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“Cooperative particles:  
Patchy colloids, active  
matters and nanofluids”  
The Geilo School 2015  
16-26 March  
Geilo, Norway:  
POSTER ABSTRACTS



Institute for Energy Technology



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Summary <p>The purpose of this Geilo School was in part at reviewing the theoretical progress in the field of active matter, placing it in the context of recent experiments. This relates to mechanical and statistical properties of living matter, like bio filaments and molecular motors in vitro or in vivo, collections of motile microorganisms, animal flocks, and chemical or mechanical imitations.</p> <p>This report contains the abstract for the posters presented at this School.</p> <p>There were altogether 16 lecturers at the School with a total of 75 participants from 18 countries. This was the 23<sup>rd</sup> Geilo School held every second year since 1971. References to earlier Geilo Schools 1971-2013 can be found at <a href="http://www.ife.no/departments/physics/projects/geilo">www.ife.no/departments/physics/projects/geilo</a>.</p>			
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## 1 Introduction

The term active matter describes diverse systems, spanning macroscopic (e.g. schools of fish and flocks of birds) to microscopic scales (e.g. migrating cells, motile bacteria and gels formed through the interaction of nanoscale molecular motors with cytoskeletal filaments within cells). Such systems are often idealizable in terms of collections of individual units, referred to as active particles or self-propelled particles. These take energy from an internal replenishable energy depot or ambient medium and transduce it into useful work performed on the environment, in addition to dissipating a fraction of this energy into heat. The individual units may interact both directly as well as through disturbances propagated via the medium in which they are immersed. Active particles can exhibit remarkable collective behavior as a consequence of these interactions, including non-equilibrium phase transitions between novel dynamical phases, large fluctuations violating expectations from the central limit theorem and substantial robustness against the disordering effects of thermal fluctuations.

Patchy materials relates to the next generation of materials and devices for molecular electronics, photonics, drug delivery and sensing, which rely on the self-assembly of synthetic nanostructures with the precision of biological organization processes. But despite tremendous advances in the fabrication of a wide range of organic and inorganic nanoscale building blocks of various sizes and shapes, control over their assembly into ordered structures remains the main obstacle to the bottom-up fabrication of these novel materials and devices.

As material systems are made smaller approaching the nano-scale, changes occur which may affect properties. The number of atoms close to surfaces increases relative to the numbers that are truly in the bulk. At the same time, thermodynamics is no longer controlled by the laws of large numbers, so dynamical fluctuations often cannot be viewed as Gaussian. Liquids flowing through narrow tubes ("microfluidics/nanofluidics") exhibit laminar flow and do not mix in the same way as fluids in macroscopic containers. In many complex fluids the relative importance of various forces depends on system size so that in biological cells, for example, dissipative forces dominate inertial forces. These and other distinctions between the properties of truly macroscopic systems and those whose spatial dimensions are constrained were explored at this School, with special emphasis on effects which occur in soft matter, where thermal and cohesive forces are of similar magnitude, in many areas of nanotechnology and advanced materials.

The theme of the School fits into the core problem areas of *Complex Systems and Soft Materials* run by the COMPLEX Coordinated Research Team (CRT) in Norway<sup>1</sup>. The COMPLEX CRT has now been working together for nearly 15 years

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<sup>1</sup> <http://www.complexphysics.org/>

and consists of physicists based at three different institutions in Norway: The Norwegian University of Science and Technology (NTNU) in Trondheim, The University of Oslo (UiO) and The Institute for Energy Technology (IFE) at Kjeller. Many of the partners and students involved in the CRT participated in the School. A significant number of international collaborators with the CRT from the Nordic countries as well as Argentina, Brazil, Cuba, France, Germany, Iran, Italy, Lithuania, Moldova, the Netherlands, Poland, Switzerland, UK, Ukraine, and USA also participated in the School.

An added feature with this School was to initiate topics relevant for the upcoming European Spallation Source (ESS) in Lund essential for European infrastructure collaboration coupled to nanotechnology.

## 2 Program Geilo School 2015

<b>1<sup>st</sup> Day Monday March 16</b>		
14:30-18:00	Arrival	Communal transportation from Oslo to Geilo
18:00-19:00	Registration	
19:00-19:30	Reception	
19:30-21:00	Dinner	
21:00-21:30	Opening	
<b>2<sup>nd</sup> Day Tuesday March 17</b>		
08:30-11:30	Francoise Brochard	Active entangled matter: from ants to cells
11:30-15:30	Outdoor activities and lunch	
15:30-17:30	Erik Luijten	Patchy colloids
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
<b>3<sup>rd</sup> Day Wednesday March 18</b>		
08:30-09:30	Erik Luijten	Patchy colloids (Ctd.)
09:30-11:30	Julia Yeomans	Active Nematics
11:30-15:30	Outdoor activities and lunch	
15:30-16:30	Julia Yeomans	Active Nematics (Ctd.)
16:30-17:30	Emanuela Zaccarelli	Patchy colloids
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
<b>4<sup>th</sup> Day Thursday March 19</b>		
08:30-10:30	Emanuela Zaccarelli	Patchy colloids (Ctd.)
10:30-11:30	Paul Dommersnes/Jon Otto Fossum	Electrodriven colloidal assembly: Patchy and active systems
11:30-15:30	Outdoor activities and lunch	
15:30-17:30	Paul Dommersnes/Jon Otto Fossum	Electrodriven colloidal assembly: Patchy and active systems (Ctd.)
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
<b>5<sup>th</sup> Day Friday March 20</b>		
08:30-11:30	David L. Hu	Fire ants as an active material
11:30-15:30	Outdoor activities and lunch	
15:30-16:30	Thomas Kiørbo	Swimmers
16:30-18:30	Poster session	Posters left on display until Wednesday March 25

<b>6<sup>th</sup> Day Saturday March 21</b>		
08:30-10:30	Thomas Kiørbo	Swimmers (Ctd.)
10:30-11:30	Ernesto Altshuler	Self-propelled particles: from bacteria to ants...or vice versa.
11:30-15:30	<i>Outdoor activities and lunch</i>	
15:30-17:30	Ernesto Altshuler	Self-propelled particles: from bacteria to ants...or vice versa. (Ctd.)
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
<b>7<sup>th</sup> Day Sunday March 22</b>		
Free	<i>Choice of excursions to nearby scenic places or various skiing events in the mountains</i>	
<b>8<sup>th</sup> Day Monday March 23</b>		
08:30-11:30	Jan Vermant	Rheology of particle suspensions in 3 and 2D
11:30-15:30	<i>Outdoor activities and lunch</i>	
15:30-17:30	Yves Meheust	The flow of an aqueous foam through a two-dimensional porous medium
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
<b>9<sup>th</sup> Day Tuesday March 24</b>		
08:30-11:30	Marcio Carvalho	Emulsions in porous media
11:30-15:30	<i>Outdoor activities and lunch</i>	
15:30-16:30	Reidar Lund	Confinement effects in self-assembled systems
16:30-17:30	Julia Yeomans	Unusual bouncing on superhydrophobic surfaces
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
<b>10<sup>th</sup> Day Wednesday March 25</b>		
08:30-10:00	Katherine Aurand	The use of nanofluids for enhanced oil recovery
10:00-11:30	Heloisa Bordallo	Neutron scattering as a tool and ESS
11:30-15:30	<i>Outdoor activities and lunch</i>	
15:30-16:30	Heloisa Bordallo	Neutron scattering as a tool and ESS (Ctd.)
16:30-17:30	Roger Pynn	Seminar
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
19:30	<i>Geilo School Closing Dinner</i>	<i>Geilo Awards, Poster Prizes etc.</i>
<b>11<sup>th</sup> Day Thursday March 26</b>		
08:00-13:30	Departure	Communal transportation of participants to Oslo

### 3 Poster Abstracts

## Diffusion of fused colloidal nanoparticles with hydrodynamic interactions

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Diffusion of colloidal nanoparticles is experimentally observed to significantly deviate from the Stokes-Einstein prediction [1, 2] but the reasons for such deviation are not properly understood yet. Here, we present results from a systematic investigation of the diffusive transport of colloidal nanoparticles, fused clusters and aggregates in a fluctuating Lattice-Boltzmann fluid [3] with explicit implementation of the microscopic no-slip and full-slip boundary conditions at the colloid-fluid interface. Results show that the translational and rotational diffusion of the colloids depend on their shape, size and the type boundary condition imposed. Further, the translational and rotational behavior of the nanocolloids are observed to deviate from the experimentally studied diffusion of submicron fused clusters [4] implying scale dependence of the diffusive transport of colloids.

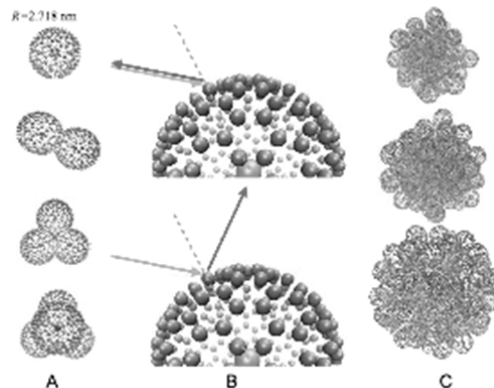


Figure 1: Graphical representation of the particles: A. fused colloidal nanoparticles and C. nanoparticle aggregates. The relative fluid-particle velocities of the no-slip (top) and full-slip (bottom) boundary conditions are illustrated in B.

