4th International Workshop on
Complex Physical Phenomena in Materials

HOTEL ARMAÇÃO - Porto de Galinhas - PE, Brazil, February 22-25, 2016

The general scope of the workshop: Scientific talks and posters on flow and dynamics of soft and complex matter, such as multi-component complex fluids, drops, emulsions and nano-fluids, in microfluidic laboratory or environmental settings. The relation between macroscopic flow patterns and underlying structures at smaller scales will be in focus. The topics are in particular relevant for energy and environment related applications such as natural fluid flow or oil-recovery including EOR.

Confirmed speakers:
Anderson S. L. Gomes (UFPE - Recife, Brazil)
Antonio Azevedo (UFPE - Recife, Brazil)
Antonio Murilo S. Macedo (UFPE - Recife, Brazil)
Aurora Pérez Gramatges (PUC - Rio de Janeiro, Brazil)
Caetano R. Miranda (Univ. Sao Paulo, Brazil)
Fernando Oliveira (Univ. Brasilia - UnB, Brazil)
Koiti Araki (Univ. Sao Paulo, Brazil)
Luca Moriconi (UFRJ - Rio de Janeiro, Brazil)
Marcio Carvalho (PUC - Rio de Janeiro, Brazil)
Maria Moura (PUC - Rio de Janeiro, Brazil)
Paulo Roberto de Souza Mendes (PUC-Rio de Janeiro, Brazil)
Peter William Bryant (IBM - Rio de Janeiro, Brazil)
Sergio Lira (UFAL - Maceio, Brazil)
Thereza A. Soares (UFPE - Recife, Brazil)
Heloisa Bordallo (Univ. Copenhagen, Denmark)
Francoise Brochard (Inst. Curie, Paris, France)
Patrick Tabeling (ESPCI-ParisTech/IPPG, Paris, France)
Josef Breu (Bayreuth Univ., Germany)
Andreas Carlson (Univ. Oslo, Norway)
Arne Skjeltorp (Inst. for Energy Tech./Univ. Oslo/GiaMag Technologies, Norway)
Paul Dommersnes (NTNU - Trondheim, Norway)
Rita de Sousa Dias (NTNU - Trondheim, Norway)
Erik Luijten (Northwestern Univ., USA)
Henri van Damme (MIT, USA)
Irep Gozen (Harvard Univ. USA)
Xiang Cheng (Univ. Minnesota, USA)

Organizers:
Jon Otto Fossum (NTNU - Trondheim, Norway)
Kenneth D. Knudsen (Inst. for Energy Tech., Norway)
Giovani Vasconcelos (UFPE - Recife, Brazil)
Romulo Tenorio (CNEN/CRCN - Recife, Brazil)
Wilson Barros (UFPE - Recife, Brazil)

Practical information to participants: The 4 day workshop starting at 3:15 pm on Monday February 22nd 2016, and ending at 1 pm on Thursday February 25th 2016, takes place in Hotel Armacao, at the beach in the beautiful village of Porto de Galinhas which is located about 50 km south of Recife, Brazil. (www.hotelarmacao.com.br). Flights directly to Recife from Europe are most easily done by airline TAP via Lisboa, or directly from USA by American Airlines via Miami. Recife may be also be reached from Europe or USA or other locations via several alternative routes.

For further information about the workshop, and for submissions of contributions, contact Jon Otto Fossum at: jon.fossum@ntnu.no. Registration deadline for submission of contributed abstracts is February 8, 2016. Submissions must include title + coauthors/affiliations + ½ page abstract, and wish for oral or poster presentation.

SIU-UTFORSK: «Soft and Complex Matter»

Departamento de Física UFPE

RCN Petromaks2 ISP: «Particle stabilized emulsions for EOR»

Abstracts

4th International Workshop on

Complex Physical Phenomena in Materials

Hotel Armação, Porto de Galinhas, PE, Brazil,
February 22 - 25, 2016

Foreword

Welcome to the **4th International Workshop on "Complex Physical Phenomena in Materials**" at Hotel Armação, Porto de Galinhas - PE, Brazil, February 22- 25, 2016. This workshop is the fourth in a series of workshops organized as follows:

The *1st International Workshop on "Complex Physical Phenomena in Materials"* in Recife, December 14-17, 2010, and organized by Prof. Mario Engelsberg, from the Physics Department of UFPE, Recife, Brazil, together with Prof. Jon Otto Fossum from the Department of Physics at NTNU, Trondheim, Norway, grew out of good and productive scientific collaborations. As it turned out, that first Workshop went well beyond the context of this bilateral collaboration and served as a venue for discussions on a wider range of complex phenomena in materials.

The *2nd International Workshop on "Complex Physical Phenomena in Materials"* in Porto de Galinhas, PE, January 31 - February 3, 2012, was organized by Prof. Giovani Vasconcelos from the Physics Department of UFPE, Recife, Brazil, together with Prof. Jon Otto Fossum from the Department of Physics at NTNU, Trondheim, Norway. In the second Workshop, we tried to follow the same guiding principles as for the first one. We also tried to expand its scope not only with respect to the scientific contributions themselves but also including a roundtable session to discuss the translation of academic research within complex matter physics into industrial applications.

The *3rd International Workshop on "Complex Physical Phenomena in Materials"* at Pontificia Universidade Católica do Rio de Janeiro (PUC-Rio), Brazil, February 17-22, 2014, was organized by Prof. Marcio Carvalho from the Department of Mechanical Engineering at PUC-Rio together with Prof. Jon Otto Fossum, from the Department of Physics at NTNU, Trondheim, Norway. The third workshop expanded the scope even further. In addition to being a regular workshop, it was also made into the intensive lecture part of a school for MSc/PhD students, as part of a "package" which also included MSc/PhD level short courses on MRI (Wilson Barros, UFPE, and Daniel Bonn, Univ. Amsterdam) and on Finite Element Methods (Marcio Carvalho, PUC-Rio). The lectures and short courses in Rio de Janeiro were followed by student distance training via Skype, so that the total package (workshop including 2 short courses + distance training) constituted a workload for the students corresponding to 7.5 CTS, and formalized through a regular registered course called FY8203 "Soft Condensed Matter" at NTNU.

The present *4th International Workshop on Complex Physical Phenomena in Materials* follows the scope of the student training defined in the third workshop (workshop + distance training), and the participating registered MSc/PhD students will receive 7.5 ESCTS through the NTNU course FY8203 "Soft Matter Physics". The success of the three previous workshops was a clear evidence of the importance of having meetings that promote interactions between scientists from (seemingly) different fields and from different working environments (universities, research institutes, and industry research centers). In this 4th Workshop, the central overall topic is on soft and complex matter phenomena in materials and related phenomena and methods. In particular we will have a focus on physical phenomena underlying (Improved) Oil Recovery ((I)OR), such as the physics of flow of complex fluids in confined and complex environments (e.g. the physics of drops, emulsions, foams, granular systems, porous structures, micro-channels and micro-fluidics).

This fourth workshop is made possible due to grants from the Norwegian agencies RCN (Research Council of Norway) - Petromaks2 Program, and SIU-UTFORSK, as well as from the Graduate Program and the Department of Physics at UFPE. We gratefully thank all our sponsors.

The last sentence of the Foreword to the Book of Abstracts of the 1st Workshop in Recife in 2010 stated: "*We hope that this is not the last workshop of its kind*." It turned out not to be the last, and we are already working towards securing funding for the 5th workshop to be held in 2018.

Welcome to Porto de Galinhas

Romulo Tenorio (CNEN/CRCN, Recife, Brazil)
Giovani Vasconcelos (UFPE, Recife Brazil)
Jon Otto Fossum (NTNU, Trondheim, Norway)

Workshop Program

4th International Workshop on "Complex Physical Phenomena in Materials"
Hotel Armação, Porto de Galinhas, PE-Brazil February 22-25, 2016.

	Sunday	Monday	Tuesday	Wednesday	Thursday	
	21/2 2016	22/2 2016	23/2 2016	24/2 2016	25/2 2016	
0900-0930			**Josef** Breu	**Henri** van Damme	**Marcio** Carvalho	**0900-0930**
0930-1000			**Koiti** Araki	**Andreas** Carlson	**Paulo** R. de Souza Mendes	**0930-1000**
1000-1030			**Rita** Dias	**Xiang** Cheng	**Heloisa** Bordallo	**1000-1030**
1030-1100			Coffee Break	Coffee Break	**Caetano** R. Miranda	**1030-1100**
1100-1130		Arrival of participants	**Aurora** Pérez-Gramatges	**Patrick** Tabeling	**Jon Otto 5 min Closing**	**1100-1130**
1130-1200			**Peter** W. Bryant	**Maria** J. B. Moura		**1130-1200**
1200-1300			Lunch	Lunch	Lunch	**1200-1300**
1300-1430			Discussions	Discussions		**1300-1430**
1430-1515		**Registration**				**1430-1515**
1515-1530	Arrival of some participants	**Jon Otto Opening**				**1515-1530**
1530-1600		**Francoise** Brochard	Poster Presentations: 3 min each poster presenter	**Arne** Skjeltorp		**1530-1600**
1600-1630		**Thereza** Soares		**Sérgio** A. Lira		**1600-1630**
1630-1700		**Irep** Gozen		**Antonio** Azevedo		**1630-1700**
1700-1730		Coffee Break	Poster session including refreshments	Coffee Break	Departure of most participants	**1700-1730**
1730-1800		**Paul** Dommersnes		**Luca** Moriconi		**1730-1800**
1800-1830		**Erik** Luijten		**Antônio** M. S. Macêdo		**1800-1830**
1830-1900		**Anderson** S. L. Gomes		**Fernando** Oliveira		**1830-1900**
1900-2000		Discussions	Discussions	Discussions		**1900-2000**
2000-2100		Dinner	Dinner	Dinner		**2000-2100**
2100 –		Discussions	Discussions	Discussions		**2100-**

Monday - February 22nd:

1430 - 1515 **Registration**

1515 - 1530 **Jon Otto** Fossum: *Welcome*

Session 1: Chair: Arne Skjeltorp

1530 - 1600 **Francoise** Brochard
How Cells Escape from Cellular Aggregates?

