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"Soft Matter Confinement: From Biology to Physics" The Geilo School 2013, 11-21 March Geilo, Norway: Poster Abstracts

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Report title

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Summary

The objective of this "Geilo School" was primarily to stimulate collaborative research between the nationally COMPLEX Coordinated Research Team (CRT) in Norway and its extensive international network of researchers as well as other research groups in Norway. The School was aimed at bringing together researchers with various interests and background including theoretical and experimental physicists, material scientists and molecular biologists to identify and discuss areas where synergism between these disciplines may be most fruitfully applied to the study of various aspects of Soft Matter Confinement: From Biology to Physics.
There were altogether 12 lecturers at the School with about 70 participants from 19 countries. This was the 22nd Geilo School held biannually since the first one in 1971. Reference to the earlier Geilo Schools 1971-2011 may be found here:

http://www.ife.no/departments/physics/projects/geilo

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Contents

1 INTRODUCTION

As material systems are made smaller, 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 will be 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 the NANO2021 and *Complex Systems and Soft Materials*[1] run by the COMPLEX Coordinated Research Team (CRT) in Norway[2]. The COMPLEX CRT has now been working together for about 12 years 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 in Norway participated in the School. A significant number of international collaborators with the CRT from the Nordic countries as well as USA, France, Brazil, Holland, Russia and Slovak Republic also participated in the School.

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

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[1] Research Council project number 191564
[2] http://www.complexphysics.org/

2 PROGRAM GEILO SCHOOL, 11-21 MARCH 2013

Theme: Soft Matter Confinement: From Biology to Physics

1st Day Monday March 11		
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*	
21.00-21.15	Arne Skjeltorp	Opening
2nd Day Tuesday March 12		
08:30-11:30	**Michael Brenner**	**Keynote address: Soft Matter Confinement**
11:30-15:30	*Outdoor activities and lunch*	
15:30-17:30	**Gemunu Gunaratne**	**Gene Regulatory Networks and their Solution Surfaces**
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
3rd Day Wednesday March 13		
08:30-09:30	**Gemunu Gunaratne**	**Of Flies and Zen: A Stochastic Analysis of *Drosophila* Exploration**
09:30- 11:30	**Eberhard Bodenschatz**	**Chemotaxis and cell migration**
11:30-15:30	*Outdoor activities and lunch*	
15:30-16:30	**Eberhard Bodenschatz**	**Chemotaxis and cell migration (ctd.)**
16:30-17:30	**Daniel Fletcher**	**Bottom-up assembly of biological systems**
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
4th Day Thursday March 14		
08:30-10:30	**Daniel Fletcher**	**Bottom-up assembly of biological systems (ctd.)**
10:30-11:30	**Paul Meakin**	**Unconventional fossil energy: opportunities and challenges**
11:30-15:30	*Outdoor activities and lunch*	
15:30- 17:30	**Paul Meakin**	**Unconventional fossil energy: opportunities and challenges (ctd.)**
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
5th Day Friday March 15		
08:30-11:30	**Patrick Tabeling**	**Microfluidics**
11:30-15:30	*Outdoor activities and lunch*	
15:30-16:30	**Poster authors**	Brief introduction to the posters by authors Abstract shown for 1 min. on screen
16:30-18:30	**Poster session**	**Posters left on display until Wedn. March 20**
6th Day Saturday March 16		
08:30- 11:30	**Heloisa Bordallo**	**Exploiting the use of quasi-elastic neutron scattering to understand confinement: From water motion in cement pastes and clays to molecular drugs**