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## Hydration state stability in Ni-fluorohectorite smectite clay

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X-ray diffraction measurements have been performed on powder samples of synthetic Ni-fluorohectorite smectite clay as a function of relative humidity for different temperatures. It is found that the basal spacings, calculated from the (001) Bragg peak positions, correspond to zero, one, two and three layers of H<sub>2</sub>O respectively, intercalated between the smectite layers. In addition, the existence of an intermediate stable state in-between one and two H<sub>2</sub>O layers, termed one-and-a-half water layers is clearly observed. The transition between the states is observed to be continuous, an observation which is markedly different from previous reported studies of Na-fluorohectorite and Li-fluorohectorite smectite clays. In the present work, average clay stack particle thickness and lattice strains were obtained from standard Williamson-Hall analysis of Bragg peak widths. The lattice strains display low values at low relative humidity of the environment, and an increase when the relative humidity is increased. It is found that the transition between the one and one-and-a-half water layer states depends on the initial sample preparation conditions, as well as on the experimental history. This kind of behaviour could possibly exist for smectite clays in general, and could thus have significant practical consequences in materials science and other areas where smectite clays are important.

## **PROGNOSTICATION OF DIRECTIONS OF DANGEROUS INFLUENCE OF RADIOACTIVE WASTES STORES**

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### **Abstract**

Under the centralized command administrative system of former USSR, the strategy of Ukrainian Nuclear Fuel Cycle development lacked proper assessment of regional and local ecological conditions. And now the radiological influence of failures of the Nuclear objects (without control radioactive wastes accumulation) of Central Ukraine can become small new repetitions of the Chernobyl Nuclear Power station catastrophe (April 04, 1986). This paper reports the use of new rules of Physics of Earth (in particular – the model of geostasy) as the new tectonical basis of prognostication the priority directions of dangerous influence of Nuclear Fuel Cycle objects and, first of all, not liquidated (not functioning) radioactive wastes stores of Central Ukraine. It's very important for concentration of necessary administrative efforts and finance for prevention of “development“ and liquidation of emergency radioactive pollution of concrete region. The using of the information about features of Earth's crust faults enables to determine the concrete azimuths of dangerous emissions of Nuclear objects, including radioactive wastes stores.

### **Main Objectives**

The new tectonical basis of prognostication of the azimuths of dangerous influence of Nuclear Fuel Cycle objects – for concentration of necessary administrative efforts and finance for prevention of “development” and liquidation of emergency radioactive pollution of concrete region

### **New aspects**

The using of new rules of Physics of Earth (in particular - the model of geostasy) as the new opportunities for the effective definition of azimuths of dangerous emissions of Nuclear objects, including not liquidated (not functioning) radioactive wastes stores.

## **Adhesion force in fluids: Effects of fingering, wetting, and viscous normal stresses.**

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Probe-tack measurements evaluate the adhesion strength of viscous fluids confined between parallel plates. This is done by recording the adhesion force that is required to lift the upper plate, while the lower plate is kept at rest. During the lifting process, it is known that the interface separating the confined fluids is deformed, causing the emergence of intricate interfacial fingering structures. Existing meticulous experiments and intensive numerical simulations indicate that fingering formation affects the lifting force, making it to decrease in intensity.

In this work, we propose an analytical model that computes the lifting adhesion force by taking into account not only the effect of interfacial fingering, but also the action of wetting, and viscous normal stresses.

The role played by the the system's spatial confinement is also considered. We show that the incorporation of all these physical ingredients is necessary to provide a better agreement between theoretical predictions and experiments.

## A microfluidic Approach to Produce Monodisperse O/W Emulsions Stabilized by Laponite nanoparticles

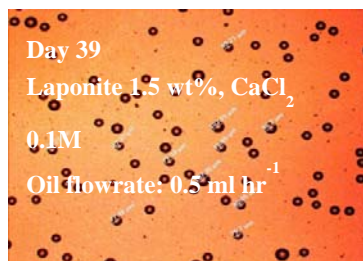
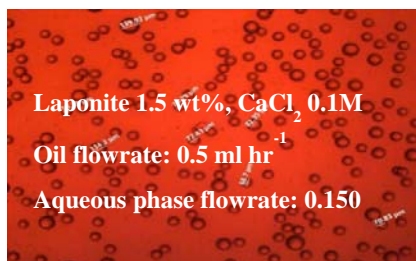
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Research on emulsions is driven by their wide-spreading use in different industries, such as food, cosmetic, pharmaceutical and oil recovery.<sup>1</sup> Emulsions are stabilized by suitable surfactants (electrostatic stabilization)<sup>2</sup>, polymers, solid particles (steric stabilization)<sup>3</sup> or a combination of them. A microfluidic emulsification is the process of droplet formation out of two or more liquids under strictly controlled conditions, without pre-emulsification step.<sup>4,5</sup> Microfluidic technology offers a powerful tool for investigating the properties of emulsions themselves.<sup>6,7</sup>

In this work stable O/W emulsions were formed with hydrophilic Laponite RD® nanoparticles adsorbed at the interface of Drakeol 7 ® as the oil phase and water in a Dolomite ® droplet T junction chip. Salt (NaCl or CaCl<sub>2</sub>) was added to flocculate the laponite particles and hence to increase the emulsion stability.<sup>8</sup> The presence of particles did not influence drop formation dynamics and thus the size of the drops generated. Different flow rates and different Laponite concentrations were examined to determine their effect on the stability of the formed emulsions. In some conditions, emulsions were stable up to 40 days. On the other hand interfacial dilational rheology studies were carried out to have an insight into the stabilization mechanism of Laponite nanoparticles. While using Laponite as well as salt, crumpling was observed upon compression.



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## **Drop breakup in turbulent flow through an orifice**

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As the two-phase oil-water mixture flows through the producing wells, risers and valves, the disperse phase may break leading to stable emulsions. The size of the dispersed oil drops has a strong effect on the flow resistance and on the phase separation process. Most of the drop breakup occurs as the oil-water mixture flows in turbulent regime through valves and narrow passages. Despite the large volume of experimental work reported in the literature, the relationship between the drop size distribution downstream of an orifice and the flow conditions is not clearly understood.

In this work, we study experimentally the drop breakup of an oil-water emulsion as it flows through an orifice. Two mineral oils of moderate viscosity were dispersed in two different continuous phases, tap water and a continuous phase formed by a mixture of substitute ocean water and the anionic surfactant STEOL® CS-330 (Stepan Company). The drop size distribution downstream of the flow restriction is measured as a function of the flow conditions, liquid properties and drop size distribution upstream of the orifice. Results show that, for each flow condition, there is a maximum stable drop diameter below which the drops do not break. Analysis of the data revealed that maximum stable drop sizes were in the inertial sub range, characterized exclusively by the energy dissipation rate per unit mass.

Details of the breakup process was studied by visualizing the breakup of a single drop using a high-speed camera. The images show that drop breakup only occurs downstream of the restriction and takes place at a certain distance from the edge of the orifice. At this breakup length, the radial velocity gradient in the flow is large enough to overcome the resistance stresses (exerted by the droplet) and produce the rupture of the droplet. The visualization has also allowed the analysis of the relative influence of interfacial tension and dispersed phase viscosity.

## Pattern formation in synthetic and living systems

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The formation of contour patterns in the heterogeneous growth of layered structures is of considerable interest for understanding the morphogenesis of many structures, including living organisms. Microorganisms, such as bacteria and fungi, exhibit characteristic patterns by forming biofilms and colonies<sup>1</sup>. Several studies show that in *Saccharomyces cerevisiae* colonies, the radial distribution of the cells varies depending on the proximity to the edge of the colony, in which younger cells are distributed along the edge and the older cells are more concentrated in the center of the colony.<sup>2</sup> We have initiated our studies by monitoring the time evolution of surface pattern formation in a swelling spherical gel using MRI of water migrating into the gel<sup>3</sup> (Fig. 1). The breaking of spherical symmetry caused by the growth of an instability produces a surface undulation and the formation of a pattern<sup>4,5</sup>. These experimental results were compared with the predictions of a nonlinear poroelastic theory<sup>6</sup> by numerically solving the nonlinear equations of evolution within a spherically symmetric approximation<sup>7</sup>. Recently, our group has started studies in imaging of microorganism colonies. Accordingly, images from different colonies of *Saccharomyces cerevisiae* were obtained and showed a characteristic patterns of formation (Fig. 2). The contrast observed on the images has its origin in the difference in magnetic susceptibility within the colony. The variation in magnetic susceptibility can be caused by the presence of paramagnetic ions, microstructure of the colony, orientation of fibers or presence of internal channels relative to the applied magnetic field, or even due to the interface effect between regions with different magnetic susceptibility.<sup>8</sup>

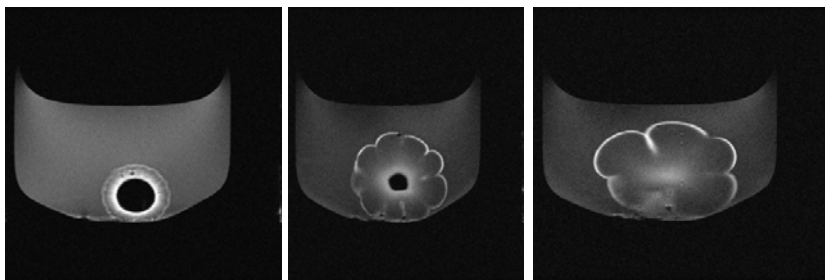


Fig. 1 MRI of initially dry gel as it absorbs water through a swelling process.