1600 - 1630 **Thereza** Soares
Computational Simulations of Bacterial Membranes

1630 - 1700 **Irep** Gozen
Effects of active particle motion on kinetics of biochemical reactions

1700 - 1730 **Coffee** Break

1730 - 1800 **Paul** Dommersnes
Physical Active Matter

1800 - 1830 **Erik** Luijten
Dynamics of Passive and Active Colloids

1830 - 1900 **Anderson** S. L. Gomes
Interplay between photonics and complex systems: Random lasers, spin glasses and Lévy flights

1900 - 2000 **Discussions**

2000 - 2100 **Dinner**

2100 - **Discussions**

Tuesday - February 23rd:

Session 2: Chair: Marcio Carvalho

0900 - 0930 **Josef** Breu
From powder to lyotropic liquid-crystalline phases

0930 - 1000 **Koiti** Araki
Nanoparticles technology for energy, environment and nanomedicine

1000 - 1030 **Rita** Dias
Monte Carlo simulations on the interaction of nanoparticles with weak polyelectrolytes

1030 - 1100 **Coffee** Break

1100 - 1130 **Aurora** Pérez-Gramatges
Surfactant, Polymer and Nanoparticle Synergy in Fluids and Biphasic Dispersions

1130 - 1200 **Peter** W. Bryant
Nanodroplets on Surfaces: Observation, Simulation, and Implications for Flow Models at Larger Scales

1200 - 1300 **Lunch**

1300 - 1530 **Discussions**

Session Posters: Chair: Jon Otto Fossum

1530 - 1700 Poster Presentations: 3 min each poster presenter

1700 - 1900 Poster session including refreshments

1900 - 2000 **Discussions**

2000 - 2100 **Dinner**

2100 - **Discussions**

Wednesday - February 24th:

Session 3: Chair: Irep Gozen

0900 - 0930 **Henri** van Damme
Looking at cities with the eyes of complex condensed matter physics

0930 - 1000 **Andreas** Carlson
Touchdown and adhesion of thin elastic sheets

1000 - 1030 **Xiang** Cheng
Granular impact cratering by liquid drops

1030 - 1100 **Coffee** Break

1100 - 1130 **Patrick** Tabeling
Designing colloidal molecules with microfluidics

1130 - 1200 **Maria** J. B. Moura
Fabrication and Mechanical Characterization of Polymeric Microcapsules

1200 - 1300 Lunch

1300 - 1530 Discussions

Session 4: Chair : Giovani Vasconcelos

1530 - 1600 **Arne** Skjeltorp
Knots and braids in physics, chemistry and biology

1600 - 1630 **Sérgio** A. Lira
Stationary magnetic fluid patterns in Hele-Shaw cells

1630 - 1700 **Antonio** Azevedo
Spintronics phenomena driven by spin orbit interaction in magnetic hybrid structures

1700 - 1730 **Coffee** Break

1730 - 1800 **Luca** Moriconi
Vortex Identification Issues in Turbulent Boundary Layer Modeling

1800 - 1830 **Antônio** M. S. Macêdo
Time Series with Fluctuating Statistical Parameters: A Dynamical Stochastic Approach

1830 - 1900 **Fernando** Oliveira
Growth model and exact solution for a 1+1 etching model

1900 - 2000 Discussions

2000 - 2100 Dinner

2100 - Discussions

Thursday - February 25th:

Session 5: Chair: Maria Moura

0900 - 0930 **Marcio** Carvalho
Flow of complex fluids through porous media

0930 - 1000 **Paulo** R. de Souza Mendes
Mechanical behavior of gels, pastes, slurries, and other yield-stress materials

1000 - 1030 **Heloisa** Bordallo
Microscopic view of hydrogen motion from neutron scattering

1030 - 1100 **Caetano** R. Miranda
Nanoscience applied to oil and gas technologies: a multiscale computational approach

1100 - 1105 **Jon Otto** Fossum: *Closing*

1200 - 1300 **Lunch**

Poster presenters (21 submitted posters):

Éverton C. Santos:
Intercalation of Ciprofloxacin into Lithium-Fluorohectorite at different pHs

Frederico C Gomes:
An asymptotic model for simulation of oil well cementing process

Frederico Pontes:
Effects of temperature, lipid structure and counterions on assembly and dynamics of Lipid A bilayers

Helton Pereira Nogueira:
Magnetic nanoadsorbents for Environmental Recovery

Iván R. Roa:
A Dynamical Approach to Time Series with Fluctuating Statistical Parameters

Jorge Avendano:
Effect of wettability in residual oil saturation within surface treated micromodels

Josue M. Goncalves:
Highly stabilized alpha-NiCE(OH)2 nanomaterials for use in electrochemical devices

Morten Stornes:
Mean Field PEM Pore Network Models: Effective Transport Properties

Nicolle Miranda de Lima:
Pore-scale analysis of oil recovery by injection of polymer solution

Ricardo Pereira Dias:
Displacement of high viscous oil using different elastic polymer solutions

Roberta M. Cardoso**:**
LTCC Microfluidic Devices applied on Synthesis and Modification of Nanoparticles

Rodrigo Bento Reboucas:
On the pressure-driven flow of suspensions: particle migration in shear sensitive liquids

Rogelma M.S. Ferreira:
Anomlous law of cooling in nano systems

Rômulo P. Tenório:
Magnetic and Wrinkles Patterns in Saccharomyces cerevisiae Colonies

Sergio L. Campello:
A new technique to prepare Metal-Organic Frameworks by laser ablation in liquid

Sergio L. Campello:
Synthesis and characterization of Fe(BTC)-iron oxide composite

Sylvia M. Mutisya:
Simulated NMR Analysis of Brine Confined in Calcite Slit Pores

Thiago A. Sobral:
Formation of loops in the packing of a flexible rod into annular cavities

Victor M. M. Alvarez:
Interfacial instabilities on rotating Hele-Shaw flows with a time-dependent angular velocity.

William O. Sosa:
Option pricing with Gaussian and non-Gaussian models: Application to the Brazilian market

Yuri M. Celaschi:
Molecular simulations of atomistic crude oil models with brine interfaces at reservoir conditions

Abstracts

Talks

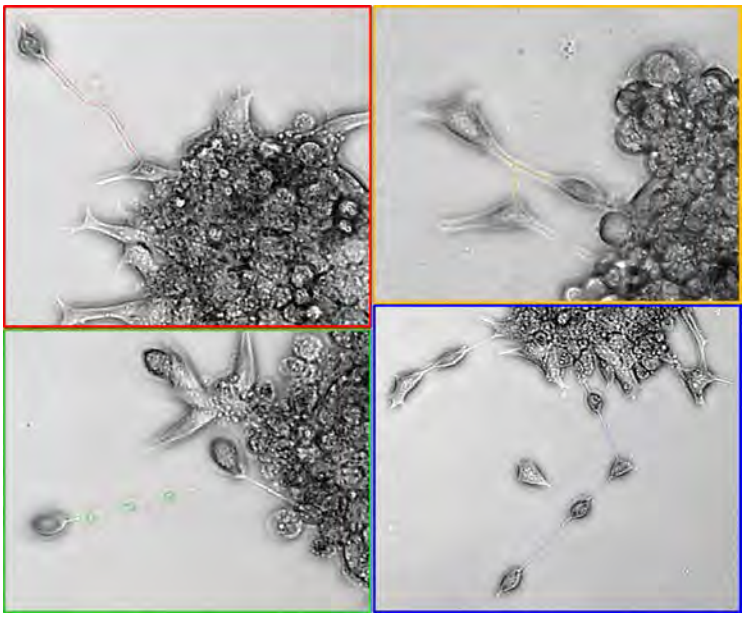
Monday 22nd 1530 - 1600

How Cells Escape from Cellular Aggregates?

Francoise Brochard-Wyart (*brochard@curie.fr*) *Institut Curie- Paris France*
Gregory Beaune and Francoise Winnik *Mana Tsububa Japan*

We first introduce the field of "Entangled Active Matter". *Active matter* describes diverse systems of self-propelling particles. But unlike swarms of fish and flocks of birds, cells are bound by transient links and can support static loads. We show that the concept of polymer physics and wetting can be applied to this living systems (1) using multicellular aggregates as a model system for tissues. We characterize the tissue mechanical properties by a new pipette aspiration technique. We apply this technic to embryonic development. Then we describe three scenarios where single cells can escape from the cell aggregate, reproducing in vitro an epithelial mesenchymal transition involved in embryonic development and tumor metastasis.
1) **by depletion of cellular adhesion molecules (CAM's).** In the spreading of aggregates (2) we observe both partial and complete wetting regimes, where a precursor film expends around the aggregate .Depending upon cell-cell adhesion, this film can be a dense cellular monolayer or consist of individual cells escaping from the aggregate.
2) **by rupture of the envelope** containing the tumor for non-adhesive cells
3) **by extrusion of membrane tubes** . We report here the formation of membrane tubes from Lymph Node Cancer Prostate (LNCaP) cell aggregates in partial wetting conditions (3): cells at the periphery are very motile, and try to escape from the aggregate, leading to the formation of tubes. Growth of tubes is followed by either its retraction or its rupture, leading to cell's escape. Our study unveil a new mechanism for tumor proliferation that do not invoke a loss of adhesion (cadherin depletion), which could be observed with other types of very aggressive cells forming cohesive tumors. Finally we show that nanostickers can glue cells together and inhibit the escape of cells

References:
1. David Gonzalez-Rodriguez et al. (2012) . Science **338**, 910; 1226418
2. Douezan, S., et al., (2011).PNAS, **108**.18
3. Gregory Beaune et al. (2014) How cells flow in the spreading of cellular aggregates. PNAS **111**.22.



Monday 22nd 1600 - 1630

Computational Simulations of Bacterial Membranes

Thereza A. Soares (*thereza.soares@ufpe.br*), Frederico J. S. Pontes, Roberta P. Dias, Denys dos Santos, Andresa Messias

Department of Fundamental Chemistry, Federal University of Pernambuco 50740-560, Cidade Universitária, Recife, Pe. dqfnet.ufpe.br/biomat

Lipopolysaccharides (LPS) are the major constituent of bacterial outer membranes, acting as an effective permeability barrier against xenobiotic agents and the host cell defence system. LPS is also a potent activator of the mammalian immune system in amounts as little as *fmol*. Variable external conditions prompt structural and chemical modifications of the bacterial outer membrane, enhancing the organism ability to evade the host immune defence and colonize specific tissues. Changes in temperature and/or specific ion concentration have been shown to trigger lamellar to non-lamellar transitions in LPS membranes. We have previously developed and validated an atomistic model of the LPS membrane of *Pseudomonas aeruginosa*, which has been used to investigate its structural dynamics, hydration and electrostatic properties. Recently, we have expanded our atomistic model to include novel LPS chemotypes expressed by *P. aeruginosa* during outer membrane remodeling. We have found that decrease in the LPS polysaccharide chain length occurs with increase in the diffusion coefficients for the Ca^{2+} counter-ions, increase in acyl chain packing (decrease in membrane fluidity), and decrease of the negative potential across the LPS surface. We have also investigated the effect of mono- and divalent cations on the stability of LPS and Lipid-A membranes. Our findings suggest that the stability of LPS membranes reflects a balance between effective membrane hydration, ionic valence and aptness to cross-link neighbouring molecules. These findings reproduce experimental trends while providing atom-level structural information on the rough LPS chemotypes that can help to rationalize antibiotic resistance and bacterial adhesion processes.

