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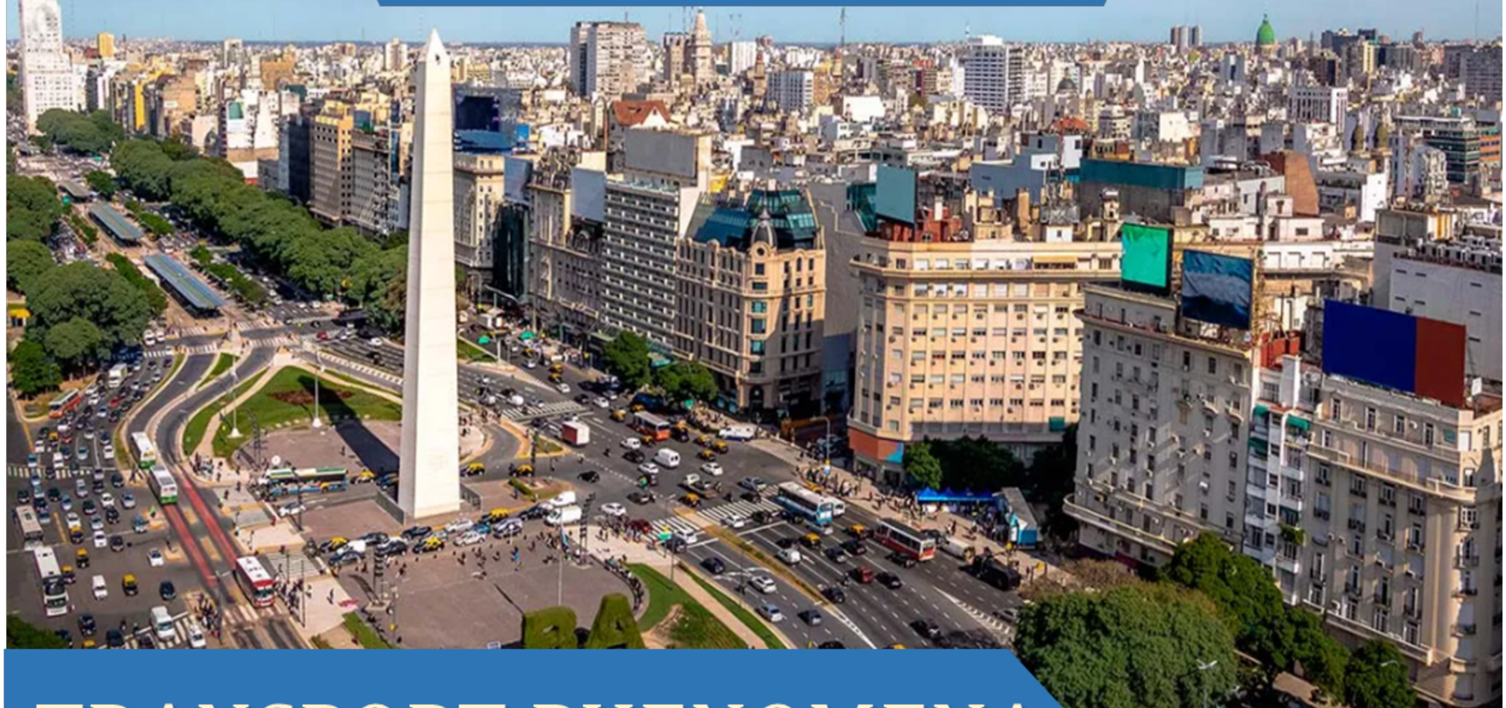

TRANSPORT PHENOMENA AND FLUCTUATIONS IN SMALL COMPLEX SYSTEMS

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MORPHOLOGICAL FLUCTUATIONS AND MECHANICAL PROPERTIES OF MITOCHONDRIA IN LIVING CELLS

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Abstract:
Mitochondria are dynamic organelles. They undergo changes in shape and size as a result of different processes, like fusion/fission events, transport, mechanical forces, and signaling cascades, which altogether affect their functionality. Molecular motors and the cytoskeleton play key roles in the structure, organization, and function of the mitochondrial network. Using confocal microscopy images of mitochondria in live Xenopus laevis melanophore cells, we analyze and characterize these different aspects of the chondriome and then build biophysical models of these organelles that can explain their behavior.