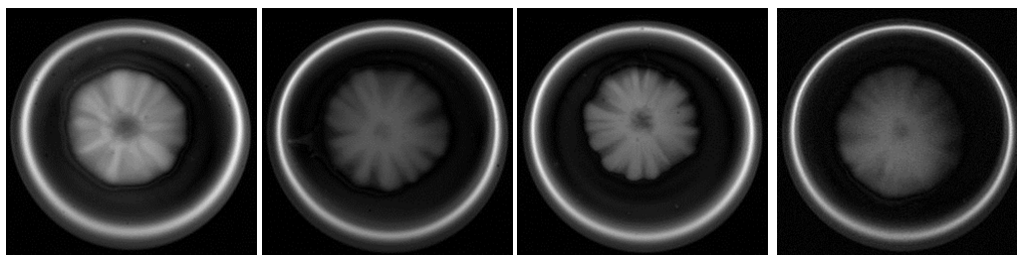


Figure 2. *S. cerevisiae* colonies images obtained by NMR weighted in magnetic susceptibility.

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## Magnetic and structural properties of cobalt-manganese ferrite nanoparticles obtained by mechanochemical synthesis

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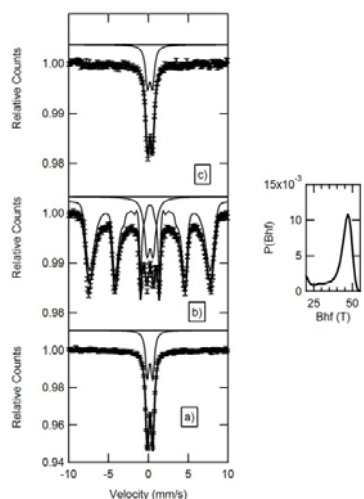
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Nanocrystalline spinel-type oxides  $MFe_2O_4$  ( $M = Co, Mn, Zn, Ni$ ) have received considerable attention because of their unique magnetic properties which significantly differ from the bulk materials. Such oxide-based magnetic nanoparticles have a great potential for technological applications: high density data storage, microwave devices etc.[1] Lately, however, magnetic nanoparticles have been extensively studied because of their possible applications in medicine: cancer therapy by hyperthermia, controlled drug delivery, cell separation and magnetic resonance imaging [2-3].

This study presents the research done on nanoparticles of  $CoFe_2O_4$  and  $MnFe_2O_4$  obtained by mechanochemical synthesis using high-energy ball mill, solid metal salts as precursor and sodium chloride NaCl as a growth agent, for further biomedical applications. *Mössbauer* spectroscopy (Fig.1), magnetization and heating characteristics for magnetic hyperthermia, atomic force microscopy (AFM) and X-ray studies were used to determine the properties of the nanoparticles depending on the conditions of the synthesis. Measurements showed that the particle size of cobalt ferrite varied from 4 nm up to ~10 nm without and with addition of sodium chloride respectively whereas no such effect of sodium chloride on manganese nanoparticles was observed.



**Fig.1.** The Mössbauer spectra

- a)  $CoFe_2O_4$  synthesized without growth agent;
- b)  $CoFe_2O_4$  synthesized with growth agent;
- c)  $MnFe_2O_4$  synthesized without growth agent.

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## EXPERIMENTAL STUDY OF SELF-ASSEMBLY OF WASTE MATERIALS

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It is considered that due to ever increasing concern for the environment the waste materials will be the most important source of raw materials in the future [1]. Today's existing waste recycling strategies can be applied only for uniform materials [2], but one of the inherent features of waste is disorder (i.e. complexity and heterogeneity) that imposes challenging problems during recycling process. The common recycling strategies lie on the processes of collection, identification, purification and etc. These processes are obviously associated with the current mass technology and production systems and restrict further material design and manufacturing alternatives. However, thinking about the new recycling design strategies ever more we look to the nature that uses continuous, closed loop recycling system. One of bio-inspired approaches is self-assembly design which agitates to reconsider all industrial processes. Self-assembly is a process in which disordered system of components under certain conditions forms the well-ordered, organized structure or patterns without the action of external forces. This concept is increasingly used in many technological branches (as physics, chemistry, biology) [3, 4] as well as design [5, 6]. The main questions that should be solved before the application of this concept in practice are origin, principles and control mechanism of self-assembly process. The understanding of these principles could provide a designer a wide variety of design and manufacturing alternatives.

The study demonstrates that in disordered waste materials the patterns emerge due to the fluctuations in particle size, compositions and shape that results in heterogeneous particles dynamics. As long as those fluctuations are small the system stays near the equilibrium, but when fluctuations become significant and reach a critical value (e.g. critical particle size distribution) the system bifurcates and spontaneously forms patterns. Using the principles of self-assembly design the materials disorder is useful feature as they impose the ability to form spatial structures which can be used to shape self-developing and self-building objects.

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## **Using Quasi Elastic Neutron Scattering to study water in confinement in different porous environments**

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By studying the energy transfer around the elastic peak in a sample it is possible to extract important information about the dynamics of that sample. Quasi Elastic Neutron Scattering (QENS) is especially good when studying water, since water is very visible for neutrons.

The dynamics of water in the porous materials depend strongly on the confinement of the water given by the pore size.

By understanding both the confinement and the related dynamics of the sample we can achieve great insight to the mechanical properties of the material.

In this study QENS has been used on two different materials, chalk and dental cement with the purpose of understanding the mechanical properties.

In the case of chalk, the mechanical properties are of great importance to the oil industry that want to improve the extraction process of oil from the chalk located world wide.

In the case of dental cement, the understanding of the dynamics of the materials currently used (Poly) can help develop a new product with better durability. This would be of great benefit to the public health.

## Self-entanglement of single protein molecules in shear flow

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While experimental evidence exists for the accelerating effect of exposure to shear flow on the process of protein aggregation, it is inconclusive as to the role of particular mechanisms potentially responsible for this phenomenon. For instance, flow-induced partial unfolding of the protein structure has been observed under relatively low shear rates in some studies, but appears to be absent in others, despite several orders of magnitude higher shear rates. Some light might be shed on this apparent contradiction by experiments indicating a cumulative character of the shear-induced effects.

To investigate this problem we perform Brownian Dynamics simulations of shear-induced unfolding of bovine serum albumin and ubiquitin. The former protein was reported to unfold at surprisingly low shear rates. Using a coarse-grained model of a protein, we track the conformational changes induced by the flow and observe that after an extended exposure to shear albumin loses its ability to refold even when the flow has been turned off. Instead, it is trapped in a metastable state characterized by a strong self-entanglement which topologically constrains the molecule to fold into the native state. This state becomes more populated with time, which can explain the cumulative effect of the shear observed in the experiments. We compare the behaviour of serum albumin with that of a small protein - ubiquitin - to analyze how the size and internal structure of a protein influence the effects of exposure to shear flow. Additionally, we investigate the impact of hydrodynamic interactions on the process of unfolding. Hydrodynamic interactions turn out to visibly change the protein dynamics and hinder the unfolding process.

## Surface molecular engineering of gold and SPIO nanoparticles for theranostics application

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Recently the Nanotechnology is been explored extensively by Medicine, combining diagnostics by multi-modal imaging and treatment by magnetic and targeted delivery of drugs, besides exploiting their special properties (high surface-area ratio, plasmon surface, superparamagnetism) and generating new materials for theranostics applications. Magnetite nanoparticles are biocompatible magnetic material that are possible for using as MRI contrast agent for imaging that can be conveniently functionalized with biomolecules, generating targeted hybrids for theranostics. Gold nanoparticles have also beneficial interactions with the organisms and can be used for the same purposes.

Folic acid is a low-cost chemical with good tumor targeting properties, because cancer cells produce more folate receptors than healthy ones. However, folate-functionatized nanoparticles are not dispersible in water and PBS, such that other polar groups must be added to improve their bioavailability and bioactivity. Among them sugars, vitamins and antitumor agents are interesting choices. Sugars are global energy sources, and most of them have high hidrofilycity. Antitumor agents can have their entrance easier by different groups attached to the nanoparticles.

Magnetite nanoparticles of about 6 nm prepared by thermal decomposition method were stabilized with phosphorylethanolamine, dopamine or sugars. The functional reactive groups on the surface were exploited to bond biomolecules using EDC and NHS as crosslinking activators generating new hybrid nanobiomaterials. Nanoparticles functionalized with more than one molecule/biomolecule were also prepared and characterized. Analysis by IR spectroscopy confirmed the binding of those biomolecules onto the surface, whereas DLS analysis confirmed the presence of narrow distribution nanoparticles with no aggregation.

The nanomaterials obtained show the possibility of multifunctionalization and tuning of their properties for selected applications. These reactions are being implemented in microfluidic systems to enhance the efficiency reduce energy consumption, and *in vivo* assays will be performed, to observe new interactions of these materials.