Related References:

Dias et al. *J. Chem. Theor. Comp.* 10, 2488. 2014;
Dias et al. *J. Comp. Chem.* 35, 1418. 2014.
Nascimento et al. *Chem. Comm.* 50, 231. 2014.
Ravi et al. *Chem. Comm.* 49, 8821. 2013.
Kirschner et al. *J. Chem. Theory Comp.* 28, 14849. 2012.

Monday 22nd 1630 - 1700

Effects of active particle motion on kinetics of biochemical reactions

Irep Gözen[1] (*irep@seas.harvard.edu*), Daniel T. -N. Chen[2], Andrew Bergman[1], Rachel Feynman[1], Viva Horowitz[1], Zachary Chambers[1], Zvonimir Dogic[2] and Vinothan N. Manoharan[1]

[1]*Harvard Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA*
[2]*Department of Physics, Brandeis University, Waltham, MA 02474, USA*

The intracellular environment is dynamic, influenced by the motion of active machinery such as cytoskeleton filaments and molecular motors. To understand whether and how such activity affects the rates of diffusion-limited reactions, we employ a model system containing active particles and diffusion limited chemical reactions. To be able to mimic the active motion, we use Janus and magnetic particles, as well as the actual biological molecular motors that are free of cargo. The model reactions include enzymatic reactions and the entropy-driven reactions involving DNA. We further aim to confine this model system in emulsions and in phospholipid vesicles which are reminiscent of biological cells. Our findings might illuminate how active motion influences cytoplasmic reaction dynamics, or may have played a role in protocell genetics.

Monday 22nd 1730 - 1800

Physical Active Matter

Paul Dommersnes (*paul.dommersnes@ntnu.no*)

Department of Physics, Norwegian University of Science and Technology - NTNU, Trondheim, Norway

Active matter is commonly defined as a system composed of "many self-driven entities". The inspiration for active matter is biology, which is inherently active on scales ranging from macroscopic to nano. Well know examples are flocking birds, colonies of self-propelled bacteria, and muscles (which work through the collective effort of many motor proteins). Studying active matter impact our understanding of biology, and at the same time gives rise to "synthetic active matter" systems. Synthetic active matter can be made in the laboratory, where the energy input comes from biochemical or chemical reactions. It is also possible to achieve "physical" active matter where the energy comes from an external field. Some of these physical active matter systems will be discussed, including work at NTNU on swimmers and colonies of particles driven by electro-hydrodynamics.

Monday 22nd 1800 - 1830

Dynamics of Passive and Active Colloids

Erik Luijten (*luijten@northwestern.edu*)

Departments of Applied Mathematics, Materials Science and Engineering, Physics and Astronomy, Northwestern University, Evanston, Illinois, U.S.A.

Flow of colloidal suspensions through microfluidic channels is ubiquitous in nature, from the transport of blood cells to the pumping of ink for 3D printing. Physically, this is a challenging and interesting problem, as the non-uniform shear effects of the flow occur on length scales comparable to the channel diameter, and the suspended colloids in turn have a similar size as well. I will discuss how these shear effects give rise to remarkable phase behavior and dynamics of attractive colloids.

In a separate development, we consider the dynamics of active colloids, propelled via induced-charge electrophoresis. This motion in alternating electric fields is now considered one of the prime model systems for self-propelled particles. However, whereas this phenomenon was predicted theoretically a decade ago and then realized experimentally, its curious dependence on the frequency of the applied field has proven difficult to explain. I will show the interesting route that allowed us to elucidate, via powerful new methods, the experimental observations.

Monday 22nd 1830 - 1900

Interplay between photonics and complex systems: Random lasers, spin glasses and Lévy flights

Anderson S. L. Gomes[1] (*andersonslgomes@gmail.com*), Ernesto P. Raposo[2] André L. Moura,[1,3] Serge I. Fewo,[4] Pablo I. R. Pincheira,[1] Vladimir Jerez,[5] Lauro J. Q. Maia,[6] and Cid B. de Araújo[1]

[1]Departamento de Física, Universidade Federal de Pernambuco, Recife-PE, Brazil, [2]Laboratório de Física Teórica e Computacional, Departamento de Física, Universidade Federal de Pernambuco, Recife-PE, Brazil, [3]Grupo de Física da Matéria Condensada, Universidade Federal de Alagoas, Campus Arapiraca Arapiraca-AL, Brazil, [4]Laboratory of Mechanics, Department of Physics, University of Yaoundé I, Cameroon, [5]Grupo de investigacion FIELDS, Universidad de Investigacion y Desarrollo, Bucaramanga, Colombia, [6]Grupo Física de Materiais, Instituto de Fïsica, Universidade Federal de Goiás, Goiania, Brazil.

Random lasers are a photonic class of open systems, which have been recently exploited as a photonic platform for studies of complex systems. This multidisciplinary approach opened up new important avenues for the understanding of random-laser behavior, including Lévy-type distributions of strong intensity fluctuations and phase transitions to a photonic spin-glass phase. In this work, we employ a solid state random laser based on a Nd:YBO powder, operating in the nonresonant feedback regime to unveil the physical origin of the complex interplay between the Lévy fluctuation regime and the photonic analogous of replica-symmetry-breaking (RSB) transition to the spin-glass phase, well studied in magnetic systems. RSB is also observed in a dye-TiO2 colloidal RL. A novel unexpected finding is also reported for the solid state system: the suppression of the spin-glass behavior for high excitation pulse energies, not observed before. The present theoretical description from first principles of this interplay unfolds new possibilities to characterize other nanolasers and small lasers, which include plasmonic-based, photonic-crystal and bio-derived nanodevices. The statistical nature of the emission provided by random lasers can also impact on their prominent use as sources for speckle-free laser imaging, which nowadays represents one of the most promising applications of random lasers, with expected progress even in cancer research.

Pontes et al., *J. Chem. Theory Comp.* 8, 3830 (2012).

Tuesday 23rd 0900 - 0930

From powder to lyotropic liquid-crystalline phases

Josef Breu[2] (josef.breu@uni-bayreuth.de), S. Rosenfeldt,[1] M. Stöter[2], T. Weiß[1], S. Förster[1]

[1]Physical Chemistry I and [2]Inorganic Chemistry I, University of Bayreuth, Universitätsstrasse 30, 95440 Bayreuth, Germany,

The intrinsically anisotropic bonding in layered materials like clay minerals may enable spontaneous delamination by osmotic swelling, where continuum electrostatic repulsion separates stacks into individual layers with high precision and a highly ordered lamellar liquid crystalline phase (Wigner crystal) is formed with basal distances from 1 – 30 nm depending only on the water/clay ratio [1]. This requires, however, a perfectly homogenous charge density only found with clays synthesized from the melt at temperatures higher than 1000 K. Utterly controlling homogeneity and thus intracrystalline reactivity, moreover, allows for synthesis of one-dimensionally crystalline heterostructures that may subsequently be delaminated into double stacks with any kind of functional molecules sandwiched between two clay layers [2]. This way emitters may e.g. be oriented in a quasi-epitaxial way allowing for polarized emission [3] or the heterostacks may be turned into Janus platelets.

1. Stöter, M., Rosenfeldt, Breu, J., *Tunable Exfoliation of Synthetic Clays***,** Annu. Rev. Mater. Res. **2015**, 45, 129–51.
2. Stöter, M., Biersack, B., Reimer, N., Herling, M., Stock, N., Schobert, R., Breu, J., *Ordered Heterostructures of Two Strictly Alternating Types of Nanoreactors*, Chem. Mater. **2014**, 26, 5412−5419.
3. Stöter, M., Biersack, B., Rosenfeldt, S., Leitl, M.J., Kalo, H., Schobert, R., Yersin, H., Ozin, G.A., Förster, S., Breu, J., *Encapsulation of Functional Organic Compounds in Nanoglass for Optically Anisotropic Coatings*, Angew. Chem. Int. Ed. **2015**, 54, 4963 –4967.

Tuesday 23rd 0930 - 1000

Nanoparticles technology for energy, environment and nanomedicine

Koiti Araki

Institute of Chemistry, University of Sao Paulo, Av. Lineu Prestes 748, Butanta, Sao Paulo, SP, 05508-000, Brazil

The large-scale production of dispersible nanoparticles and the development of mild functionalization processes to attach different types of molecules, biomolecules and transition metal complex catalysts/photocatalysts on the surface, while maintaining the colloidal stability, are the bottlenecks for development of new functional hybrid nanoparticles and nanocomposites. In this presentation we will discuss on an efficient chemical approach for large-scale production of nanoparticles suitable for energy, environment and nanomedicine applications. Also, adsorbents for removal of undesirable contaminants such as heavy metals, hormones, pesticides, and dyes will be presented.

Keywords: Nanoparticles, hybridization, nanocomposites

References:

1. M. K. Uchiyama *et al.*, Ultrasmall cationic superparamagnetic iron oxide nanoparticles as nontoxic and efficient MRI contrast agent and magnetic-targeting tool. *Int J Nanomed* **10**, 4731 (2015).
2. S. H. Toma, J. J. Santos, K. Araki, H. E. Toma, Pushing the surface-enhanced Raman scattering analyses sensitivity by magnetic concentration: A simple non core-shell approach. *Anal Chim Acta* **855**, 70 (2015).
3. M. K. Uchiyama *et al.*, In vivo and In vitro Toxicity and Anti-Inflammatory Properties of Gold Nanoparticle Bioconjugates to the Vascular System. *Toxicol Sci* **142**, 497 (2014).
4. U. Condomitti *et al.*, Silver recovery using electrochemically active magnetite coated carbon particles. *Hydrometallurgy* **147**, 241 (2014).
5. P. R. Martins *et al.*, Highly stabilized alpha-NiCo(OH)(2) nanomaterials for high performance device application. *J Power Sources* **218**, 1 (2012).