11:30-15:30	*Outdoor activities and lunch*	
15:30-16:30	**Dimitri Argyriou (Seminar)**	**About the European Spallation Source (ESS)**
16:30-17:30	**Roger Pynn (Seminar)**	**Probing Confined Colloids with Neutrons**
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
7th Day Sunday March 17		
Free	***Choice of excursions to nearby scenic places or various skiing events in the mountains***	
8th Day Monday March 18		
08:30- 11:30	**David Pine**	**Colloidal atoms & molecules**
11:30-15:30	*Outdoor activities and lunch*	
15:30- 17:30	**Robin Bruinsma**	**Theory, physical models for biological macromolecules and self-assembled structures**
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
9th Day Tuesday March 19		
08:30- 09:30	**Robin Bruinsma**	**Theory, physical models for biological macromolecules and self-assembled structures (ctd.)**
09:30- 11:30	**Carlos Marques**	**Bio-adhesive lipid membranes on DNA carpets:** **Confinement, depletion and localized pressure**
11:30-15:30	*Outdoor activities and lunch*	
15:30- 16:30	**Carlos Marques**	**Bio-adhesive lipid membranes on DNA carpets:** **Confinement, depletion and localized pressure (ctd.)**
16:30-17:30	**Mogens H. Jensen(Seminar)**	**Life in Turbulence**
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
10th Day Wednesday March 20		
08:30- 11:30	**Julia Yeomans**	**Swimming and stirring at low Reynolds number (ctd.)**
11:30-15:30	*Outdoor activities and lunch*	
15:30-17:30	**Joel Stavans (Seminar)**	**Fluctuations in Biological Cells**
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
19:30	***Geilo School Closing Dinner***	***Geilo Awards, Poster Prizes etc.***
11th Day Thursday March 21		
09:30-13:30	*Departure*	*Communal transportation of participants to Oslo airport and Oslo*

3 POSTER ABSTRACTS

Dynamics of Humidity in Iron-Fluorohectorite

Altoé, M. A. S.[*1], Grassi, G.[1], da Fonsêca, c. l. s.[1], Michels, L. E.[2], Droppa JR, R.[3], Fossum, J. O.[2,4] and da Silva, G. J.[1]

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Keywords: **Clays, Diffusion, Humidity, Synchrotron, X-ray Diffraction.**

The sample we utilize in this experimental study is a synthetic clay which has nominal chemical formula per half unit cell Fe^{+2}_x–$[Mg_{(3-x)}Li_x]Si_4O_{10}F_2$, called Iron-Fluorohectorite (Fe-Fh). It is a 2:1 phylossilicate, meaning that the platelets are formed by two inverted silicate tetrahedral sheets, sharing their apical oxygens with one octahedral sheet sandwiched in between. It is classified as a trioctahedral smectite since Li^+ substitutes for Mg^{2+} in the octahedral sheet sites, which are fully occupied. Fluorohectorites differ from natural hectorites in that the OH groups have been replaced by F. The platelets are held together in the stacked structure by an interlayer cation, which in this case, the Fe^{+2} is the novelty. Previous studies were done for different cations, for example Na (da Silva *et al.*, 2002), Ni (Ribeiro, 2009) and Li (Michels *et al.*, 2012).

As this clay absorbs water, the distance between the layers can expand and such expansion or swelling can be described accordingly to the interactions described elsewhere (da Silva *et al.*, 2002). Monolayers of water intercalated can be stabilized in accordance with the relative humidity within the environment where the sample is.

For this work the experiments were performed in a synchrotron source of Brazilian Synchrotron Light Laboratory (LNLS). These measurements enable a more in-depth study of the water transport process. In this research we focus in the transitions of the clay powder, and also investigate in detail the Fe^{2+} dependence of this process, as innovation. With this information we will be able to understand dynamics of the diffusion process in the clay nano-porous, comparing with others studies performed with the same structure, but with other cations, as da Silva *et al*. (2002), Michels (2012) and Ribeiro (2009).

Keeping the temperature fixed and varying the ambient relative humidity, we have previously found small reproducible d-spacing changes also within the hydration states. The reproducibility and reliability of this relative humidity controlled d-shift enables use of the interlayer repetition distance-d as a measure of the local humidity surrounding the clay particles.

The experimental procedure consists in put the clay powder inside a small hole in a cooper piece within a sample cell close to the humidity sensor. Humidity-regulated air is pumped into this chamber by controlling the fluxes from the two sources of dry and humid air that is merged before entering the sample chamber.

References

da Silva, G. J.;Fossum, J. O.;DiMasi, E.; Maløy, K. J.; Lutnæs, S. B. (2002) *Physical Review E*, **66**, 011303

Michels, L. E.; Hemmen, H.; Droppa Junior, R.; Grassi, G.; da Silva, G. J. and Fossum, J. O. (2012) Synchrotron X-ray scattering studies of Li-Fluorohectorite synthetic clay: Random intercalation states. Proceedings of 2nd International Workshop on Complex Physical Phenomena in Materials.Porto de Galinhas-PE, Brazil.