## Stationary patterns in centrifugally driven interfacial elastic fingering

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A vortex sheet formalism is used to search for equilibrium shapes in the centrifugally-driven interfacial elastic fingering problem. We study the development of interfacial instabilities when a viscous fluid surrounded by another of smaller density flows in the confined environment of a rotating Hele-Shaw cell. The peculiarity of the situation is associated to the fact that, due to a chemical reaction, the two-fluid boundary becomes an elastic layer. The interplay between centrifugal and elastic forces leads to the formation of a rich variety of stationary shapes. Visually striking equilibrium morphologies are obtained from the numerical solution of a nonlinear differential equation for the interface curvature (the shape equation), determined by a zero vorticity condition. Classification of the various families of shapes is made via two dimensionless parameters: an effective bending rigidity (ratio of elastic to centrifugal effects), and a geometrical radius of gyration.

## **Oil-Fluid (CO<sub>2</sub> and CH<sub>4</sub>) interfaces confined in silicate nanoporous: a molecular dynamics study**

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James Moraes Almeida and Caetano Rodrigues Miranda.

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In our work the effects of CO<sub>2</sub>, CH<sub>4</sub> and oil confinement in silica nanopores (1 to 4 nm diameter) were explored. The structural, thermodynamic and transport properties of the confined fluids were

studied using classical molecular dynamics, at 300 K temperature and pressures ranging from 50 to 200 atm, in order to mimic a geological environment. Also, the surface passivation was varied, by adding SiOH and Si(OH)<sub>2</sub> terminations to the surface dangling bonds (from [13% SiOH

- 87% Si(OH)<sub>2</sub>] to [87% SiOH - 13% Si(OH)<sub>2</sub>]). The chosen force fields were: EPM-2 for CO<sub>2</sub>, Cruz-Chu for silica, CHARMM for oil and CH<sub>4</sub>. We have simulated the infiltration of the fluids to the nanopores, by modeling a reservoir adjacent to a silica block with the nanopore. The molecules of the fluid were free to enter the nanopore, until it reached an equilibrium density. Thus, a reservoir with CO<sub>2</sub> and CH<sub>4</sub> was simulated, then an oil interface is also added, to explore how soluble are the CO<sub>2</sub> and CH<sub>4</sub> under supercritical conditions. We have obtained the radial pair distribution functions, diffusion coefficients, density profiles and interfacial tensions of the CO<sub>2</sub>/Silica, CH<sub>4</sub>/Silica and Oil/Silica interfaces.

## **Solid Particle Transport in Laminar Flow**

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The use of directional wells became frequent in the development of oil fields, allowing great progress in exploration. This scenario, however, brings great challenges to operations related to wellbore cleaning, that consists in the removal of cuttings from within the annular through the circulation of drilling fluid. As they are denser than the circulating liquid, the cuttings tend to sediment. Due to the inclination of the well, they may form a stationary bed, which blocks part of the annular, leading to lower flow rate that causes operational problems, such as reduced rate of penetration, higher torque and drag, trapped column and others.

This research studies the laminar two-dimensional flow of solid particles suspended in a liquid due to a pressure gradient between two parallel plates, representing a simplified description of the flow that occurs in an annular during drilling process. The mathematical formulation leads to a coupled system of three differential equations: mass and momentum conservation and particle transport equation, which includes the effects of particle diffusion due to the frequency of interaction between particles, the gradient of viscosity and the density difference between the liquid and the particles. The coupled system is solved by the Galerkin/finite element method. The profile of the particle bed along the channel and the flow rate pressure difference relationship for different flow conditions are determined.

Keywords: Particle transport; viscous resuspension; finite element method; drilling

**SYNERGISTIC ANALYTICAL ASSAYS FOR MICROFLUIDIC DIAGNOSTICS**

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Quantitative analytical assays are important in many fields of medical diagnostics and research where they are used to estimate quantitatively the concentration of analytes in samples. In the state of art there are multiple 'analogue' assays [1,2] that use a known correlation between the amplitude of a measured signal (e.g. absorbance of light through a sample cell, electrical conductivity of the sample, time of passage of a sample through a porous bed, intensity of fluorescence, amplitude of force exerted on the sample, etc.) and the concentration of analyte in the sample. In the state of art there are also known 'digital' [3,4] assays in which the concentration of the molecules of analyte, or more generally of target particles being either molecules or colloids, is established with the use of a statistical calculation on the basis of the number of binary (negative or positive) signals recorded from a set of independent partitions of the sample. In the digital assays usually the presence of a single, or a known threshold number of particles, or a threshold concentration of particles in the partition of the sample is amplified to a measurable positive signal.

The method presented here bridges the advantages of the analogue and digital assays in an innovative way to provide for high precision of the estimate of concentration of the analyte while requiring a relatively small number of partitions of the sample. In particular the method relates to quantitation assays that i) provide amplification of a finite number (or concentration) of particles to a measurable signal, and ii) provide a signal, the amplitude of which is related to the number of particles (or their concentration) in the inspected volume. The only requirement for the amplitude is that it is an univocal and monotonically increasing function of the number of particles. The functional dependence may be of many different types, e.g. amplitude being linear in the concentration of particles, square in the concentration of particles, or exponential in the number of particles, or any other kind that satisfies the requirement.

This method is applicable to suitable particles selected from the group comprising or consisting of nucleic acids, peptides, proteins, receptors, enzymes, bacteria, pesticides, drugs, steroids, hormones, lipids, sugars, vitamins or any other suitable particles or combinations thereof.

Here we show the performance of the method for quantitative DNA and RNA assessments based on Polymerase Chain Reaction (PCR) [5]. We propose algorithms of division of the sample into compartments that allow to run diagnostic tests using standard Real Time and digital PCR techniques. Also, we provide analytical tools that synergistically bridge information from analogue and digital signals for improved data analysis and show the experimental and numerical verification of the proposed algorithms.

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## 6. **Minimization of Viscous Fluid Fingering: A Variational Scheme for Optimal Flow Rates**

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Viscous-fingering instability has been actively studied for over half a century. This phenomenon occurs when a less viscous fluid displaces another fluid of higher viscosity in a porous medium or in a confined geometry of a Hele-Shaw cell. In this situation, the fluid-fluid interface become unstable and gives rise to complex interfacial morphologies. It is known that the emergence of this ramified fingering caused by viscous driven instability is a major factor in degrading oil recovery from underground petroleum reservoirs. In this work, we propose a simple mechanism to prevent the development of the viscous fingering instability by just manipulating the pumping rate of the less viscous fluid. In this circumstance, a fundamental question is asked: if one wishes to inject a certain amount of fluid in a given time, what would be the optimal time dependent injection rate  $Q(t)$  for which the perturbation amplitudes could be truly minimized? In order to answer this question, we use an analytical variational scheme to look for the precise functional form of such an optimal flow rate. Experiments and nonlinear numerical simulations support the effectiveness of this particularly simple, but nontrivial, pattern controlling process.



## **Experiments on oil recovery by injection of polymer solution**

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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.

In this work, we study oil displacement by polymer solution with the goal of relating the amount of displaced oil and rheological properties of the solution. In a first experiment, a sandpack was initially saturated with a synthetic oil. After that, part of the oil present in the sandpack was displaced (until no more oil being produced) by substitute ocean water (SW). Afterwards, three partially hydrolyzed Polyacrylamide (HPAM) SW solutions, containing increasing concentrations of HPAM, were consecutively injected in the same sandpack and the amount of recovered oil factor was progressively increased. In a second experiment, using a similar sandpack saturated by the same oil, SW wasn't initially injected in the sandpack. However, the same three HPAM solutions were injected as described above. The same final recovery factor was observed in both experiments but it was achieved much faster in the second experiment.

## **Study of Collective Behavior via Rotating Spinners**

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In active matter, dissipative, steady-state structures far from equilibrium can emerge in systems of particles by converting energy to particle motility. In the Glotzer Group, we have modeled rotating spinners to study collective phenomena in various aspects. In the model, each spinner experiences a constant internal torque in either a clockwise or counterclockwise direction. We have observed simulation results of phase separation via spinodal decomposition and self-organization into rotating crystals due to increasing density and activity. With cooperative, superdiffusive motion along interfaces, inactive test particles can be transported.

## Droplet morphological transitions and solvation forces in nanochannels

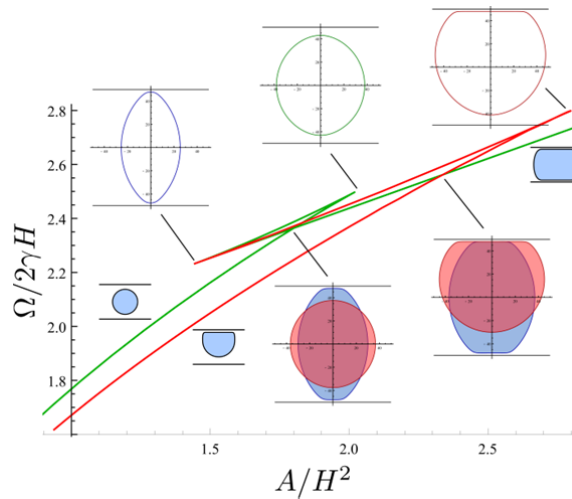
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The morphological phase transition between sessile and lenticular shapes of a droplet placed in a nanochannel is observed upon increasing the droplet volume. The phase diagram for this system is discussed within the macro- and mesoscopic approaches, Fig. 1. On the mesoscopic level, the van der Waals forces are taken into account via the effective interface potential acting between the channel walls and the droplet. We discuss the contact angle dependence on the droplet volume and the distance between the walls; this angle turns out to be smaller than the macroscopic Young's angle. The droplet presence induces the solvation force acting between the channel walls. It can be both attractive and repulsive, depending on the width of the channel.