Tuesday 23rd 1000 - 1030

Monte Carlo simulations on the interaction of nanoparticles with weak polyelectrolytes

Rita Dias[1] (*rita.dias@ntnu.no*), Morten Stornes[1], Per Linse[2]

[1]*Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway*
[2]*Division of Physical Chemistry, Center for Chemistry and Chemical Engineering, Lund University, Lund, Sweden*

Systems comprising of nanoparticles and oppositely charged polyelectrolytes have a great technological interest, being major components in formulations used in pharmaceutical, food, cosmetics, detergents, and paint industries. The stability of colloidal suspensions and the interaction of its constituents are important issues in formulations, and a large effort has been made to understand how the properties of each individual component affect the overall characteristics of the formulations.
Weak polyelectrolytes are especially interesting since their properties can be tuned resorting to pH variations. An additional characteristic of weak polyelectrolytes is the fact that protons can also migrate along the chains and between different chains [1]. It has been shown, using experimental and theoretical tools, that such type of charge correlations enhances the interaction between oppositely charged species. Examples are the adsorption of DNA [2-4] and proteins [5,6] onto lipid membranes and the interaction between annealed polyacids and micelles [7,8].

In this work we have systematically studied the effect of charge mobility (quenched vs. annealed) on the adsorption of polyacids to a nanoparticle. The effect of polyacid chain length and number is also evaluated.

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Tuesday 23rd 1100 - 1130

Surfactant, Polymer and Nanoparticle Synergy in Fluids and Biphasic Dispersions

Aurora Pérez-Gramatges[1] (*aurora@puc-rio.br*), Ana M. Percebom[1], Regina S. V. Nascimento[2]

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Interactions between surfactants, polymers and nanoparticles in complex fluids give rise to the formation of association structures that can modify the solution and interfacial properties. This is the underlying reason behind a great number of applications in world-wide industries such as cosmetics, detergents, pharmaceutics, petroleum and others. In particular, the synergistic effects observed in their adsorption at interfaces, compared to individual behavior, allow for tuning properties of interest for potential applications in fields dealing with control of surface activity and interfaces. In this work, three tailored systems will be discussed: amphiphilic polymer and non-ionic surfactants, silica nanoparticles and surfactant mixtures, and Janus nanoparticles with interfacial activity. In the first case, the hydrophobic segments in the macromolecule strongly associate with surfactants, promoting micellization and encapsulation in the presence of salt [1]. Second, mixtures of silica nanoparticles and different surfactants enhance interfacial properties, while amphiphilic Janus nanoparticles allow controlled self-assembly and high interfacial activity [2].

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Tuesday 23rd 1130 - 1200

Nanodroplets on Surfaces: Observation, Simulation, and Implications for Flow Models at Larger Scales

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As a consequence of demands in the petroleum and biomedical industries, the behavior of fluids and how they interact with solids must be understood at the smallest possible length scales. Recent and future advances require investigation at sub-micrometer lengths. At these scales, intermolecular interactions are sufficiently strong that fluids cease to behave as they do in bulk, and their interactions with surfaces can be dominated by the dynamics of individual molecules. Even the applicability of traditional metrics for characterizing fluid-solid interactions, such as wettability, contact angle, and line tension must be investigated. Understanding how nanoscopic phenomena affect macroscopic flow properties promises to lead to new technologies.

To these ends, we have developed a platform with which we observe nanodroplets on manufactured surfaces using a combination of Atomic Force Microscopy and optical measurements. In conjunction with experiments, we perform Molecular Dynamics simulations of the droplets to gain insight into molecular-level phenomena between the droplets and the surfaces, as well as within the droplets themselves. We observe and characterize the departure from the typical shape of macroscopic droplets as well as the formation of a precursor film that spreads along the surface. We also perform thermodynamical studies to determine the extent to which droplet shapes can be understood in terms of bulk properties, such as internal and surface energies, along with an effective potential to model surface interactions. As a result, we gain perspective on methods for the inclusion of salient nanoscale phenomena in simulations of fluid flow at larger scales. We will present both the experimental platform as well as experimental and simulation results.

Wednesday 24th 0900 - 0930

Looking at cities with the eyes of complex condensed matter physics

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[4]*CINAM, CNRS and Aix-Marseille Université, Marseille, France*

In an increasingly urban world, large and mega-cities are emerging as the focal points of several of the greatest challenges that we have to face, from affordable housing, mobility, energy and food resources to infrastructure and communities coexistence. Therefore, a science-based understanding of the dynamics, growth, organization, energetic metabolism, and "livability" of cities is urgently needed. Surprisingly good universal scaling "laws" affecting a wide variety of metrics such as wealth, crime, or patents, have recently been evidenced, which suggest that relatively simple parameters may control a wide variety of complex urban phenomena. While many of the physical approaches to city structure are devoted to fractal aspects, centrality, or street networks, we adopted a condensed matter physics perspective, considering buildings as "molecules". It was observed that the toolbox of crystal and glass physics apply remarkably well to North American cities. Focusing on the so-called urban heat island effect, we found that the excess temperature observed in cities centers is primarily related to a local order parameter controlling energy dissipation. All other factors frequently invoked (green areas, building materials,…) are of second order.

Wednesday 24th 0930 - 1000

Touchdown and adhesion of thin elastic sheets

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[2]*Paulson School of Engineering and Applied Sciences, Harvard University*

The dynamics of contact between a thin elastic film and a solid arises in many scientific and engineering applications, from the simple saran-wrap to cellular adhesion to grounding lines in ice sheets. Elastohydrodynamic lubrication theory allows us to derive a partial differential equation coupling the elastic deformation of the sheet, the microscopic adhesion and the viscous thin film flow. We use a combination of numerical simulations of the governing equation and a scaling analysis to describe the self-similar solution of the touchdown and spreading of an elastic sheet on a solid substrate. Our analysis generalizes similar approaches for rupture in capillary thin film hydrodynamics and suggests experimentally verifiable predictions for a new class of singular flows linking elasticity, hydrodynamics and adhesion.

Wednesday 24th 1000 - 1030

Granular impact cratering by liquid drops

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Department of Chemical Engineering and Materials Science, University of Minnesota

Granular materials are large conglomerations of discrete macroscopic particles. Examples include seeds, sand, coals, powder of pharmacy, etc. Though simple, they show unique properties different from other familiar forms of matter. The unusual behaviors of granular materials are clearly illustrated in various impact processes, where the impact-induced fast deformation of granular materials leads to emergent flow patterns revealing distinctive granular physics. Here, we investigated impact cratering in granular media induced by the strike of liquid drops—a ubiquitous phenomenon relevant to many important environmental, agricultural and industrial processes. Surprisingly, we found that granular impact cratering by liquid drops follows the same energy scaling and reproduces the same crater morphology as that of asteroid impact craters. Inspired by this similarity, we develop a simple model that quantitatively describes various features of liquid-drop imprints in granular media. Our study sheds light on the mechanisms governing raindrop impacts on granular surfaces and reveals an interesting analogy between familiar phenomena of raining and catastrophic asteroid strikes. The research was partially supported by the NSF Faculty Early Career Development (CAREER) Program (DMR-1452180).

Wednesday 24th 1100 - 1130

Designing colloidal molecules with microfluidics

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MMN (Microfluidique, MEMS, Nanostructures) at ESPCI-ParisTech & IPGG, Paris, France

The creation of new colloidal materials involves the design of functional building blocks. Here we introduce a microfluidic method for designing building blocks one by one, at high throughput, with a broad range of shapes. The method exploits a coupling between hydrodynamic interactions and depletion forces that controls the configurational dynamics of droplet clusters traveling in microfluidic channels. Droplet clusters can be cross-linked *in situ* with UV. By varying the flow parameters, clusters are prescribed a given size, geometry, chemical and/or magnetic heterogeneities enabling local bonding. We produce compact structures (chains, triangles, diamonds, tetrahedrons,...) and non-compact structures, such as crosses and T, difficult to obtain with current techniques. Size dispersions are small (2 %) and throughputs are high (25000/hour). The work opens a new pathway, based on microfluidics, for designing colloidal building blocks with a potential to enable the creation of new materials.

Wednesday 24th 1130 - 1200

Fabrication and Mechanical Characterization of Polymeric Microcapsules

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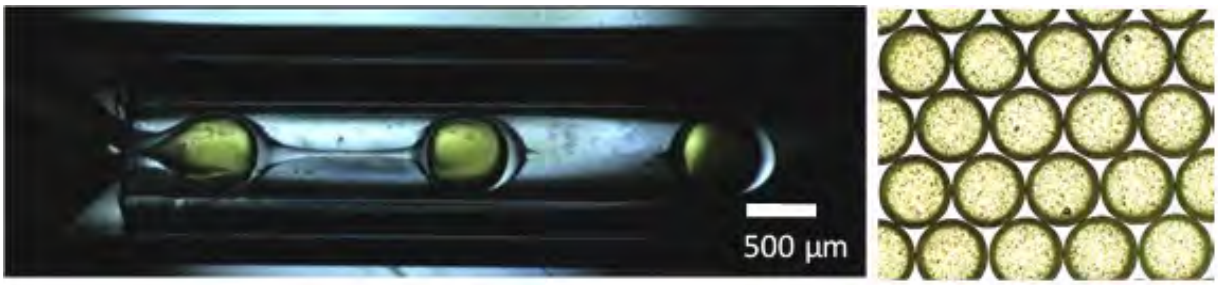
Microcapsules are commonly used in the pharmaceutical, cosmetics, and food industries. Here we present a method for generating polymeric microcapsules with tunable elasticity, as well as a study of their mechanical properties. The microcapsules we produce consist of an inner phase of water, a middle phase (the shell) of PDMS (SYLGARD 184: pre-polymer base with a cross-linker), and an outer phase of PVA solution in water 10wt%. The microcapsules are formed using a glass capillary microfluidic device. The capsules produced are monodispersed and are ~700 microns in diameter. Our fabrication technique allows us to produce capsules with different shell thicknesses, by adjusting the injection rates, and with different stiffness, by adjusting the degree of polymer cross-linking. The stress-strain curves of the microcapsules were obtained by squeezing the capsules between two parallel plates. We have also performed experiments of flow of the microcapsules through a constricted capillary, measuring the pressure drop and the deformation of the capsules. Our final goal is to design and fabricate microcapsules to control water mobility through heterogeneous porous media.