Ribeiro, L. (2009) *Estudo dos processos de intercalação e difusão de água em nanosilicatos sintéticos por espalhamento e absorção de raios X de sincrotron*, (Tese de Doutorado), UnB.

Migration of Chemical Elements in Soft Plant Tissues

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Research object – bastard acacia (Robinia pseudoacacia L.) in urban ecosystems and in rural area. The subject of study is peculiarities of chemical elements (heavy metals) migration in the soft plant tissues. Research methods of biogeocenology, variational statistics, atomic absorption spectrophotometry had been used. Difference of the chemical elements migration in plants in industrial city and in rural area (conditions of different influence of human activities) had been detected.

Features are: urban plants absorb of chemicals in excess from environment; vacating elements from migration increases due to the removal of fall leaves and dry leaves out of ecosystems.

Productivities indicators (addition of biomass for leaves, auxiblasts, offsprings), biomass of leaves, offsprings and roots in the city are 1.4 times less than in the village, auxiblasts, branches - 1.2, the mass of fall leaves - 1.5, and dry leaves - in 6.5 times less.

To annual accumulation of organic and mineral substances in the village is 3.7 times more than in the city. The chemical elements migration depends on biological productivity. The primary importance of the elements accumulation belongs to the green leaves. Leaves, offsprings and auxiblasts (organs with soft tissues) accumulate of metals 100 times more than the organs with dense tissues (wood, bark, tree branches).

The Influence of Deformation Non-uniformity on the Buckling of Woven Structures under Tension

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The thin-walled structure which one dimension is small compared to the other two is probably the most common form of soft fibrous networks (textile, paper, biological membrane). From the amazing range of textile structures the most ancient and by far the most commonly used are woven structures, formed by interlacing two sets of yarns. The unique feature of woven fabrics is large shear deformations very different from that of continuous materials. On the one hand low shear rigidity warrants the excellent formability properties, while on the other hand – buckling instabilities. This phenomenon is mainly considered as result of lateral compressive forces raised because of tensioned structure contraction. Whereas, the studies in the field of dynamics of non-equilibrium systems have shown that instabilities are related with the structure non-uniformity and localisation phenomena. Nevertheless, buckling during tension phenomena in thin-walled textile structures was not investigated from this point of view.

The aim of this work was to study the influence of deformation non-uniformity on the buckling during woven structures tension and to propose the methods to solve these problems. The desirable solution lies on the development of textile structures that can retain shape stability without sacrificing performance.

The uniaxial bias sample tension test combined with the image analysis technique was carried out to study strain variation during woven fabric tension. Because of the yarns fixation peculiarities the well defined sample zones with different degree of movement freedom can be separated, that cause non-uniform stress and strain distribution along the direction of applied load. At the zone where the highest stress values are obtained, the stress localisation points will occur. Between these points the strain distributes non-uniformly and determines buckling instability formation. When the difference between strain values in different sample zones (i.e. strain non-uniformity) increases, the buckling instability will increase as well, until yarn self-locking in highly deformable zones is attained. As the further strain increase in highly deformable zones is prevented, the more intensive deformation behaviour in zones with slight deformations is observed. This mechanism will decrease deformation non-uniformity and buckling instability in the sample. To avoid appearing of instability defects the woven fabric was stitched. Coincident with sample tension direction oriented stitching pattern introduced as the inverse reflection of the high-stress zone ensured specimen form stability because of the lower deformations non-uniformity and avoided stress localisation. In addition such stitching pattern will not change sample deformation behaviour.

Correlating signaling cascade with movement in *Dictyostelium discoideum*

Christoph Blum, Kaumudi Prabhakara, Marco Tarantola, Eberhard Bodenschatz

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Actin cytoskeletal dynamics provide the fundamental basis of eukaryotic cell motility. The cross-linked actin network at the front of a cell pushes the leading edge of the membrane towards the source of attractant. It is our aim to provide a quantitative understanding of the spatio-temporal dynamics of the actin cytoskeleton within the actin cortex.

We have developed experimental methods to address single *Dictyostelium discoideum* cells with well-controlled mechanical and chemical stimuli [1]. Our experimental techniques are based on microfluidic devices, such as flattening device and micromixer, and fluorescence microscopy (Confocal, TIRF).