**Figure 1** Surface energy  $\Omega$  in units of surface

tension coefficient  $\gamma$  as function of volume  $A$  for

symmetric (green line) and asymmetric (red line) shapes for the Young's angle  $\theta = \pi/4$ .

## Brownian motion of particles with arbitrary shapes

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An example will be discussed of research which originated from specific questions of chemists, who wanted to determine conformation of proteins from measurements of their self-diffusion and intrinsic viscosity. It turned out that to answer these questions, fundamental problems in microhydrodynamics need to be solved. Within microhydrodynamics, based on solutions of the Stokes equations, it is possible to determine the relation between the particle conformation and the parameters which can be measured – such as the hydrodynamic radius or intrinsic viscosity. However, derivation of such relations is often challenging for theoreticians, because it requires solving conceptual problems. For example, are the mean square displacements of different particle points the same? While evaluating the self-diffusion coefficient of a non-symmetric particle, and averaging its mobility, which reference point should be chosen? In Ref. [1], this problem has been solved, and in Ref. [2], these theoretical results have been applied to evaluate numerically the hydrodynamic radius of fibrinogen at different conformations, what allowed for comparison with the corresponding experimental data.

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## **Single and double emulsions assembled with microfluidics and applied as polymeric drug delivery systems**

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Polymeric single and double emulsions are some of the most promising approaches for the development of more effective and compliant medicines. The present work shows the development of these systems to improve the release of actives. We intend to study the influence of the composition and structure of polymeric drug delivery vehicles on the release kinetics of encapsulated drugs [1, 2].

Microfluidics devices were used to assemble monodisperse aqueous single emulsion drops and w/o/w double emulsions. The single emulsion contained a polymer such as alginate (ALG), poly(ethylene glycol) (PEG), chitosan (CHT) and studied their interactions with isoniazid (INH). We changed the crosslink density of alginate microcapsules by modifying the calcium concentration, and varied the drug loading and compared with the other polymers. Encapsulants were released within 30 min. PEG and chitin showed a slightly slower release of isoniazid compared to alginate. The double emulsion contained ALG and a fluorescent dye (sulforhodamine B) at the inner phase, fluorinated oil and surfactant at the middle phase, and poly(vinyl alcohol) (PVA) at the outer phase. We varied the thickness of the shell to analyse the influence on the release of the dye by measuring the fluorescent intensity. It was possible to observe that the systems were promising for different applications: They single emulsion could be used to release the drug within short period of time, while the double emulsion could be applied for long period of release.

## **Synchronization of beating cilia and propagation of metachronal waves on ciliated spherical bodies.**

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Volvox and paramecium are spherical and ellipsoidal microorganisms with their size not exceeding a few 10  $\mu\text{m}$  and their bodies is covered with thousands of cilia. Each cilium works independently but the movement of one cilium affects other cilia via hydrodynamic interactions. Observations show the propagation of a wave called metachronal wave on the surface of ciliated microorganisms. The metachronal wave is formed due to a significant phase lag between two neighboring cilia.

We have theoretically calculated and modeled the hydrodynamic interaction between two cilia, beating on the surface of a sphere. We found different state of synchronization between two cilia and understood final state depends on initial phase difference of them. By numerically calculating the nearest neighbor interaction for a cilium we were able to produce symplectic and counter symplectic metachronal wave for 44 cilia on the equator of a sphere.

## **Polymorphism and chirality in the formation of fibrous aggregates**

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Things are twisted, particularly if one looks at the biological matter. Starting with amino-acid sequences yielding helical conformations, through DNA entwined in the double helix, and coiled coils of alpha-helical proteins such as tropomyosin, to microtubules or fibrillar aggregates of misfolded proteins. The morphology of these macromolecules or their aggregates depends typically on two major interplaying forces - the attractive interactions balancing the elastic strains. Using a simple coarse-grained numerical model we study a polymorphic nature of a small cluster of chiral elastic polymers, capable of forming helicoidally twisted fibers, flat, raft-like structures and hollow, tubular forms, all of which are also observed experimentally, in particular during the protein aggregation.

## **Properties of nano-track-containing foils**

(Current activities and the goal of research)

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I am a post-graduate student. The topic of my research is linked to physical processes in track-containing foils.

The tracks are formed as a result of the bombardment of thin dielectric films by fast heavy ions. The diameter of tracks is of nanosize. Such structures formed the basis of new electronics, so called “track electronics” (TE). To create novel track devices it’s important to study physical mechanisms of tracks formation, the properties of the internal surfaces of tracks, the processes of penetration of electrolytes through the tracks of different size and shape, peculiarities of ion currents in tracks and so on.

In our theoretical work a model of the track system is created. The proposed model is designed on the base of classical molecular dynamics (MD). We developed an appropriate computer program and improved the standard MD approach. In our model quantum effects are accounted.

The model is applied to describe ion current pulsations in track-containing foils. Typically pulsations of the ion current are observed in experiments in which the track-containing polymer foils are embedded in electrolytes, and AC voltage is applied. The interacting currents in tracks are simulated by two-dimensional system of oscillating model particles located in the nodes of a plane lattice. In the model external discontinuous forces are introduced to simulate an application of AC voltage. Interaction between models particles is varied to clarify its influence on pulsation effect. It is assumed that the average amplitude of oscillations of model particles is proportional to the average amplitude of current oscillations in real track structure. The model describes adequately the main features of the pulsation effect that were found experimentally. The obtained results are useful for creation and improvement of sensors and other devices of track electronics.

Now we continue this work to clarify the influence of geometry parameters and other features of tracks on the characteristics of ion currents through the tracks. We show how to use the results of nanotracks study to create new biosensors.

The work is closely coordinated with investigations of experimental groups in European universities.



## Steadily translating parabolic dissolution fingers

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Dissolution fingers (a.k.a. wormholes or solution pipes) are large-scale ( $\sim 1\text{m}$ ) karst forms formed as a result of nonlinear feedbacks between the flow, transport and chemical reactions at pore surfaces. We analyze theoretically the shapes and growth velocities of such fingers within the thin-front approximation (i.e., the reaction is assumed to take place instantaneously with the reactants fully consumed at the dissolution front). Using the Ivantsov Ansatz and conformal transformations we find the family of steadily translating fingers characterized by a parabolic (in 2D) or paraboloidal (in 3D) shape. We derive the reactant concentration field and the pressure field inside and outside of the fingers and show that the fluid flow within them is uniform. The advancement velocity of the finger is shown to be inversely proportional to its radius of curvature in the small Péclet number limit and constant for large Péclet numbers.

## **Estimation of neutron dose rate in the biological sample saturated with local dose converters irradiated with PuBe neutron source**

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Boron neutron capture therapy (BNCT) is based on the selective uptake of non-radioactive  $^{10}\text{B}$  by the tumor cells and subsequent irradiation with low energy ( $<0.025$  eV) thermal neutrons ( $n_{\text{th}}$ ). Irradiation results nuclear capture and fission reactions ( $^{10}\text{B} + n_{\text{th}} \rightarrow [^{11}\text{B}] \rightarrow ^4\text{He}(\alpha) + ^7\text{Li} + 2.31$  MeV) yielding high linear energy transfer (LET) alpha particles ( $^4\text{He}$ ) and recoiling lithium ( $^7\text{Li}$ ) nuclei, which have path lengths of  $\sim 9$  and  $5$   $\mu\text{m}$ , respectively.

For the successful BNCT, the sufficient amount of  $^{10}\text{B}$  (20–35  $\mu\text{g/g}$  or  $\sim 10^9$  atoms/cell) must be selectively delivered to the tumor tissue and enough thermal neutrons must be absorbed by them to sustain a lethal  $^{10}\text{B}(n, \alpha)^7\text{Li}$  capture reaction.

In order to choose optimal conditions for irradiation of biological sample, neutron flux intensity and energy distribution should be determined. Neutron activation analysis (NAA) and MCNP6 simulation was used for identification of neutron flux parameters. Experiments were carried out using isotopic PuBe neutron source at total activity  $4.5 \times 10^7$  n/s. For the experimental cross-checking of the MCNP6 simulation samples of V, Mn, Fe, Al have been irradiated. After irradiation, the samples were measured by the high purity germanium (HPGe) detector and the activities of neutron induced isotopes were obtained. According to the experimental neutron activation results, the certain adjustment of parameters of neutron source intensity has been performed for exact neutron source representation. MCNP6 has been used for neutron transport calculation, energy deposition, assessment of the reaction rates and dose rates in the biological sample with local dose converters.

Boron containing nanoparticles are studied as local dose converters for BNCT. Relying on existing neutron source, the optimal boron content in biological sample was obtained.

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

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Waterflooding is the most commonly used oil recovery method in the industry. However, the high mobility ratio limits the amount of oil displaced by the water phase.

An effective alternative to minimize this limitation 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 contribute to a better pore level oil displacement, reducing the residual oil saturation. This pore level behavior is not clearly understood.