Wednesday 24th 1530 - 1600

Knots and braids in physics, chemistry and biology

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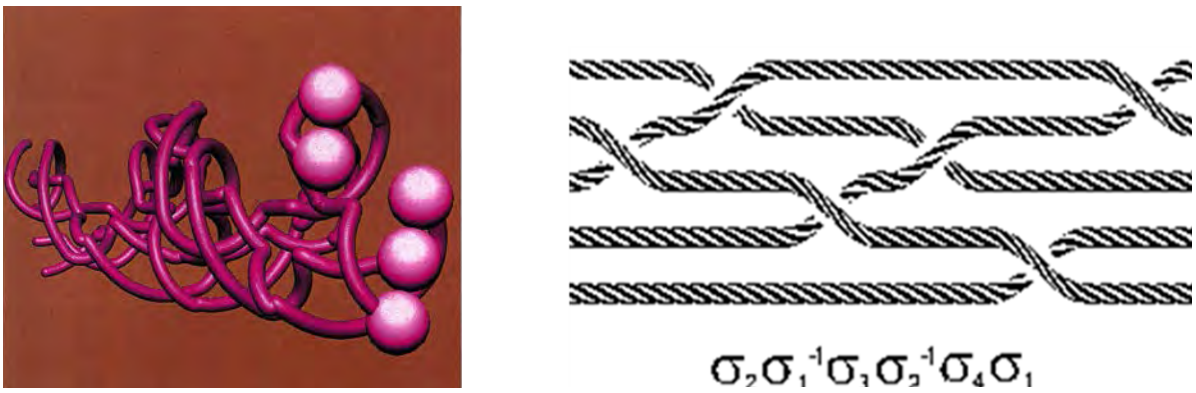
Knot and braid theory is a subfield of mathematics known as topology. It involves classifying different ways of tracing curves in space. Knot theory originated more than a century ago and has been an active area of mathematics. The study of knots and braids has led to interesting applications in physics, chemistry and biology. Some aspects will be reviewed.



A space-time plot of the motion of magnetic particles subject to external magnetic fields (left), which can be classified by a braid notation (right).

Wednesday 24th 1600 - 1630

Stationary magnetic fluid patterns in Hele-Shaw cells

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We investigate a quasi-two-dimensional system composed by an initially circular ferrofluid droplet surrounded by a nonmagnetic fluid of higher density [1]. These immiscible fluids flow in a rotating Hele-Shaw cell, under the influence of an in-plane radial magnetic field. We focus on the situation in which destabilizing bulk magnetic field effects are balanced by stabilizing centrifugal forces. In this framing, we consider the interplay of capillary and magnetic normal traction effects in determining the fluid-fluid interface morphology. By employing a vortex-sheet formalism [2] we have been able to find a family of exact stationary *n*-fold polygonal shape solutions for the interface. A weakly nonlinear theory is then used to verify that such exact interfacial solutions are in fact stable.

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Wednesday 24th 1630 - 1700

Spintronics phenomena driven by spin orbit interaction in magnetic hybrid structures

Antonio Azevedo[1], J. B. S. Mendes[2], O. Alves Santos[1], L. M. Meireles[3], R. G. Lacerda[3], L. H. Vilela-Leão[4], F. L. A. Machado[1], R. L. Rodríguez-Suárez[1,5], and S. M. Rezende[1]

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The rich physics driven by the spin-orbit interaction in systems with translational symmetry breaking has been shown to be effective at magnetic metallic surfaces and has stimulated many research activities, leading to the discovery of a variety of phenomena in the area of spintronics. This is a very active and multidisciplinary field, in which the main subject is the generation, manipulation and detection of spin currents in hybrid magnetic nano-structures. Spin currents can be mostly generated by means of the spin Hall effect, ferromagnetic resonance (FMR) driven spin pumping, and spin Seebeck effect. Detection of spin currents is usually done through their conversion into charge currents by means of the inverse spin Hall effect (ISHE) or the inverse Rashba-Edelstein effect (IRRE), and also by the spin-transfer torque exerted on the magnetization of attached magnetic layers. In this talk we will give a brief introduction about the generation, manipulation and detection of spin current as well as present very new results in which spin current is injected and detected in different materials. We will show that in heterostructures made with the insulating ferrimagnet yttrium iron garnet (YIG), spin-pumped spin current can be efficiently converted into electric signals in an attached nanometer thick layer of Pt, Ta, permalloy (Py) or $Ir_{20}Mn_{80}$, a high-temperature antiferromagnetic metal that is commonly employed in spin-valve devices. We will also show that spin current can be injected in single layer of graphene deposited onto a layer of YIG and its conversion in charge currents is attributed to the inverse Rashba-Edelstein effect.

Wednesday 24th 1730 - 1800

Vortex Identification Issues in Turbulent Boundary Layer Modeling

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A structural description of turbulent boundary layers (TBLs) has been a promising direction of research, strongly supported by an increasing number of fluid dynamicists along recent years. We discuss in this talk a particularly simple statistical vortex model, inspired by the picture of the TBL as a "gas" of hairpin-vortex configurations, which is able to reproduce, with remarkable agreement, important qualitative features of streamwise velocity fluctuations. In order to refine the model, with the help of numerical and experimental feedback, it is absolutely necessary to work with vortex identification methods, which, however, lose accuracy in a dramatic way in the inner layer of TBL flows. Focusing on one of the most popular vortex identification methods - the swirling strength criterion - we critically discuss its main problematic issues as (i) vortex image deformation and suppression due to the near presence of intense vortical structures; (ii) artificial vortex merging; (iii) introduction of "ghost" vortices in many-vortex configurations and (iv) in the presence of background shear. We, then, propose an alternative vortex detection criterion, based on the curvature properties of the vorticity profile, which is shown to clearly improve over the results obtained with the swirling strength criterion in a number of relevant two-dimensional case studies.

Wednesday 24th 1800 - 1830

Time Series with Fluctuating Statistical Parameters: A Dynamical Stochastic Approach

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Time series distributions in complex physical systems may show strong deviations from Gaussian statistics which can be understood as a superposition of different dynamics with well separated time scales. In this interpretation, Gaussian statistics holds on short time scales as a quasi-equilibrium distribution with parameters that change on larger time scales. Averaging over these fluctuating parameters with a suitable statistical model yields a compounding that provides a description of non-Gaussian distributions of physical observables, such as velocity increments in turbulent flow. This scheme, known in physics as superstatistics, has had great successes in describing phenomena as diverse as turbulence in classical fluids, microwave propagation through disordered cavities, quantum transport through ballistic cavities with mixed dynamics and price variations in financial time series. An interesting multiscale extension of superstatistics was introduced recently by Salazar and Vasconcelos (Phys. Rev. E 86, R050103, 2012) via the stationary solution of a hierarchy of coupled stochastic differential equations (SDE) which achieved good agreement with experimental data on classical turbulence. In this work we extend this EDE approach in two ways: (i) we focus on time-lagged increment distributions, as opposed to marginal stationary distributions; (ii) we account for long time-lagged Gaussian asymptotic behavior in the increment distributions by inserting time-dependence on some EDE parameters. In addition, we provide a novel procedure to extract the time series of the fluctuating parameter of the short-time Gaussian statistics, which describes well heavy-tailed long-time compounding distributions. Our numerical results show good qualitative agreement with experimental data on Eulerian turbulence.

Wednesday 24th 1830 – 1900

Growth model and exact solution for a $1+1$ etching model.

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2-Instituto de Física, Universidade de Brasília, CP 04513, CEP 70919-970, Brasília, DF, Brazil
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We present a method to derive analytically the growths exponents of a eroded surface whose dynamics is ruled by cellular automata. Starting from the automata, we write down the time evolution for the height's average and height's variance (roughness). We apply the method to the etching model[1,2] of $1+1$ dimensions, than we obtain the dynamical exponents, which perfectly match the numerical results obtained from simulations. Those exponents are exact and they are the same as those exhibited by the KPZ model[3] for this dimension. Therefore, it shows that the etching model and KPZ belong to the same universality class[4].

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Thursday 25th 0900 - 0930

Flow of complex fluids through porous media

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The most common oil recovery method used for displacing the oil and maintaining the reservoir pressure is water injection. However, in most cases, the recovery efficiency of this method is limited by the high fluid mobility ratio and reservoir heterogeneities. The non-linear flow properties of complex fluids through porous media give rise to multiphase flow displacement mechanisms that operate at different scales, from pore-level to Darcy scale. Experiments have shown that injection of oil-in-water emulsions and viscoelastic polymer solutions can be used as an effective enhanced-oil recovery (EOR) method, leading to substantial increase in the volume of oil recovered. The mechanisms responsible for increasing the recovery factor in different EOR methods are not fully understood.

We study the effect of complex fluids (dispersions and viscoelastic polymer solution) both at pore and Darcy scale. Visualization of the flow of complex fluids through a transparent network of micro-channels, which serves as a model of a porous media, reveals how the flow behavior improves the pore-level displacement efficiency, leading to lower residual oil saturation. Oil recovery results during complex liquids flooding in tertiary mode (after water flooding) in sandstone cores and sandpacks show how the improved oil recovery varies with flow conditions and fluid properties.

Thursday 25th 0930 - 1000

Mechanical behavior of gels, pastes, slurries, and other yield-stress materials

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In this lecture we will describe the mechanical behavior of soft solids like gelled crudes, drilling muds, cement pastes, tooth paste, hair gel, mayonnaise, ketchup, yogurt, butter, and many other. We present the most recent phenomenological models that can predict the macroscopic behavior observed in these materials: elasticity, plasticity, shear thinning, and time dependence (thixotropy). We then describe the main rheological tests that should be done to characterize these materials in order to employ the models to simulate flows of practical interest.