First, we studied the transport of mitochondria along microtubules to explore the performance of the different motor teams responsible for retrograde and anterograde transport. In order to do this, we tracked individual rod-like mitochondria and recovered their trajectory. By calculating the size of the organelle along the trajectory, we verified that they retract during retrograde transport, whereas they maintain their size during anterograde transport1. This suggests that the molecular motor teams have a different mechanism of action. These results were interpreted using a one-dimensional stochastic numerical model that considers the action of motors anchored to different regions of a flexible organelle2.

Second, we investigated how the integrity of the cytoskeleton affects the cellular organization, morphology and motility of mitochondria3,4. We performed several cell treatments that selectively affect different networks of the cytoskeleton (microtubules, F-actin and vimentin filaments). We observed that the distribution and orientation of mitochondria depend mainly on microtubules, which also favor more elongated organelles. In contrast, vimentin and actin filaments have a greater effect on mitochondrial curvature. In addition, we found that microtubules transmit their jittering to the organelles, whereas actin restricts their mobility. These results imply that there is mechanical interaction between the cytoskeleton and mitochondria, affecting their shape and movement.

Finally, we used a numerical worm-like chain model to simulate the behavior of a filamentous mitochondrion, assuming that it is immersed in a viscous medium and in the presence of thermal noise. To understand how forces affect the evolution of the organelle shapes, external forces are applied at different points of the filament with random direction and duration. Preliminary analyses show that the simulated mitochondria require the action of active forces to exhibit behaviors similar to those observed in living cell mitochondria.

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2. Intracellular motor-driven transport of rod-like smooth organelles along microtubules. A. B. Fernández Casafuz, M. C. De Rossi and L. Bruno. Physical Review E 101, 062416 (2020)

3. Morphological fluctuations of individual mitochondria in living cells. A. B. Fernández Casafuz, M. C. De Rossi and L. Bruno. Journal of Physics: Condensed Matter. 34 094005 (2021)
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THERMAL RECORDING IN MICROCHANNELS

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Abstract:
In this work we present tests on microfluidic platforms to study heat transport and thermal monitoring of the devices. We use microfluidic devices in PDMS with copper inserts and thermistors as control points. Copper inserts, connected to a current source, allow modeling thermal processes in electronic systems. The variation in the applied current generates different temperature conditions, as well as the variation in the fluid flow properties in the microchannel (mainly flow variation) generates different heat transport conditions. In order to monitor the process, we worked with fluorescence techniques, in particular we worked with rhodamine B solutions, whose fluorescence is highly dependent on temperature. The emission of a line generator laser, with a frequency of 532 nm, was focused on the microchannels of the devices to be studied and through which the rhodamine B solution flows, which when excited by the laser emits fluorescence and whose intensity is a function of the temperature of the fluid sample. Intensity levels were recorded with a high sensitivity camera. Recording the fluorescence intensity gives a very precise record of the temperature map in the microchannels. An image analysis was carried out by determining temperature profiles along the channel for different values of applied current and for different flow rates of the conveying fluid. The fluorescence intensity was calibrated at control points with NTC-type thermistors inserted for this purpose into the device. In order to keep the ambient temperature controlled, a Peltier cell was coupled to the system, simultaneously recording the response of the thermistors, the fluorescence intensity, the current applied to the copper insert, the ambient temperature outside the device and the flow rate. The images were contrasted with results obtained through simulations using the finite volume technique in the "NEP &TP group of the Institute of Sciences - UNGS" replicating the same characteristics and operating conditions of the microfluidic device, which allowed obtaining a detailed thermal mapping of the walls. of the channel and the heat flow exchanged in them. The studies performed in this work show that fluorescence thermometry has clear potential for temperature measurements and mapping in microfluidic devices that can optimize thermal transfer capabilities.

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THE CONNECTION BETWEEN SECOND-ORDER MEMORY KERNEL IN VISCOELASTIC MEDIA AND NORMAL OR ANOMALOUS DIFFUSION BEHAVIOR

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Abstract:
We present a simple criterion based on the Einstein relation for determining whether diffusion in systems governed by a generalized Langevin equation with long-range second-order memory is normal ,superdiffusive, or subdiffusive. Also we derive the asymptotic behavior of the velocity autocorrelation function in terms of the asymptotic behavior of the second-order memory kernel. We support our analysis with the application of our results in the relevant case of the Mittag-Lefller noise.