Here, a glass microfluidic chip is used as a two-dimensional model porous space. This device has the principal features of a porous media and provides means for pore level flow visualization. The evolution of the water phase as it displaces oil is recorded. Three different water phases were used: pure water, a high molecular weight PEO 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 polymer solution can modify the liquid distribution in the porous media, improving the displacement efficiency at pore scale and consequently the final oil recovery factor.

Keywords: polymer, enhanced oil recovery, viscoelasticity, porous media, micromodel

## **Actin-based motility of lamellar fragments at arbitrary viscous contrast: a phase-field approach**

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Lamellar fragments are pieces of lamellipodia, the actin-based locomotion machinery of crawling cells. These fragments have been shown to exhibit spontaneous, sustained motion if properly deformed [1]. Despite its relative simplicity, a theoretical understanding of the minimal ingredients to explain this phenomenon is still lacking. A challenging question is how the treadmilling dynamics of actin, which polymerizes at the boundary, is coupled to the shape of the fragment to sustain motion, in particular in the absence of molecular motors [2]. Here we present a phase-field description [3] of this free-boundary problem, as a tool to numerically integrate the fully nonlinear dynamics of this problem, aiming at a systematic study of the different families of steady propagating solutions, their stability and their basins of attraction [4].

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## **Experiments on oil recovery by emulsion injection**

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Emulsion flooding oil recovery mechanisms involve partial blockage of the pore throats by the emulsion disperse phase, creating new water paths, leading to mobilization of trapped oil, and consequently increased oil production. The benefit of using water-alternated-emulsion (WAE) injection has been observed for both consolidated media and unconsolidated sand pack. Detail information on the necessary emulsion characteristics to optimize the oil recovery is still unknown. It is a function of the resident oil and porous space properties.

Here, we analyze the effect of emulsion drop size distribution and wettability characteristics of the porous media on the efficiency of emulsion injection as an enhanced oil recovery method. The porous media used in the experiments was glass bead packs with grain size diameter between 53-100 microns. Experimental results shows if the drop size is much smaller than the pore throats, they flow through the porous space without strong changes on the water phase mobility. On the other hand, if the drop diameter is much larger than the pore throats, most of the emulsion drops are retained close to the injection point, reducing its effect on the rest of the porous space. Higher oil recovery was obtained for drop to pore size ratio close to unity. As expected, when the glass beads were treated becoming hydrophobic, there was a reduction of 10% of the amount of oil recovery by water flooding. However, emulsion injection after water flooding was still effective.

Keywords: emulsion, wettability, unconsolidated porous media, enhanced oil recovery

## **Flow of viscoelastic polymer solution through constricted micro capillary**

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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. Because of the complexity of the flow, different mechanisms for residual oil mobilization have been proposed. The relative importance of each of these mechanisms is not clear.

The geometry of a single pore throat resembles that of a constricted micro capillary. Here, we study experimentally the flow of viscoelastic solution in this geometry. The goal was to determine the pressure drop – flow rate relation as a function of geometry and rheological properties of the liquid. Results show that, above a certain flow rate, the pressure drop is not fully described by the viscous flow and elastic effects need to be taken into account. The reduced mobility of the water phase due to the extension of polymer molecules, as they flow through the converging-diverging channel, can be used to improve oil displacement in porous media.

## **Intercalation and Retention of Carbon Dioxide in a Smectite Clay promoted by Interlayer Cations**

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A good material for CO<sub>2</sub> capture should possess some specific properties: (i) a large effective surface area with good adsorption capacity, (ii) selectivity for CO<sub>2</sub>, (iii) regeneration capacity with minimum energy input, allowing reutilization of the material for CO<sub>2</sub> adsorption, and (iv) low cost and high environmental friendliness. Smectite clays are layered nanoporous materials that may be good candidates in this context. Here we report experiments which show that gaseous CO<sub>2</sub> intercalates into the interlayer nano-space of smectite clay (synthetic fluorohectorite) at conditions close to ambient. The rate of intercalation, as well as the retention ability of CO<sub>2</sub> was found to be strongly dependent on the type of the interlayer cation, which in the present case is Li<sup>+</sup>, Na<sup>+</sup> or Ni<sup>2+</sup>. Interestingly, we observe that the smectite Li-fluorohectorite is able to retain CO<sub>2</sub> up to a temperature of 35 °C at ambient pressure, and that the captured CO<sub>2</sub> can be released by heating above this temperature. Our estimates indicate that smectite clays, even with the standard cations analyzed here, can capture an amount of CO<sub>2</sub> comparable to other materials studied in this context

## Mechanics and rheology of Pickering films

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The phenomenon of colloidal particle adsorption at interfaces between two immiscible liquids has been known and investigated for more than a century, and interest in this field has recently increased because of the many promising applications<sup>1</sup>. Drops fully covered by particles, so called Pickering emulsion drops, are (among other applications) used to stabilize emulsions and are ideal templates for producing particles and advanced capsules<sup>2</sup>. Recent studies show how electrohydrodynamic circulation flows in drops can structure free particles on drop surfaces<sup>3</sup>, but there appear to be few studies on the dynamics of Pickering drops subjected to electric field.

Understanding flow and rheology of emulsions is essential in a vast range of industrial applications. A fundamental problem in emulsion flow is the response of single emulsion droplets to shear flow, which induces flow, stretching of drops, and breakup at high shear, all depending on shear rates, surface tension, and viscosity ratio of the droplet and surrounding liquid. Pickering drops are covered with colloidal particles, which add an additional complexity to the system. The colloidal layer imposes a conservation law in the fluid dynamics, i.e. the surface flow is no longer free. The colloidal layer can be considered as a quasi-two dimensional solid or fluid. Much remains to be explored on the dynamics of Pickering emulsion fluid dynamics, and a deeper understanding of this field is of fundamental interest as a basic complex soft matter science problem, and for exploiting Pickering emulsions in industrial applications.

We investigate both the rheology and dynamics of Pickering drops subjected to DC E-fields. Like leaky-dielectric drops in E-fields, free surface charges accumulate at colloidal capsule surfaces and create an electric stress forcing the capsule to deform. By using different particle packing and drop geometries, we examine how stiffness and shape of Pickering droplets influence the macroscopic emulsion yield stress. Although there have been some studies on the response of particle covered drops or bubbles to shear flow<sup>4</sup> or other mechanical forces<sup>5</sup>, there are very few reports on the plasticity of Pickering drops. Here we demonstrate plasticity of leaky-dielectric capsules by the utilization of a uniform DC E-field which offers great control of the compressive stress exerted on capsules as the applied stress can easily be adjusted, reversed or turned off.

We find that there is a capsule geometry dependent critical E-field corresponding to the deformation yield point of the capsule above which the capsule plastically deforms. Below this yield point, we observe electro-orientation, weak capsule deformation and crumpling. The crumpling of the Pickering drop surface supports the capsule in absorbing the compressive electric stress. The results are discussed in relation to existing rheology theories, and we use a simple model to estimate the electric properties of the particle layer.

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## Synthesis and Application of Engineered Nanoparticles

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The Laboratory of Supramolecular Chemistry and Nanotechnology of University of Sao Paulo (LSCN-USP) is focusing efforts on the syntheses, characterization and application of metal and metal oxide nanoparticles in areas such as environmental remediation, metal recovery, catalysis and biocatalysis, solar energy and sensors, nanomedicine and oil exploration.

Large-scale processes for production of superparamagnetic iron oxide nanoparticles by both coprecipitation and thermal decomposition methods, as well as robust strategies for chemical functionalization of surface to control interaction and dispersibility/compatibility properties, were developed. Nanoparticles modified with mercaptopropyltriethoxysilane and magnetic composites were employed for the capture and analysis of mercury ions from aqueous solution and crude oil, providing efficient materials for decontamination of water.<sup>[1]</sup> In addition, these nanomaterials have been used advantageously in hydrometallurgy processes to get pure metal from dilute solutions of the respective metal ions.<sup>[2]</sup> Analogous nanoparticle derivatives also have been used as support for attachment of enzymes improving their stability and catalytic performance.<sup>[3]</sup>

In the sensors area, gold nanoparticles modified with trimercaptotriazine were successfully applied to produce ultrasensitive SERS nanoprobess<sup>[4]</sup> to quantify hazardous metal ions; and more recently new reproducible and simple substrates based on self-assembly of AuNPs with substrates and magnetite nanoparticles, followed by magnetic concentration, suitable for analyses of organic molecules was developed. Sensors based on mesoporous titanium dioxide nanoparticles were shown to be versatile visual detectors as they instantly change color when exposed to vapor of organic solvents. Titanium dioxide was also used to prepare ultraviolet radiation dosimeters and devices for *in vitro* evaluation of solar protection factor<sup>[5]</sup>, as well as for assembling dye-sensitized solar cells.<sup>[6]</sup>

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## **Exploring Oil Extraction by Smart Nanofluids in Pore Network Models: A combination of Molecular Dynamics and Lattice Boltzmann simulations**

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Wetting properties in pore-scale media play a significant role in the oil extraction process. Transport properties such as capillary pressure and relative permeability are directly affected by the wettability. Recently, the use of smart nanofluids has become an interesting alternative to modify the wetting properties with a potentiality to improve the oil extraction process. Particularly, dispersed nanoparticles solutions have shown the ability to control and modify the interfacial and wetting properties of liquid-liquid and liquid-solid interfaces. Although the recent advances in experimental techniques, the determination of the interfacial tension and wetting properties at nanoscale continues to be a challenge. Molecular dynamics simulations (MD) are a good alternative to determine the interfacial properties of a system. However, such atomistic simulations are limited to the nanoscale (ns and nm), and it is not possible to scale-up the fluid information to larger scales, where industrial process may take place. Based on this, we have proposed a hierarchical computational protocol combining MD and Lattice Boltzmann Method (LBM) simulations to investigate the role of functionalized SiO<sub>2</sub> nanoparticles to the oil extraction process at both nano and micro scales. Our previous studies have shown that functionalized SiO<sub>2</sub> nanoparticles dispersed brine solution interfaced with crude light oil phase modifies the interfacial tension between oil and brine at the nanoscale. Also, an increase of the contact angle and a small reduction in oil viscosity are observed when in contact with clay (Montmorillonite) surface. At the nanoscale, due to the inclusion of nanoparticles, these physical-chemical modifications lead to a more efficient oil extraction process in a pore doublet model at the microscale. Here, based on the combined MD and LBM simulations, we study the oil displacement process in different clay covered pore network models. The improvement in oil recovery was evaluated for different rock geometries, porosity and permeability.