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- A unified approach to model elasto-viscoplastic thixotropic yield-stress materials and apparent-yield-stress fluids, P. R. de Souza Mendes and R. L. Thompson, *Rheol Acta*, 52(7) 673-694 (2013)
- A unified approach to model elasto-viscoplastic thixotropic yield-stress materials and apparent-yield-stress fluids, P. R. de Souza Mendes K. R. Rajagopal and R. L. Thompson, *Intl. J. Non-Linear Mech*, 55 48-54 (2013)
- Thixotropic elasto-viscoplastic model for structured fluids, P. R. de Souza Mendes, *Soft Matter* 7 2471-2483 (2011)
- P. R. de Souza Mendes, R. L. Thompson, A. A. Alicke, R. T. Leite, The quasilinear large-amplitude viscoelastic regime and its significance in the rheological characterization of soft matter, Journal of Rheology 58(2), 537-561 (2014)

Thursday 25th 1000 - 1030

Microscopic view of hydrogen motion from neutron scattering

Marcella C. Berg[1,2], Murillo L. Martins[1], Martin K. Rasmussen[1,], Éverton C. dos Santos[1,4] , Ana R. Benetti [3], Markus Strobl[1,2], Jon Otto Fossum[4] and **Heloisa** N. Bordallo[1,2] (*bordallo@nbi.ku.dk*)

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Neutron science is the science of everyday life, providing a microscopic view of the materials we rely on for modern life. Neutrons, similarly to X-rays, penetrate matter. However, unlike X-rays, neutrons interact with matter in a different manner, thus allowing the identification of elements with very low molecular weight, including hydrogen. While X-rays allow the characterization of the micro-structure of materials, neutron imaging provides information on proton distribution within the structure. For this reason, both X-rays and neutron imaging, complemented by neutron spectroscopy, which brings information about hydrogen mobility, can contribute for better understanding of complex structures.
In this talk I will discuss on this promising approach by presenting a couple of specific examples. The first is related to the investigation of the highly intricate pore structure of dental cements [1] and the second to a recent study of the encapsulation of the HBsAg protein, used in the Hepatitis B vaccine, into the SBA-15 adjuvant [2]. Finally I will give a brief overview in how solid-state techniques can in general be used in studying encapsulation process and release of drugs [3].

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[2] Martin Kjærulf Rasmussen, BSc thesis: *"Localization of hepatitis B vaccine in SBA-15: A new method of delivery". http://xns.nbi.ku.dk/student_theses/Mastert_martinkj_rulfrasmussen.pdf*
[3] Murillo L. Martins, PhD thesis: *"Synthesis and!characterization of a bio-nanocomposite for cancer treatment"*http://xns.nbi.ku.dk/Murillo_Martins_PhD_2014.pdf

Thursday 25th 1030 – 1100

Nanoscience applied to oil and gas technologies: a multiscale computational approach

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Departamento de Física dos Materiais e Mecânica, Instituto de Física, Universidade de São Paulo (DFMT-IFUSP), São Paulo, Brazil.

With emergence of nanotechnology, it is possible to control interfaces and flow at nanoscale. This is of particular interest in the Oil and Gas industry, where nanoscience can be applied on processes such as Enhance Oil Recovery and asphalthene aggregation. Currently, our group is exploring the applications of Nanoscience in the O&G industry using three strategies:
i) Nano-EOR, based on surface drive flow, where mobilization of hydrocarbons trapped at the pore scale can be favored by controlling by the chemical environment through "Wettability modifiers", such as functionalized NPs and surfactants;
ii) Nano-IOR, through pressure driven flow, by controlling the spatial confinement and fluid flooding in nanoporous media and
iii) understanding the nano-aggregation mechanisms of asphaltenes. In this talk, we will explore the application of molecular simulations to characterize oil recovery and nano-aggregation processes under broader oil reservoir conditions through an integrated multiscale computational protocol ranging from first principles calculations, molecular dynamics and Lattice Boltzmann method (LBM). This proposed multiscale approach can be a useful tool to explore potential chemical additives for EOR and investigate the effects of the interfacial and wetting properties on fluid behavior at both nano and micro scales. Additionally, it also unveils the nature of nano-aggregation mechanisms of asphaltenes and their interactions within rock-water-oil interfaces from an more fundamental perspective.

Abstracts

Posters

Poster

Intercalation of Ciprofloxacin into Lithium-Fluorohectorite at different pHs

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Over the last decade, different porous materials have been used as hosts for drug encapsulation, and recently, due to its swelling properties and cation-exchange capacity, clays have been added to this list. Additionally to its swelling properties and cation-exchange capacity, clays have been shown to be non-toxic for trans-dermal application and oral administration.
In this poster are presented an initial analysis of the intercalation of Ciprofloxacin (CIPRO, C17H18FN3O3), a broad-spectrum antibacterial agent, into the layers of the synthetic smectite Lithium – Fluorohectorite (LiFh, Li1.2[Mg4.8Li1.2]Si4O10F2) at different PHs. TG experiments together with Infrared spectroscopy confirms that the CIPRO molecules are at least mixed with the clay particles and indicates that the intercalation process might change the Clay/water interactions. X-ray measurements indicates the presence of CIPRO into the clay layers and shows that this intercalation process is strongly dependent of the pH, being more effective at lower than higher pHs.

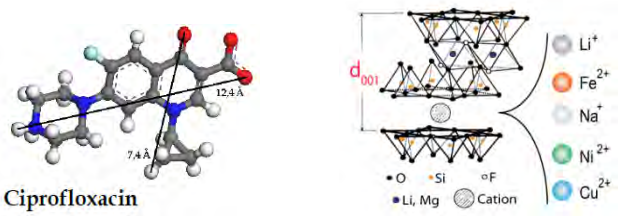

Figure 1: CIPRO molecule (left) and a sketch of the hectorite presenting some of the possible interlayer cations (right).

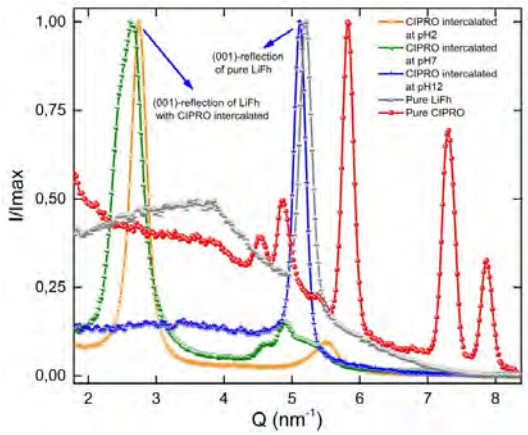

Figure 2: X-ray pattern of the pure drug, pure clay and of the drug intercalated into the clay at acid, neutral and basic pH.

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Poster

An asymptotic model for simulation of oil well cementing process

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In the construction of oil and gas wells the cementing process is an important step. Displacing fluids in downhole conditions and for long distances is a complex task, affecting several steps on well construction. Cementing gains relevance in the moment that fluid contamination compromises cement sheath integrity and consequently zonal isolation. Hence, fluid properties and process condition should be designed to minimize non-uniformities on the displacement front. A complete analysis of the annular flow that occurs during cementing is extremely complex, because of the presence of different liquids that often present non-Newtonian characteristic and the flow is three dimensional and transient. In some cases, the flow in the lower viscosity liquid phase may become turbulent. A complete model has a prohibitive high computational cost. Simplified models are available in the literature and are used by the oil industry in commercial simulation software for cementing. The available models are not able to accurately describe turbulent flow regime. In this work, we extend the lubrication based model in cylindrical coordinates developed before to include turbulent flow regimes and inner cylinder rotation.

Poster

Effects of temperature, lipid structure and counterions on assembly and dynamics of Lipid A bilayers

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Lipopolysaccharides are the main component of extern membrane of Gram-negative bacteria and main responsible for the structural integrity and bacteria adhesion. The structure, dynamics, phase transition and general assembly of Lipid A bilayers (main responsible for the bacteria endotoxicity) were investigated in this work through atomistic molecular dynamics simulations. A range of temperature (278K, 300K, 328K and 343K), cations (mono- and bivalentes: Mg^{2+}, and Na^{+}) and phenotypes of Lipid A (hexa-, penta- and tetraacilated) of two different Gram-negative bacterias (*Pseudomonas aeruginosa* e *Escherichia coli*) have been tested in order to characterize the membranes and its properties. Phase transition induced by temperature from gel to liquid-crystalline phase was characterized. Moreover, our findings show that Lipid A bilayers undergo from a lamellar to non-lamellar rearrangement in the presence of monovalent ions. This is due to the inability of these ions to crosslink phosphate groups from neighboring Lipid A units. Our findings support two dominant aspects governing Lipid A bilayer membrane assembly: the shape of Lipid A units (conical vs cylindrical) and the ability of the counter ion to crosslink between different phosphate groups. Analysis of simulated trajectories do not support quantitatively the experimental proposition that correlates the tilt angle between the glucosamines rings of Lipid A and the membrane plane with acyl chain phenotypical variation. The GROMOS53A6 force field were used to build the topologies and all simulations were performed with the GROMACS software package.

Poster

Magnetic nanoadsorbents for Environmental Recovery

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Chemistry Institute – University of Sao Paulo

The demand for low cost and high efficiency methods for removal/recovery of heavy metals, pesticides and nitrogen compounds from water bodies is increasing as a function of the intalled industrial capacity and more rigorous environmental laws regulating the maximum concentration of polutants in the efluents, assuring the health and safety of the population. The application of well-established materials such as activated charcoal, chitosan and zeolites combined with superparamagnetic iron oxide nanoparticles emerge as a viable strategy for the treatment of large volumes of wastewater decreasing the process time and cost by magnetic precipitation/separation.
Magnetizable activated charcoal and zeolite were applied for treatment of industrial waste water in order to make them suitable for disposal in water bodies according to the current environmental law requirements. The designed process allow cutback the nitrogen (NH3) content from 300 ppm (diluted slurry source) to less than 36 ppm (Ion Selective Electrode Potentiometric Measure), hexavalent chromium (chromate source) from 50 **ppm** to 9 **ppb** and undetectable die color in industrial wastewater sample (UV-visible absorbance measurement). The present research work has as focus the demand for new materials for treatment of industrial wastewater.

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Poster

A Dynamical Approach to Time Series with Fluctuating Statistical Parameters

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Time series distributions in complex physical systems may show strong deviations from Gaussian statistics which can be understood as a superposition of different dynamics with well separated time scales. In this interpretation, Gaussian statistics holds on short time scales as a quasi-equilibrium distribution with parameters that change on larger time scales. Averaging over these fluctuating parameters with a suitable statistical model yields a compounding that provides a description of non-Gaussian distributions of physical observables, such as velocity increments in turbulent flow. This scheme, known in physics as superstatistics, has had great successes in describing phenomena as diverse as turbulence in classical fluids [1], microwave propagation through disordered cavities [2] and price variations in financial time series [3,4]. Recently [5], an interesting multiscale extension of superstatistics was introduced by studying the stationary solution of a hierarchy of coupled stochastic differential equations (EDE) which achieved good agreement with experimental data on classical turbulence. In this work we extend this EDE approach in two ways: (i) we focus on time-lagged increment distributions, as opposed to marginal stationary distributions; (ii) we account for long time-lagged Gaussian asymptotic behavior in the increment distributions by inserting time-dependence on some EDE parameters. In addition, we provide a novel procedure to extract the time series of the fluctuating parameter of the short-time Gaussian statistics, which describes well heavy-tailed long-time compounding distributions. Our numerical results show good qualitative agreement with experimental data on Eulerian turbulence.