Here we present correlations of important proteins in the signaling cascade, namely the Ras-GTP, with the actin polymerization as well as correlations of Ras-GTP localization with the formation of pseudopods and their dynamics. The localization is visualized by the Ras binding domain probe (RBD-GFP). The pseudopod formation is analyzed by curvature maps. The polymerization of actin is shown by the filamentous actin marker LimE.

[1] C. Westendorf, A.J. Bae, C. Erlenkamper, E. Galland,C. Franck, E. Bodenschatz, and C. Beta,PMC Biophys.3 (2010) 9.

Coarse-grained simulation of bovine serum albumin unfolding due to shear flow

Agnieszka Budek and Piotr Szymczak

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Shear flow is known to speed up the protein aggregation process. This can occur for a variety of reasons, including partial unfolding of the protein structures induced by the flow. However, the experimental evidence regarding the influence of shear flow on the protein tertiary structure is rather contradictory. Some studies indicate unfolding of protein under relatively low shear rates, other do not show any impact on protein structure even after exposure to shear rates which are a few orders of magnitude higher. To investigate this problem we perform Brownian Dynamics simulations of shear-induced unfolding of several proteins using a coarse-grained Go model. In
particular, we analyze shear-induced conformational changes in bovine serum albumin.

Separation of paramagnetic beads from droplets in microfluidic devices

Paweł Rafał Dębski, Sławomir Jakieła and Piotr Garstecki

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We present the technique of separating paramagnetic material on demand from droplets in microfluidic devices. The technique is based on the division of the droplet into two separate droplets, one of which containing most of the volume without paramagnetic material and the other containing only paramagnetic material. Paramagnetic material in the form of beads can be used as a solid medium in diagnostic assays (based on PCR methods or ELISA). The use of microfluidic devices allows to shorten the time needed to run such tests, reduce the amount of reagents and the sample volume where the reaction takes place. To run such tests effectively, it is important to introduce reliable methods of manipulation of the solid medium, i.e. paramagnetic beads, including their separation from droplets [1]. The idea of using paramagnetic beads as a solid medium is well known [2,3], however, it is difficult to achieve high efficiency (determined as the ratio of the amount of separated magnetic material and the amount of magnetic material initially put in the droplet). We present the technique of the on-demand separation of paramagnetic beads that provides the efficiency up to 99%. Paramagnetic beads are separated using an electromagnet located close to the microfluidic channel with modified profile.

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3. Anal. Chem. 2001, 73, 5896-5902

The influence of self-assembled organic monolayers on DNA stretching on the substrate

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Different organic molecules as alkanes derivatives self-assemble on some crystal surfaces like highly oriented pyrolytic graphite (HOPG) [1,2]. Such self-assembled monolayers, or molecular nanopatterns, possess unique spatially periodic physicochemical properties like charge, hydrophobicity, roughness, ability to form H-bonds. These molecular nanopatterns were shown to influence the adsorption of polymeric molecules [3] including DNA [4-5]. In this work we have studied the adsorption of DNA molecules on several molecular nanopattens, differing by the functional group of the modifier and the length of its carbon tail. We have shown several effects of self-assembled organic monolayers on DNA molecules such as DNA self organization and stretching on molecular nanopatterns as well as the partial unfolding of the double helix. The adsorption was characterized by the analysis of statistical fluctuations of the contours of the deposited DNA molecules obtained from the atomic force microscopy (AFM) images.

Acknowledgement. This work was funded by RFBR, research project No.12-02-31289.

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Humidity Intercalation Processes in Synthetic Nanosilicates by Synchrotron X-Ray Scattering

Grassi, G.[1], Michels, L. E.[2], Droppa JR, R.[3], da Silva, G. J.[1] and Fossum, J. O.[2].

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The aim of this research is to study the processes of water diffusion in the synthetic clay Lithium-Fluorohectorite (Li-Fh) as a function of relative humidity in a fixed temperature by mapping out the X-ray higher order peaks.

Li-Fh is a layered phyllosilicate clay. Its basal structural unit is formed by two inverted silicate tetrahedral sheets, sharing their apical oxygen with one octahedral sheet sandwiched in between. Due to its structure, water can be intercalated in between each platelet causing the clay to swell. This intercalation process, which can be controlled, yields hydrodynamically stable hydration states which are quite well ordered along the stacking direction. The unit cell along the stacking direction is given by the repetition of the "d" distance between the stacked platelets. With the change in humidity, the d-spacing suffers small variations which can be followed by an x-ray diffraction experiment.