## **Model of oil recovery by macro-emulsion flooding**

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In the oil industry, a variety of emulsion types are commonly produced along with the crude oil stream. Moreover, several chemical EOR methods used for heavy oil recovery, including alkaline and alkaline-surfactant flooding, involve the formation of in situ emulsions. To design or use produced oil in water-oil emulsions successfully as selective plugging agents after waterflooding, the associated EOR recovery mechanism must be understood and properly represented in reservoir simulators to upscale pore-level effects to the continuum in porous media. In this work, we have incorporated two known effects of emulsion flooding, namely an increased pore-level displacement efficiency and secondly, a macroscopic mobility control, through a parametrization of the relative permeability curves as functions of the dispersed phase concentration. In the first mechanism, relative permeability endpoint saturation is parameterized with respect to the dispersed phase concentration to allow mobilization of residual oil after waterflooding. The latter mechanism is modeled through changes of the water relative permeability end-point. A quarter of a five-spot model was used to evaluate oil recovery improvement corresponding to each mechanism as well as the timing for the injection of the emulsion slug for a light oil under water-alternating emulsion (WAE) injection in a weakly water wet media. In this model, the effect of heterogeneity in the permeability field was studied to evaluate the performance of the emulsion mobility control. A 1D model was simulated to study oil production and water saturation profiles for a light as well as a heavy oil by modifying the shape of the relative permeability curves.

Numerical results show that displacement efficiency is responsible for the extra oil recovered during WAE injection. However, pure mobility control leads to acceleration of the oil production for an early slug injection. Similar oil production acceleration trends are observed for WAE injection in homogeneous and heterogeneous permeability fields under pure mobility control even for a very unfavorable mobility ratio. 1D simulations reveal that the higher the oil mobility, the more the oil recovery acceleration, which suggests that fractional flow behavior prevails on the observed early oil recovery over oil viscosity and mobility ratio alone.

**Keywords:** *Emulsions, Dispersed flow, Porous media, Mobility control, Enhanced oil recovery.*

## **A simple approach to forming long conductive pearl-chains by utilizing dipolar and capillary interactions**

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We present a simple approach to form long conductive pearl-chains by utilizing dipolar and capillary interactions. Electrostatic dipolar interactions were used to both assemble particles into a chain-like structure and to pull particles out from dispersion. Capillary liquid bridges stabilized the chain. As we demonstrated, such conductive pearl-chain wire can be then embedded, e.g. into an epoxy resin or paraffin-wax. The chains can be formed very fast, around 1 meter per minute, and this velocity depends on the size of particles used. Here we show the results from the experiments, in which particles with radii of around 10 to 100  $\mu\text{m}$  were used.

We also studied the influence of both the liquid viscosity and the quantity of mobile charges on threshold frequencies above which the formation of conductive chains is feasible. The conductive model for ER chaining was used for estimation of dipolar forces. We also calculated the capillary forces of plane-particle bridges and particle-particle bridges and confronted the theoretical estimations with the experimental results. Finally, we investigated the dependence of the velocity of pulling particles out from the interface on the magnitude of the volume of the liquid sphere-sphere bridge. The volume of the liquid sphere-sphere bridge influences the stability of a pearl-chain, since the force of adhesion is a function of that volume.

## **Cooperative behavior of molecules inside the inhomogeneous nano-fluctuations of the order parameter near the phase transitions of the second kind**

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For an integrated description of the properties of complex collective system, critical fluid, and substance near the phase transition of the second kind, a new approach, named “comprehensive scaling” [1,2], has been proposed. The symmetric algebra of fluctuating variables has been proposed in the frame of this approach for the critical fluid in the fluctuation region with the asymmetric equations of state. The resulting equations of state and three-dimensional phase diagrams of state adequately describe the experimental data for thermal and calorific quantities, thermodynamic responses and kinetic coefficients for all close vicinity of the critical point.

Based on the symmetric algebra of fluctuating variables for critical fluid the correlation functions of different orders have been proposed. When transferring of thermodynamic variables from critical fluid to the Ising model the obtained pair correlation functions in direct and reciprocal space transfer to the correlation functions, proposed by M.Fisher [3], and unary correlation functions for the local density and the local energy (entropy) transfer to the functions proposed by L.Kadanoff [4].

Interactions of the molecules within the fluctuations of the order parameter are indirect collective interactions [5]. The proposed unary correlation function of the local density is a density profile within the nano-scale fluctuation of the order parameter. It has been shown that for the critical fluid the average density of the collective ensemble of particles inside of fluctuation of the order parameter is  $\rho_a > 2\rho_c$ . Here  $\rho_c$  is the critical density (it is  $\rho_a = 2\rho_c$  for symmetric Ising model). This conclusion is in agreement [6] to the conclusions based on the van der Waals model of real gas of fluctuations ( $\rho_a \approx 3\rho_c$ ) and with the results of spectroscopic experiments for liquids near the critical point.

Based on the “comprehensive scaling” [1,2] equations the method of modeling and expert evaluation of collective behavior of complex systems (biological, ecological, economic) with positive and negative feedback has been proposed. The special electrical circuit (with the serial and parallel conductors and sources) which is described by the equations of “comprehensive scaling”, can be considered as an example of such system with positive and negative feedbacks.

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## Capture and release of drug molecules by clays

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Conventional release dosage forms are known to providing an immediate release of drug, with little or no control upon the release rate, leading to significant fluctuations in the concentration of the drugs in the organism. Additionally, the use of drug encapsulation offers protection against chemical degradation, drug hydrolysis and drug toxicity, increasing the efficiency of the drug and, at the same time, reducing the side effects. 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. In addition, clays have been shown to be non-toxic for trans-dermal application and oral administration, and several studies have shown that the administration of medicines with clays decreases the oral absorption, making clays a promising material for drug delivery systems.

## **Numerical studies of the relaxation in cavities for a glass former lattice glass model**

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While the Biroli Mezzard (BM) lattice glass model exhibits crystallization, the t-154 Darst variation of the BM model, in which the proportions of 3 types of particles are fixed, does not. In this setting we performed a measurement of relaxation times in non-elastic cavities for equilibrium configurations. Although the system does not possess a high density, the tridimensional cubic cavity size acts as a constrain and slows-down the dynamic. Using kinetic montecarlo we are able to study, in a fast computational manner, relaxations of self overlap time correlation functions and thus determine information regarding length correlation and configurations where samples exhibits aging.

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## Modeling of Asphaltenes Interaction with Carbonate Surfaces

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Asphaltenes are a fraction of the oil that can be the primary adsorbing species in oil mixtures, reducing the oil recovery process in natural reservoir. For the reason, to produce high quality treated oil, many alternative methods are used to ensure the rejection of the most of the asphaltenes, such as the selective adsorption. Calcite (10-14) surface is regarded for retaining asphaltene molecules, mainly in natural reservoirs. Therefore, using first principles calculations based on density functional theory (DFT) within the generalized gradient approximation (GGA) for exchange–correlation functional with van der Waals (vdW) dispersion correction, models of asphaltene-surface interactions with calcite surface (10-14) were investigated to understand what are the main forces related in this adsorption process. The asphaltene models were obtained in collaboration with Edo S. Boek from the work Thomas F. Headen, Edo S. Boek, and Neal T. Skipper, *Energy & Fuels* 2009, 23, 1220-1229. Accordingly, adsorption energy, projected density of states, charge density difference and HOMO-LUMO analysis were calculated. Although there is steric hindering in interaction of the aromatic ring region on the surface, the organic chains in asphaltene molecule are fundamentals to the adsorption process, mainly through vdW interactions used in our calculations.



## **Bubble Break up Model with Elastic Interface**

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To show the influence of the surface elasticity on snap off, a mathematical model of an inviscid bubble surrounded by a water phase inside a constricted capillary tube was developed based on lubrication theory. To account for the elastic interface, a linear constitutive equation was used to relate the tension acting on the deformed surface to the surface elastic modulus and to surface tension. The model lead to an equation of evolution of the bubble surface profile, which was discretized in space using the centered finite-difference method and a 4<sup>th</sup> order Runge-Kutta method for the initial value problem. Results show that the bubble profile tends to break up at the constriction after a certain time called break up time, which is a function of the capillary geometry, the initial film thickness, and the fluid material properties, namely viscosity, surface tension, and surface elastic modulus. Results show that the break up time increases with the surface elasticity monotonically.