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ON COHERENT STATES DESCRIPTION OF EXCITON SYSTEMS: NLSE EQUATIONS AND HYDRODYNAMICS

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Abstract:
The exciton system is described by means of specially constructed coherent states (CS), according to an idea of L.V. Keldysh long ago. The system is analyzed from the geometric point of view and from the relevant symmetry group contained in the displacement operator as generador of the CS system in the Klauder-Perelomov sense. Explicitly important quantities involving the quantum statistics of the system (partition function, mean density n and the Yuen limit) are calculated and briefly discussed in relation to the known case of pure bosons (e.g. photons). The Bogoliubov type transformations for the field operators of the Wannier-Mott type exciton system are presented in an exact way (in sharp contrast with other proposals where only a rough approximation was given) showing how these transformations induce non linearity (cubic at first order) in the Schrodinger equation of the system. The conditions for a hydrodynamic description of the original Keldysh model, as the possibility of a BEC (Bose-Einstein Condensation), are discussed.

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EXPLORING THE DEPTHS OF PINUS RADIATA WOOD: A JOURNEY OF MORPHOLOGICAL AND MECHANICAL DISCOVERY THROUGH VACUUM IMPREGNATION WITH PHASE CHANGE MATERIALS

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Abstract:
Wood impregnation with phase change materials (PCM) is a process that may be used in the timber industry to enhance the thermal properties in applications such as temperature regulation, energy savings, and structural improvement of wood. We believe that including PCM in the porous structure of Pinus radiata wood will stabilize and enhance its mechanical properties for use as a building material. For this reason, the project focused on (a) Analyzing the mechanical properties of wood, examining the variation in Young's modulus in samples of 140 mm x 9 mm x 8 mm, previously dried at 103 ±2 °C, before and after the impregnation process with oleic acid and octadecane, using the pulse excitation technique. (b) Analyzing the effect of vacuum pressure, temperature, and the type of PCM on impregnation capacity. In the latter point, emphasis was placed on the morphological properties of wood, such as porosity, and transport properties, such as linear permeability (which quantifies the ease with which fluids flow along the longitudinal axis of wood cells and fibers) and tangential permeability (a parameter that quantifies fluid flow in the direction perpendicular to the growth rings), which were correlated with the impregnation ratio through a Pearson correlation. Regarding the mechanical properties, the percentage variation of Young's modulus ranged from 6.19% to 29.99%, which was notably higher in wood subjected to higher impregnation pressure and longer PCM process duration. In other words, there is a proportional relationship between pressure and impregnation time, which are fundamental variables in the process. As for the impregnation variables, the study found that the impregnation percentage ranged from 18% to 80%, with higher values in samples with higher average porosity. It depended solely on the difference in applied vacuum pressure for both PCM substances. This highlights the critical role of wood pore structure in the impregnation process. In this regard, from a structural and PCM transport perspective through wood, the number of tracheids per cm2 was correlated with the impregnation ratio through a Pearson correlation. The correlation coefficient was 0.17162, indicating a weak correlation between these variables. This shows that as the number of tracheids per cm2 increases, the proportion of impregnated PCM increases slightly. In contrast, for the relationship between the number of pits and the impregnation ratio, the coefficient was -0.49105, indicating a moderate negative correlation. This shows that fewer pits result in a higher proportion of impregnated PCM. As for the relationship between linear permeability and the impregnation ratio, the coefficient was -0.024092, indicating a very weak negative correlation, suggesting that linear permeability does not significantly influence impregnation. In contrast, the tangential permeability, with a coefficient of -0.41704, indicates that lower tangential permeability results in higher PCM impregnation.

Acknowledgment: The authors would like to express their gratitude for the financial support of the project ANID/Chile Fondecyt 1201520.

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MAGNETIC STRATEGIES FOR NON-MAGNETIC PARTICLE CONTROL IN SURFACE AND MICROCHANNEL ENVIRONMENTS

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Abstract:
Our investigation explores the domain of magnetic particle behavior in aqueous environments when subjected to external excitations. It examines the dynamics and self-organization of these systems, particularly in response to time-dependent excitations, which have profound implications in both fundamental physics and practical applications.

To explore this domain, the study adopts an innovative method, utilizing three Helmholtz coils to create elliptically polarized magnetic fields. These fields are harnessed to manipulate micrometer-sized nickel and iron particles positioned at the base of a container filled with an aqueous medium. An analysis of video-microscopy images is conducted to scrutinize the time-dependent displacement patterns of these particles.
We observed the emergence of chain structures referred to as 'rollers.' These formations exhibit controllable movement along the vessel's bottom plane in response to the applied magnetic field. Moreover, the introduction of glass microspheres into the system induces motion due to the displacement and drag exerted by these magnetic structures. This phenomenon opens up new avenues for particle manipulation. We demonstrates successful control of the movement of glass beads within these microchannels, presenting exciting prospects for targeted cargo delivery using this effective magnetic approach.