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Poster

Effect of wettability in residual oil saturation within surface treated micromodels

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Enhanced oil recovery methods are highly influenced by the wetting affinity of the rock containing oil. We present an experimental study of oil being displaced by water through visualization of the flow in a glass microfluidic chip that is used as a two-dimensional porous space. Two different devices are used, one preferentially wetted by water and the other by the oil phase. The porous micromodels, whose network is composed by 100 microns channels with different constrictions ranging from 60 microns, are initially saturated with Drakeol 7 oil (white mineral oil, 17.8cP @ 25C). The oil contained in the micromodels is then displaced by deionized water, which is injected using syringe pumps at various constant rates, covering capillary numbers between 3.10^{-7} and 5.10^{-5}. Using an inverted microscope, the micromodel is swept in its entirety and image analysis (coupled with the fact that injected water is colored) allows us to calculate the residual oil saturation after two porous volumes water are injected. The results allow us to affirm that there are two completely different displacement patterns, influenced by the micromodel surface wettability. Understanding these mechanisms is the first step to improve several experiments regarding enhanced oil recovery in real porous systems.

Figure: Water phase distribution after injection of 2 pore volumes in a (a) water-wet porous media and (b) oil-wet porous media.

Poster

Highly stabilized alpha-$NiCe(OH)_2$ nanomaterials for use in electrochemical devices

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The nickel hydroxide ($Ni(OH)_2$) have been widely studied as electroactive materials for batteries and devices. The $Ni(OH)_2$ presents the α and β polymorphs, where the first one has superior electrochemical properties. However, the α-$Ni(OH)_2$ is not stable and convert to the β form easily[1]. In this context, we propose the synthesis and characterization of the highly stabilized α-$NiCe(OH)_2$ nanoparticles in order to increase the performance of NiMH batteries. The combination of cerium, as additive, and nanostructured materials revealed a very promising approach for this purpose. Thus, we prepared the new α-$NiCe(OH)_2$ nanoparticles electrodes with large specific charge/discharge capacity and high structural stability, withstand up to 2000 redox cycles without any significant phase transformation, as confirmed by cyclic voltammetry and transmission electron microscopy.

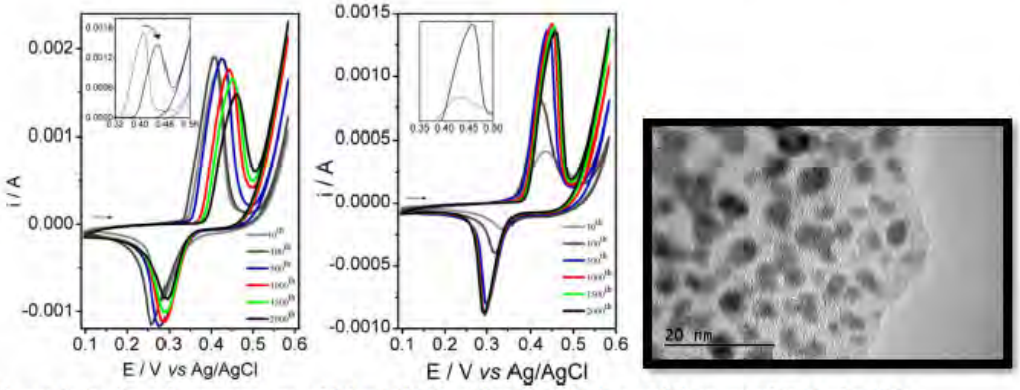

Figure 1: Cyclic voltammograms of (A) α-$Ni(OH)_2$, (B) α-$NiCe(OH)_2$ and (C) Image of TEM of α-NiCe.

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Poster

Mean Field PEM Pore Network Models: Effective Transport Properties

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Polymer electrolyte membranes (PEM) are a crucial component in PEM fuel cells due to their role as proton conductors. The PEM itself consists of water-filled domains which facilitate the transfer of protons through the membrane by proton exchange between acidic surface groups and water molecules in the domains. These nanopores, forming a complex pore network, all have varying, random properties (e.g. geometries, radii, surface charge density) which influence the flow of water and ions. Therefore, studying the flow both through a single nanopore as well as through the network, is needed to derive effective transport characteristics of the PEM.
In this contribution, we use a mean field pore network model to investigate effective transport properties of the PEM. This is done combining thermodynamically consistent equations for the water and ion fluxes [1, 2] with a pore network described at equilibrium [3, 4]. Using randomised surface charge densities, this forms the basis for large-scale simulations, which allows us to reproduce important equilibrium (water sorption, swelling) and non-equilibrium properties of the membrane (electro-osmotic drag, conductivity).

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Poster

Pore-scale analysis of oil recovery by injection of polymer solution

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Water flooding is the most commonly used oil recovery method in the oil industry. However, the high mobility ratio between the water and oil phases limits the amount of oil displaced by the water phase. An effective alternative to minimize this problem is the application of technologies that act as mobility control agents. Polymer solution is used in many cases as a way to increase the water phase viscosity and consequently reduce the mobility ratio. Experimental evidences have shown that the elastic behavior of some polymer solution may not only improve the mobility ratio but also contribute to a better pore level oil displacement, reducing the residual oil saturation. This pore level behavior is not clearly understood. In this work, a glass microfluidic chip made of a 2-D array of channels is used as a two-dimensional porous space. This device has the principal features of a porous media and provides means for pore level flow visualization. A microscopic is used to monitor the evolution of the water phase as it displaces oil and images of the saturation profiles can be made. Three different water phases were used: pure water, a high molecular weight poly(ethylene oxide) solution and a glycerol-water mixture with the same viscosity of the polymer solution. Flow visualization provides specific information about the presence of the trapped oil phase and the movement of the oil/water interface in the network. Results show that the viscoelastic forces modify the liquid distribution in the porous media, improving the displacement efficiency at pore scale and consequently the residual oil saturation.

Poster

Displacement of high viscous oil using different elastic polymer solutions

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The injection of polymer solution is used as an Enhanced Oil Recovery method in many fields. The addition of polymer molecules to the injected water increases its viscosity, leading to a better mobility ratio between the oil and water phases and consequently larger volumes of produced oil. However, despite recent progress, the fundamental understanding on how elastic properties of a polymer solution improve oil recovery is still not complete, mainly when the displaced oil presents a high viscosity.
The oil displacement experiments were performed using silica sandpack and different water phases were used to displace the high viscous oil present in the sandpack: different types of water (deionized, intermedium and high salinity) and two high molecular weight polymer (PEO or HPAM) solutions dissolved in the mentioned different types of water. The different polymer solutions had the same shear viscosity at the characteristic shear rate from the flow in order to study the role of extensional viscosity.

Poster

LTCC Microfluidic Devices applied on Synthesis and Modification of Nanoparticles

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Microfluidics has brought diverse advantages on chemical processes improving the control on chemical processes; enhancing mixing and heat and mass transfer processes; increasing the safety; decreasing energy, time and reagent consumption; and making possible the use of portable and tailor-made devices. Among the different type of materials used for microfluidic devices, ceramics have special characteristics: suitable thermal, mechanical and electrical properties, high chemical resistance, and low cost. Low temperature co-fired ceramics (LTCC) have additional advantages as compared to conventional ceramics, like easiness to integrate with optical and electrical components, low processing temperature, good control of thickness and low surface roughness.
Nanomaterials are currently used in diverse areas such as catalysts, cosmetics, medicines, fuel, sensors and additive of polymers. However, there are many problems associated with controlling the synthesis of nanomaterials, which can lead to irreproducible results or low-quality materials (non dispersable, polidisperse nanoparticles, with wrong surface functionalization). The conjugation of LTCC technology with microfluidics allows the development of micrometric sized channels and reactors exploiting the advantages of fast and controlled mixing and heat transfer processes, essential for the synthesis and surface functionalization of nanoparticles. In fact, it is possible to dream with one step bottom up synthesis, in a continuous and highly controlled and homogeneous process, generating nanoparticles with high monodispersity, and low reagents consumption. Accordingly, we are focused on the development, test and optimization of microfluidic systems for fabrication of nanoparticles, using the Brust-Schiffrin and Turkevich method for synthesis of gold nanoparticles as model systems. The preliminary results will be presented in the workshop.

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Poster

On the pressure-driven flow of suspensions: particle migration in shear sensitive liquids

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Fundamental understanding of flows of suspensions is key in many different areas such as bioengineering, oil, food, pharmaceutical and cosmetic industries. Two important phenomena may occur in the flow of particle suspensions. The first is associated with the relaxation process of particles towards a rest state after the flow is stopped that leads to shear-sensitive viscosity. The second is associated with particle-particle interaction that leads to shear-induced migration. The intensity of each of these effects is directly associated with particle size and imposed deformation rate. The available analyses are usually limited to one of these phenomena. A common approach is to consider that the suspension viscosity varies with shear rate, using a viscosity function to describe this dependency, and that the particle concentration is uniform throughout the flow. Most of the studies that consider shear-induced particle migration assume that the viscosity varies only with the local particle concentration and is not a function of shear rate. The range of validity and accuracy of these two approaches is not well understood. In this work, we analyze the fully developed flow of particle suspensions in a tube using different flow models to evaluate the effect of both particle migration and shear dependent viscosity. The results show that, at certain conditions, accurate predictions on the flow rate-pressure gradient relation can only be made by considering both phenomena in a fully coupled, non-linear flow model.

Poster

Anomalous law of cooling in nano systems

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We analyze the temperature relaxation phenomena of systems in contact with a thermal reservoir that undergoes a non-Markovian diffusion process[1]. From a generalized Langevin equation, we show that the temperature is governed by a law of cooling of the Newtons law type in which the relaxation time depends on the velocity autocorrelation and is then characterized by the memory function[2]. The analysis of the temperature decay reveals the existence of an anomalous cooling in which the temperature may oscillate. Despite this anomalous behavior, we show that the variation of entropy remains always positive in accordance with the second law of thermodynamics[3-4].

