RADIATION

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M. Florencia Carusela (Instituto de Ciencias, Univesidad Nacional de General Sarmiento, Buenos Aires, Argentina)
Alejandro G. Monastra (Instituto de Ciencias, Univesidad Nacional de General Sarmiento, Buenos Aires, Argentina)

Abstract:
Energy and entropy balances are studied in many-body systems exchanging heat through thermal radiation. We consider local thermal equilibrium conditions in which each body has its own temperature and acts as a source of thermal radiation. In addition, we analyze situations including semiconductors biased by the action of an external voltage, for which the emitted photons can acquire a nonvanishing chemical potential. This allows us to describe systems that exploit electroluminescence to control the radiative heat exchange between its components. To quantify dissipation in the bodies, the irreversible entropy production can be identified from energy and entropy balances in general scenarios. This approach is particularly useful for studying near-field radiative energy converters and heat pumps, as the entropy production provides valuable information about the device's performance.
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THERMAL MONITORING IN MICROCHANNELS

Name: Freytes Mariana
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Author: Mariana Freytes (Grupo de Medios Porosos, FIUBA, UBA)

Abstract:
The development of technologies to enhance the thermal management performance of electronic architectures is a topic of particular interest in the industry. There is currently a growing focus on research and development in the field of chip-level thermal management, driven by increasing power and, size reduction of electronic systems. Microfluidic devices emerge as a solution to this problem because the reduction in hydraulic diameter increases the surface area per flow volume unit, leading to an improvement in the heat transfer coefficient. The analysis of potential architectures should include some basic factors, defining optimal materials and geometries for microdevice structures. The study of thermal monitoring schemas in the devices is also crucial. We present a basic discussion of microfluidic devices as heat exchangers and will explore the feasibility of different thermal monitoring systems on these platforms, with a particular focus on fluorescence-based systems for mapping temperature variations within a microchannel.