**CRACK PATTERNS IN DRY DROPLETS OF ALBUMIN SUSPENSIONS: EFFECT OF IONIZING RADIATION AND TEMPERATURE.**

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Colloidal suspensions are physical-chemical systems widely found in nature and with a great technological and scientific importance. A common feature of colloidal suspensions is that the evaporation of a droplet leaves a circular ring on a solid surface at the end of the process, an annular structure formed by the accumulation of colloidal particles present in the suspension at the periphery of the drop. This physical-chemical phenomenon is popularly known as coffee ring effect. The coffee ring effect is characterized by radial flow of colloidal particles present in the drop towards the edge during the evaporation process. This effect gives rise to characteristic distribution patterns that depend on the physicochemical properties of the solid surface, as well as the size and shape of colloidal particles. Studies have shown that the patterns formed by the deposition of constituents of biological fluids, have potential use as markers of disease processes. Together with this picture described above, some colloidal suspensions undergo sol-gel phase transition, during the drying process, that builds up an unusual pattern of cracks on the edge of the ring. To understand the effect of the tridimensional structure of the colloidal particles, we did experiment with protein Albumin suspension subjected to different doses of  $\gamma$  radiation and heated in microwave. Our results shows that the cracks observed strongly depend on the concentration of the samples and on the structure of the protein previously subjected to  $\gamma$  or microwave radiation. In this work, it is included the preliminary results of the attempt to use deposition patterns obtained by coffee ring effect as makers of physico-chemical changes.

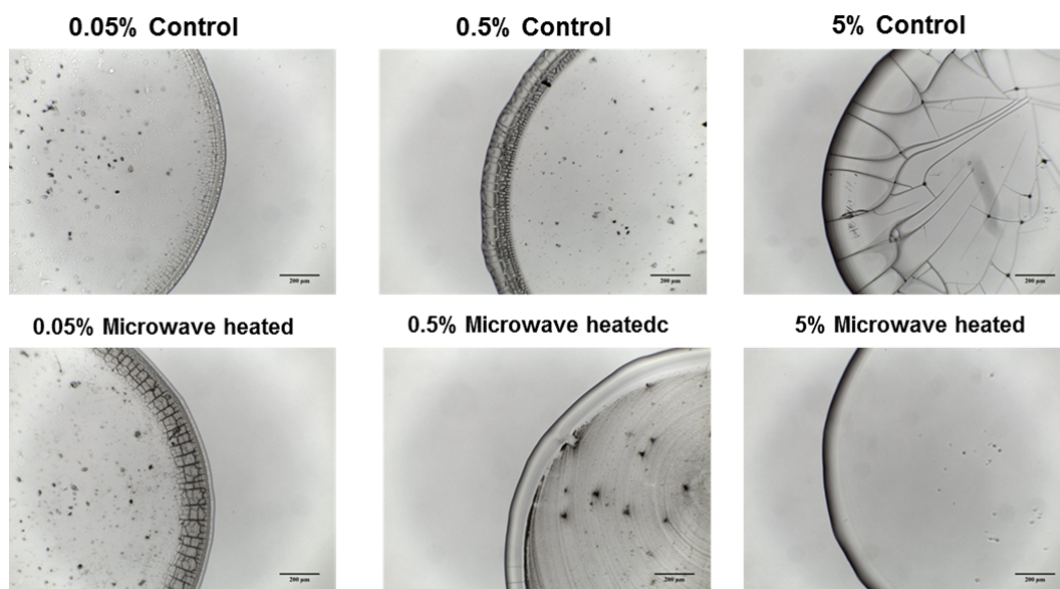


Figure 1. Microimages of the edges of Albumin suspension dried droplets as a function of concentration and microwave radiation.

**LIGHT SCATTERING PATTERN IMAGES OF MICROBIAL COLONIES: APPLICATIONS  
IN THE STUDY OF IONIZING RADIATIONS IN BIOSCIENCES**

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The light scattering pattern images of microbial colonies has been successfully used recently as a new way to do bacterial identification at level of species. Since the light scattering pattern depends almost all on the morphological characteristics of colonies, which are unique from each species, the use of tools of pattern recognition together with feature extraction method could be applied to make clustering and classification based on these characters. In this work, we extend this idea to study morphological changes in microbial colonies subjected to low doses of ionizing radiation. We used *Saccharomyces cerevisiae*, *Saccharomyces boulardii* and *Bacillus cereus* as model microorganisms. Suspensions of each one were prepared contain  $10^6$  CFU/mL. The suspensions were exposed to a dose of 2 Gy by irradiating the samples with Cs-137, with a mean energy of 661 keV. After that, the colonies were cultivated in plates contain solid sabouraud culture medium, and then incubated by 48 hours at 23°C. The images of light scattering were obtained by passing through each microbial colony the beam of a He:Ne laser of 633 nm (1 mW). The scatter pattern was projected to a plane surface and the images collected with the aid of a digital camera of high definition. The scatter images obtained showed different features in colonies irradiated and non-irradiated. The images obtained from colonies of *Saccharomyces cerevisiae* were subjected to a pattern recognition methodology. First, the images were pre-processed with the aid of a wavelet transform to extract the most import features and make data reduction. The next step involved the treatment of this data with a principal component analysis (PCA) approach. In this analysis, were used 14 scatter images of non-irradiated and 07 scatter images of irradiated *Saccharomyces cerevisiae*. The first three principal components explained all together 84% of the total variance of the data. The bi-dimensional plot of the projections of the original matrix features on the first principal component and on the third principal component showed a satisfactory graphical clustering and separation between irradiated and non-irradiated colonies, revealing the potential of this experimental approach to analyze ionizing radiation effects on microbiological colonies. Future works are being conducted to improve the optical and image acquiring system, and other mathematical methods are also being tested to make a more efficient extraction of the main features from images.

## **Direct modeling of particle suspensions**

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Modeling particle suspensions in incompressible fluids is of interest in fields ranging from crystal rich magmatic intrusions to swimming microbes and flow of proppant packings. This is a particularly challenging task when modeling the regime of large volume fractions, which is dominated by particle interactions. Here we present an adaptive unstructured finite element model for two-dimensional particle-laden flows at low Reynolds numbers, and propose an upscaling approach of close particles using Schur complements and lubrication theory. We then use the model to study shear induced mixing and particle dispersion in porous media.

## Incorporation of Ciprofloxacin into NaFh clays: slow release systems

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In the last years, smectite clays charged with organic molecules have attracted the attention of the scientific community, since their physical and chemical properties allow numerous applications. Reports on the use fluorohectorite (Fh), a commercially available synthetic smectite, as a drug hosting material, can be found in the literature [1]. Several authors have reported the incorporation of drugs and their slow release from Fh. We have recently demonstrated the successful incorporation of Ciprofloxacin (Cipro) in a Li-Fh clay [2]. Based on that, in this work the optimization of the Cipro intercalation into NaFh, as well as its release from system are evaluated [3]. The influence of different physical parameters in the process allowed us demonstrating that the drug intercalation into the clay depends of the temperature, the initial drug concentration and the pH of the medium. The optimal conditions for the preparation of the NaFh-Cipro composite were established. The characterization by infrared spectroscopy (IR) and X-ray diffraction (XRD) indicated that the drug molecules were actually incorporated between the clay layers. The drug release profile from the composite –in simulated gastric fluid (SGF) and simulated intestinal fluid (SIF) – showed that the Cipro incorporation is reversible. It also confirmed that the drug release profile corresponds to a diffusion (or zeroth-order) mechanism. Thus, it is possible to design slow release formulations based on NaFh which meet the pharmaceutical standards for these kinds of systems.

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## **Structure and dynamics of a layer of sedimented microspheres near a horizontal planar wall**

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Structure and dynamics of a sedimented layer of silica microspheres is investigated using computer simulations and confocal-microscopy measurements. The system is characterized by the particle area fraction and the dimensionless sedimentation parameter which is proportional to temperature and inversely proportional to buoyancy-corrected weight and diameter of sphere. The range of area fraction between 0 and 0.62 is explored in our experiments. The near-wall particle distribution exhibits a layered structure, with the second layer developing at area fraction around 0.4. Particle distribution is well described by a phenomenological model that involves equilibration of a quasi-two dimensional chemical potential. The effective self-diffusivity of the first and second particle layer has been determined. We find that the suspension microstructure is significantly affected by particle polydispersity, whereas the self-diffusivity is only moderately affected.

## **Viscosity of dumbbells with overlapping spheres.**

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We present a method to calculate viscosity of complex particles constructed from overlapping spheres. An arbitrary shaped particle can be constructed from overlapping spheres in Corrected Rotne-Prager-Yamakawa approximation and mobility matrix stays positive definite. We present suitable correction for the Stresslet components of mobility matrix. The Brownian trajectories are calculated in periodic Lees Edwards boundary conditions. Finally the Stresslet is averaged over the trajectory and gives the additional component to bulk viscosity.

We illustrate the method with dumbbells, that can have overlapping beads.

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