Regarding the number of water layers, i.e. the possible states of hydration, Li-Fh samples owns zero (0WL), one (1WL), one and half (1.5WL), two (2WL) and three (3WL) water layers, with discrete jumps in d-spacing at the transitions between the hydration states [1, 2]. For a given hydration state monotonous d-distances changes as a function of controlled relative humidity and temperature are one order of magnitude smaller than the shift in d-spacing typically of the transition in between two hydration states.

These diffusion process experiments were done by the X-ray technique at the XRD1 Beamline at Brazilian Synchrotron Light Laboratory (XRD1/LNLS) at Campinas SP, Brazil, under proposal #12479. The X-ray wavelength of 0.103284 nm and a focused beam spot at sample of about 0.5 mm high and wide was utilized. The relative humidity was monotonically increased from 0% to 92.5% at a constant temperature of 23°C. The sample was left to equilibrate for 15 minutes after each small increase in the humidity, which in turn, readings of temperature and humidity were measured before and after each X-ray scan. Because of hysteresis, decreases in humidity were avoided. High order peaks analysis also permits to investigate the coexistence of hydrations Hendrix-Teller type-like states.

[1] Tenório, R. P.; Engelsberg, M.; Fossum, J. O.; da Silva, G. J., Langmuir, ***26****(12), 9703 (2010).*

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Actin Dynamics in Myosin II-null Dictyostelium Discoideum

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Starved *D. discoideum* show chemotaxis to cAMP. The directed migration is driven by the assembly and disassembly of actin filaments. In addition to the actin dynamics the contraction of Myosin II plays an important role in the effective movement. Cells lacking Myosin II show frequent protrusions of the membrane. Here we investigate the dynamics of actin filament (labeled by LimE-GFP) in the AX2 cells without Myosin II heavy chain. We observed Myosin II mutants show spontaneous periodic actin dynamics even without external stimulation of cAMP. We further investigate this phenomenon by perturbing the system with different periodic pulses of cAMP created by flow photolysis. Our observation showed Myosin mutants show more instability of actin networks than wild-type cells.

Modeling of scientific paradigms spreading

Pawel Kondratiuk

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Recently a simple model was introduced [Phys. Rev. Lett. 106 058701 (2011)], which attempts to describe the process of emergence, expansion and decline of scientific ideas. It is an agent-based model, which takes into account the agents' memory. Possible interactions between the agents are defined by the interaction network. We try to develop an analytical description of the dynamics, in the case of two competing ideas, considering different topologies of the interaction networks (including homogeneous networks, such as the chain graph, as well as heterogeneous networks, e.g. Barabási-Albert graphs). We examine the pace of an innovative idea expansion, as well as the time after which a new idea replaces the old one. Our analytical results agree with the results of the simulations.

Reference to our paper: [Phys. Rev. E, 85(6), 1–11 (2012)].

Near-Wall Dynamics of Spherical Brownian Particles: Translational and Rotational Diffusion

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Evanescent Wave Dynamic Light Scattering (EWDLS) is an experimental technique that gives an insight into near-wall diffusion of submicron-sized particles. In a system of optically anisotropic spherical colloids one can trace either their translational or rotational diffusion. As hydrodynamic interactions with the wall have a pronounced effect on the dynamics of the particles, it has a reflection in the structure of scattered electric field correlation function which is measured in the experiment, rendering the interpretation of data more involved. EWDLS seems to be the first experimental technique available to probe spatially-resolved rotational diffusion of nanoparticles in the vicinity of the wall. We present theoretical approach leading to analytic expression for the initial decay of measured correlation function and results of experiments in agreement with those predictions.

Self-assembled structures with tunable interface in tethered nanoparticle systems

Ryan Marson

University of Michigan, USA

In many materials, interfaces are responsible for dictating a host of properties, and can provide a means of subdividing space for separating or confining fluid domains. Finding ways to effectively "tune" these interfaces can allow us to dial in desired behavior, or isolate and remove behavior that is undesirable. On the nanoscale, immiscible polymeric, surfactant, and tethered nanoparticle self-assembly offers an effective route to such structures. We highlight a few examples of this type of structure from our work in tethered nanoparticle telechelics, including gyroids and other networks, and discuss how we can alter various aspects of our system to create structures with tunable interfaces and crystal symmetries.