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CHARACTERIZATION OF THE DYNAMICS OF A VERTICAL JET IN THE PRESENCE OF A GRANULAR BED

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Abstract:
In this work, the behavior of fluid flow in a model fracture in the presence of a layer of grains of initial height hg, is analyzed. A vertical jet is injected, with flow rate Q, at the bottom of a square Hele Shaw cell of width L, through an orifice of width a ($a \ll L$) and presents the structure of a hydrodynamic jet altered by lateral confinement. The cell is partially filled with glass beads (grains) with mean diameter d = 1 mm up to an initial height hg and with water up to an initial height hw (with hw > hg). As hw < L the system has a free surface which is disturbed from below by the jet.
In the absence of grains (hg = 0) and a certain lateral confinement L, the jet oscillates laterally in a certain range of values of Q and hw. The amplitude and frequency of the longitudinal oscillation of the jet were analyzed as a function of Q and hw. A strong correlation was observed with the frequency of the odd modes of the transverse oscillations of the free fluid surface (analogous to the so-called sloshing oscillations for a rectangular box).
In the presence of grains (hg > 0), the granular bed becomes fluidized above a critical flow rate Qc, which depends on hg, and the jet presents longitudinal oscillations. For supercritical flows, the oscillatory dynamics of the jet was analyzed by studying the oscillation frequency as a function of the control parameters hw, hg and Q and results are also compared to those obtained without grains.

Financial support: UBACyT Project subsidy (20020170100697BA, "Fluidización de lechos granulares en recintos confinados")

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CHARACTERIZATION OF CALCIUM SIGNALS IN NORMAL AND TUMOR CELLS IN RESPONSE TO PHYSICAL/CHEMICAL MODIFICATIONS OF THE MICROENVIRONMENT

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Abstract:
Cellular calcium signals are ubiquitous and involved in numerous physiological processes in various cell types. Cytosolic free calcium concentration affects different signaling cascades1. The present work focuses on the study of calcium (Ca2+) signals in response to physicochemical modifications of the microenvironment. Normal (MCF10A) and tumor-derived (MCF-7) human mammary epithelial cells were used which respond to mechanical stimuli under normal physiological conditions2. Changes in cytoplasmic calcium were visualized in the confocal microscope using the fluorescent sensor Fluo-43, a plasma membrane-permeable fluorophore that increases its fluorescence intensity by binding Ca2+. The response of cytosolic Ca2+ in normal and tumor cells was analyzed in response to variations in extracellular Ca2+ concentration. We also studied the intercellular calcium waves generated by a scratch on a monolayer of normal or tumor cells using a glass microcapillary. These strategies allowed us to contrast the calcium signals generated by normal and tumor cells in response to different stimuli in their environment. The effect of increasing extracellular calcium resulted in an increase of cytoplasmic calcium, where the MCF10A cells responded faster than MCF-7 cells. Furthermore, the intracellular calcium wave generated in MCF10 propagates faster than in MCF7 monolayer.

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EVALUACIÓN COMPUTACIONAL DE LAS INTERACCIONES ACE2-SPIKE EN DIFERENTES ANIMALES Y EL ROL COMO HOSPEDADORES INTERMEDIOS EN LA TRANSMISIÓN DEL SARS-COV-2 A HUMANOS

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Abstract:
El SARS-CoV-2 es el agente patógeno que causa la enfermedad de COVID-19, se estima que este virus tuvo un origen animal y que saltó a la población humana (Zhou et al., 2020). No obstante, aún no se ha establecido ni la fuente exacta del SARS-CoV-2 ni la ruta de introducción en la población humana, ni se confirmaron los hospedadores intermedios (Li et al., 2020; Hobbs et al., 2021). Distintos tipos de estudios han demostrado que el SARS-CoV-2 mediante la proteína Spike se une a la enzima convertidora de angiotensina tipo 2 (ACE2), con lo cual se postula como la principal vía de entrada del virus (Low-Gan et al., 2021). Si bien se han logrado avances todavía hay mucha incertidumbre en el mecanismo de acción del SARS-CoV-2, por lo tanto en este trabajo presentamos un análisis sistemático basado en extensas simulaciones de dinámica molecular para estudiar a nivel atómico y molecular los factores que determinan la eficiencia de interacción entre la proteína Spike, a través del dominio de unión al receptor RBD, de una cepa de SARS-CoV-2 (wild-type) y la proteína ACE2 de diferentes especies que son gato, perro, cerdo, hurón, pato y gallina. El análisis

se centro en las interacciones no covalentes entre estás proteínas, y de este modo identificamos los aminoácidos clave que interactúan en la formación del complejo ACE2/RBD, lo cual aporta otro enfoque para entender diferencias de susceptibilidad que podrían ayudar tanto a reconocer potenciales huéspedes del SARS-CoV-2, como también a explicar porque diferentes poblaciones humanas exhiben diferentes susceptibilidades.