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Poster

Magnetic and Wrinkle Patterns in *Saccharomyces cerevisiae* Colonies

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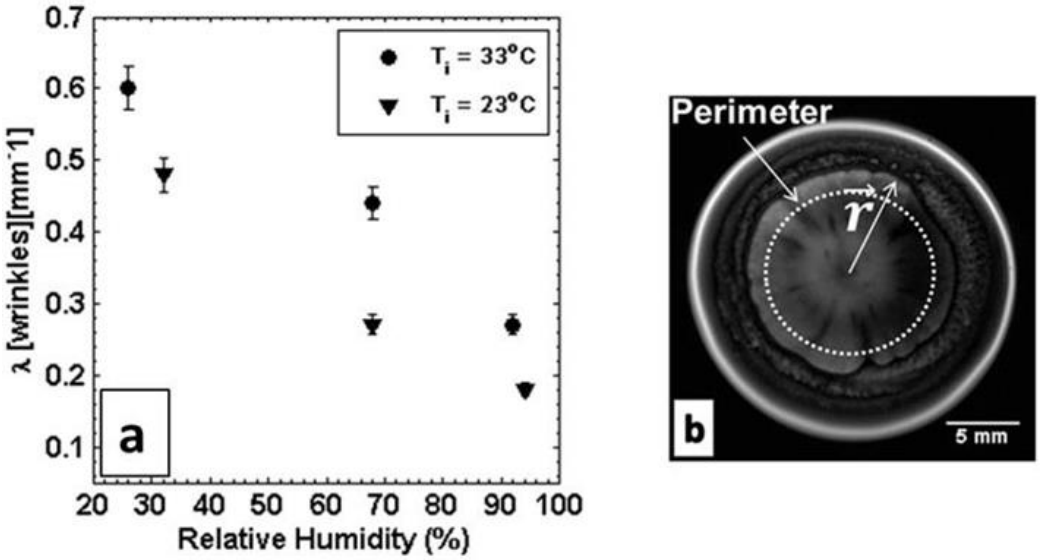
Here we investigate the magnetic pattern of colonies of the yeast *Saccharomyces cerevisiae* observed with Nuclear Magnetic Resonance (NMR) imaging. The quantification of the effects were done by producing the respectively $\mathbf{T_2}$ and $\mathbf{T_2^*}$ maps. This is simply done by fitting of the collections of images, obtained by each sequence with different $\mathbf{T_E}$, to the equation $\mathbf{S = S_o exp(-T_E/T_2)}$. Our results indicate a large demagnetization effect distributed spatially in specific regions of the colony with respect to others. The observed patterns are due to the discontinuity of the magnetic susceptibility ($\boldsymbol{\chi}$) in the colony. The variation in the magnetic susceptibility ($\boldsymbol{\Delta\chi}$) induces a loss in the NMR signal that scales with ~ $\mathbf{exp(-i\gamma g \Delta\chi B_o T_E)}$, where $\boldsymbol{\gamma}$ is the gyromagnetic constant, $\mathbf{g}$ is a geometric factor of the magnetic susceptibility and $\mathbf{B_o}$ is the applied magnetic field. Our findings were applied to study the wrinkle patterns seen in the surface of the colony as a function of relative humidity (RH) and temperature (T).



Poster

A new technique to prepare Metal-Organic Frameworks by laser ablation in liquid

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Metal organic frameworks (MOFs) belong to a class of polymeric material composed by three-dimensional (3D) metal coordination network structures consisting of metal ions or clusters linked together by organic bridging ligands. The high surface areas presented by these materials, combined with an uniform small porous architecture make MOFs promising materials for a large range of applications [1]. Regarding to the sample preparation, almost all methods used for MOFs preparation are time consuming, except for the Microwave-assisted processes, and therefore new methods should be developed. On the other hand a non-conventional and less used synthesis technique for sample preparation is laser ablation in liquid (LAL) medium. This technique has been extensively used in the past two decades. The reason to use this technique nowadays is that LAL can be considered a chemically clean and an one-pot synthetic route, which is able to prepare a variety of functionalized new nanostructures and more recently chemical compound [2] . Also it is a low cost experimental technique, which presents few controlled parameters and provides extreme confined conditions of high temperature and pressure that favor the formation of metastable phases[3]. This work presents a chemical bottom-up synthesis of highly crystalline sub micro structured metal organic framework $Cu_3(BTC)_2(H2O)_3$ (HKUST-1, BTC=benzene-1,3,5-tricarboxylate) prepared for the first time by Laser ablation technique in liquid. The experiment consists of the ablation of a Cu metal target in a solution of DMF/H_2O (1:1) containing benzene 1,3,5, benzene tricarboxilic acid and $NaNO_3$ with a high power second harmonic of a Nd:YAG laser. The x-ray and SEM measurements showed that high crystalline $Cu_3(BTC)_2(H_2O)_3$ with octahedral morphology and dimensions in the range of 200 nm - 2 μm were obtained in a high yield [4].

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Poster

Synthesis and characterization of Fe(BTC)-iron oxide composites

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Metal Organic Framework (MOF) form a class of crystalline materials having high porosity and because of this property become important for applications in the storage of gases and in catalysis[1]. A chemical synthesis of Fe(BTC) (BTC = 1,3,5-benzenetricarboxilic acid) metal organic framework was prepared by three different techniques: assisted by ultrasonic radiation, solvothermal and eletroquemichal methods. All experiments were realized by the same initial reactants conditions (except for eletroquemichal method), which consists in a solution of DMF/H2O (1:1) containing BTC and NaNO3 with iron powder (α-Fe). The x-ray and SEM measurements showed that sample x-ray patterns is similar to those found in the literature and has a rods likes morphology. The magnetic measurements indicates a paramagnetic characteristic strongly dependent of the initial parameters.

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Poster

Simulated NMR Analysis of Brine Confined in Calcite Slit Pores

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Nuclear Magnetic Resonance (NMR) is a powerful tool for analyzing the dynamic properties of liquids confined in a porous matrix. In this work, we use classical molecular dynamics simulations to predict NMR spin-spin relaxation time T2. We investigate the effect of temperature, concentration of ions and confinement in calcite slit pores (1-6nm) on the relaxation time of water, salt and brine. We observe that the T2 relaxation time increases with increase in temperature. The presence of Na+, Cl- and Ca2+ ions slow down the dynamics of water with this effect more pronounced for solutions with high concentration of ions. The water and brine dynamics in the calcite pores splits into two different behaviors depending on the location in the slit pores: water and brine located on the surface of the calcite relax slowly compared to molecules located far from the surface. It was found that the strong surface interactions lower considerably the surface relaxation time. Compared to bulk water/brine, water/brine confined in the 1 and 2 nm slit pores has a shorter T2 relaxation time while for larger pores, the relaxation times are comparable to values obtained for the bulk systems. These results are expected to be relevant for enhancing the understanding of the pore size distribution in carbonate reservoir rocks.

Poster

Formation of loops in the packing of a flexible rod into annular cavities

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The injection of a filamentous object inside confined environments is a very interesting non equilibrium problem which is related to several biological and technological applications. In order to investigate this process we performed experiments of injection of a thin rod into annular cavities. Each self contact of the rod splits the total area of the cavity in cells with a given number of vertexes. The cell that is formed by one vertex is called "loop". In such a way, the problem can be analyzed by both continuum and discrete approaches. Although the system presents several important features as jamming transition, morphological phases, and order-disorder transition, the study of the dynamic process of creating loops was still lacking. We find that an exponential hierarchy describes the total length needed to create each loop in the geometrical pattern. An extrapolation to infinite loops shows that the fraction of the area covered by the rod would be fixed irrespective the width of the annulus. The experiment also allows us to observe stick-slip instabilities near the tight packing. Furthermore, comparisons with results for the simply connected cavity shows the impact of the topology of the cavity in the number of accessible states for the flexible rod.

Poster

Interfacial instabilities on rotating Hele-Shaw flows with a time-dependent angular velocity.

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The impact of time-dependent angular velocity on the interfacial instability of two immiscible, viscous fluids of different densities, confined in a rotating Hele-Shaw cell is investigated. Linear and weakly nonlinear stages of the dynamics are described analytically through a mode coupling approach. We found that the linear dispersion relation is a complex quantity, where the imaginary part represents a travelling wave, with speed in the θ direction. Thus, the inertial force tends to move the fingers "backwards", deviating them from the purely radial growth. We also examine how finger competition dynamics is affected by this inertial force.

Poster

Option pricing with Gaussian and non-Gaussian models: Application to the Brazilian market

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We present an empirical analysis of different option pricing models as applied to options on the Ibovespa index of the São Paulo Stock Exchange. Besides the standard Black-Scholes for option pricing model which assumes that the returns are Gaussian distributed, two non-Gaussian models are analyzed, namely, the exponential model [1,2] and the model introduced by Borland [3] which assumes that the returns follow a distribution with power-law tails, the so-called Tsallis distributions. We compare the predictions of these models with the actual market prices for options on the Ibovespa index during a period spanning two years of trading (2005-2006). It is found that the exponential model performs better than both the Black-Scholes and Borland models, in the sense that it fits the empirical data better than does the other two models. In addition, it is observed that the Borland model performs better than the Black-Scholes, as expected since the former model is based on a more general non-Gaussian distribution which has the Gaussian as a special case. In all cases analyzed, the q parameter of the Tsallis distribution was found in the range $1 < q < 5/3$, suggesting a distribution with heavy tails. The central part of the empirical distribution of returns follows, however, an exponential distribution [2], and this explains why the exponential model describes better the option data in spite of the power-law tails of the distribution of returns.

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Poster

Molecular simulations of atomistic crude oil models with brine interfaces at reservoir conditions

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The understanding of molecular mechanisms underlying Enhanced Oil recovery processes becomes essential for their optimization and new developments. Experimentally, the characterization of wettability and interfacial properties at reservoir conditions can be time consumed and expensive. Here, molecular simulations of oil-brine interfaces have been performed and their thermodynamical properties characterized at both ambient and reservoir (337 K and 547 atm) conditions. Molecular dynamics (MD) was applied to simulate light and medium oil models interfaced with API brine and sea water. The light oil is a combination of alkanes, cycloalkanes and aromatic hydrocarbons, while the medium oil was based on the dead oil composition found in the Brazilian Pre-Salt. To describe the interactions between these systems, the following interatomic potentials have been used: SPCE/FH for water, CHARMM for oil, while the ions were described by point charge model and a flexible model for sulfates. Density profile shows the accumulation of aromatics in interface, which leads to a lowering interfacial tension between aromatics and water. The medium oil was found to have a lower interfacial tension than light oil at both conditions, mainly due to a higher concentration of aromatics with a higher molecular weight. The diffusivity of the molecular species was determined and the effects of brine composition on the transport properties elucidated. Our proposed atomistic oil and brine models with their interfacial characterization based on MD leads to an interesting cost-effective way to test new EOR processes at reservoir conditions.

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