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MOLECULAR DYNAMICS SIMULATIONS OF T. CRUZI'S ALDO-KETO REDUCTASE: ANALYZING AGGREGATION AND LIGAND INTERACTIONS

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Abstract:

Disease is a tropical illness, considered by the World Health Organization as one of the major neglected diseases. It is caused by the protozoan Trypanosoma cruzi and affects more than 8 million people worldwide. The enzyme Aldo-Keto reductase of T. cruzi (TcAKR) is a biologically relevant target due to its potential involvement in the activation of trypanocidal drugs. Experimental kinetic studies have shown that TcAKR exhibits both aldo-keto reductase (AKR) and quinone reductase (QOR) activities, with hyperbolic and sigmoidal kinetics, respectively. In line with the sigmoidal kinetics and some experimental techniques, we have proposed that TcAKR can form oligomers. However, the literature does not provide a clear understanding of TcAKR aggregation or its physiological role. In this context, our objective was to characterize the aggregation and stability of TcAKR's multimeric forms at an atomic and molecular level using computational molecular dynamics (MD) simulations. We discovered that TcAKR molecules are stable in dimeric forms and can also form stable supramolecular structures. In the case of supramolecular arrangements, we found a central monomer interacting with three neighboring monomers as the preferred motif. Additionally, we conducted an exhaustive

exploration of TcAKR's interaction with the substrates 4-Nitrobenzaldehyde (a typical substrate for AKRs) and Benznidazole (the primary therapeutic drug). Preliminary analysis of the molecular dynamics simulations allowed us to identify a second binding site. This finding is intriguing because the atomic and molecular interaction mechanism of trypanocidal drugs with TcAKR is currently unknown. Furthermore, the presence of an additional binding site may open up new possibilities for exploring new ligands that can appropriately modulate the activity of trypanocidal drugs in the chronic state,

Keywords: Chagas disease supramolecular structure molecular dynamics, T. cruzi.

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MODELING SULFATE-REDUCING BIOFILM GROWTH AND CORROSION UNDER THE VARIATION OF ORGANIC MATTER: A HYBRID DIFFERENTIAL-DISCRETE APPROACH

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Abstract:

Microbiologically influenced corrosion (MIC) is estimated to account for 20% of total corrosion damage. Since sulfate is present in many environments, biofilms formed by sulfate anaerobic reducing bacteria (SRB) are responsible for MIC. In oilfield water flood systems, SRB cause the largest number of recorded instances of corrosion problems.

Current risk-factor probability models are useful for predicting the likelihood of MIC. However, a reliable prediction of the progression of MIC pitting and the subsequent changes between sessile (biofilms) and planktonic (motile) bacterial populations under different nutritional conditions observed in the oil field has not been reported. Most models only utilize a specific strain of bacteria to simulate corrosion. To reflect the realistic environmental conditions observed in the oil field, it is necessary to consider a complex environment with hundreds of microorganisms. This work presents an experimental and theoretical approach to obtaining the empirical biological parameters of a consortium of SRB, aiming to achieve this desired complexity.

A mathematical model was developed in this study to investigate the interactions between SRB biofilms and a metallic surface under different nutritional conditions (variation of organic matter) for a 21-day period. The experimental conditions mentioned above were carried out to collect corrosion test data for model calibration. Lactate consumption (organic matter) or iron as electron donors, and sulfate as the electron acceptor were considered as SRB metabolism. The distribution and consumption of organic matter, sulfate, and bacterial growth were based on Fick's Law and the Monod equation. A growth limitation hypothesis was implemented by deactivating the duplication of sessile cells once a growth threshold was reached and by reducing the metabolic rate inversely related to the distance from the metallic surface. The model was developed using the free programming language Python, employing a hybrid differential-discrete approach. The output of the model accurately predicted parameters such as colonization, growth of sessile and planktonic populations, consumption of sulfate, and corrosion of the steel surface. Computer simulations indicated that under the set conditions, the presence of organic matter favored the free-living planktonic state over the biofilm state (sessile), in contrast to the prediction for starvation conditions where planktonic bacteria are not favored. While the corrosion rate increased significantly in the presence of organic materials, the maximum pit depths calculated by the model did not indicate any significant changes across nutritional circumstances.

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