Fluid Entrainment by a Micro-Swimmer near a Surface

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Because of their size bacteria and fabricated micro-swimmers swim at low Reynolds number. As they move they set up velocity fields which stir the surrounding fluid. We have recently shown that as a swimmer moves along an infinite straight trajectory tracer particles far from the swimmer move in closed loops, whereas those close to the swimmer are entrained by its motion[1]. Most experiments on microswimmers are performed in finite geometries and therefore here we extend these results to describe the tracer trajectories when an individual swimmer is close to a no-slip boundary. Our work is a step towards understanding biofilm formation, and how swimmers enhance diffusion and hence increase nutrient uptake.

1. Dmitri O. Pushkin, Henry Shum, Julia M. Yeomans, Fluid transport by individual microswimmers, arXiv:1209.3329 (2012).

Diffusion through layered clay monitored by small angle neutron scattering

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A Ni-fluorohectorite (NiFH) suspension was heat pressed at 120 °C by exerting me-chanical force onto a disc shaped sample volume. The load used was 10 000 kg, giving a pressure of approximately 26 MPa. The final result was a smectic dehydrated clay where the clay platelets (~1nm thick) were stacked with preferential orientation such that the main platelet direction was perpendicular to the axis of compression. The disc was cut into small, prism shaped samples either perpendicular or parallel to the stacking, measuring 10x3x2 mm. The samples were loaded into 2mm quartz cuvettes open at the top. The SANS pattern for the perpendicular sample (oriented with the stacking direction perpendicular to the neutron beam) showed distinct anisotropy, where the other parallel sample produced an isotropic pattern.

The experiment consisted of two parts, where the first was drying of the sample, while the second was water absorption in a humidity gradient. The drying was performed in-situ inside the sample chamber which was under vacuum (~1 mbar). The samples were first hydrated in a humid atmosphere, for several hours, before they were measured with SANS. The total intensity of a scattering pattern was used as a relative measure of water desorption, since the total intensity decreases when there is less water due to change in contrast. The parallel-oriented sample dried faster than the perpendicular one.

In the second part a small quantity of water was put at the bottom of the cuvette, and the samples, now completely dry, were inserted into the cuvette ca. 5 mm above the water surface. SANS was performed immediately after the samples had been inserted. The water at the bottom lead to a humidity gradient, and it was possible to see from the total intensity in each scattering pattern that the water content of the samples increased. Both samples showed absorption in two steps; at first a quick increase followed by a plateau, and subsequently a slow increase in water content until the experiment was stopped. The parallel-orientated sample had a relative increase in total intensity of 100% while the perpendicular sample only showed a 45 % relative increase.

These results demonstrate that water vapor permeability is limited perpendicular to clay layers. The observed plateau during absorption indicates that water absorption happens in two steps, and that this is related to the clays' microstructure. The rapid absorption at the beginning may be attributed to filling of pores between clay tactoids, while the subsequent absorption of water is into the interlayers. The latter is limited by diffusion through narrow pathways, and to swelling of the clay.

Dynamics of humidity uptake by meso-, and nano-porous clay

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Keywords: diffusion, fluorohectorite, relative humidity, transport, porous, x-ray diffraction.

Abstract: The swelling of layered smectite clay particles consists of a change in the interlayer repetition distance (d-spacing) as a function of temperature and humidity. In this work, a fine scan of the relative humidity under room temperature was done for the synthetic clay Lithium Fluorohectorite (Li-Fh). This sample has hydrodynamically stable hydration states with zero, one, one and a half, two and three intercalated monolayers of water [1] which are described in a similar work for the Sodium Fluorohectorite [2] with discrete jumps in d-spacing at the transitions between the hydration states. The reproducibility and reliability of this relative humidity controlled d-shift enables us to use the interlayer repetition distance d as a measure of the local humidity surrounding the clay particles. We provide an example of application of this observation: imposing a humidity gradient over a quasi-one-dimensional temperature-controlled sample and using x-ray diffraction to record the d-spacing, we are able to extract profiles of the relative humidity along the sample length. Their time evolution describes the transport of water through the mesoporous space inside the clay [3].

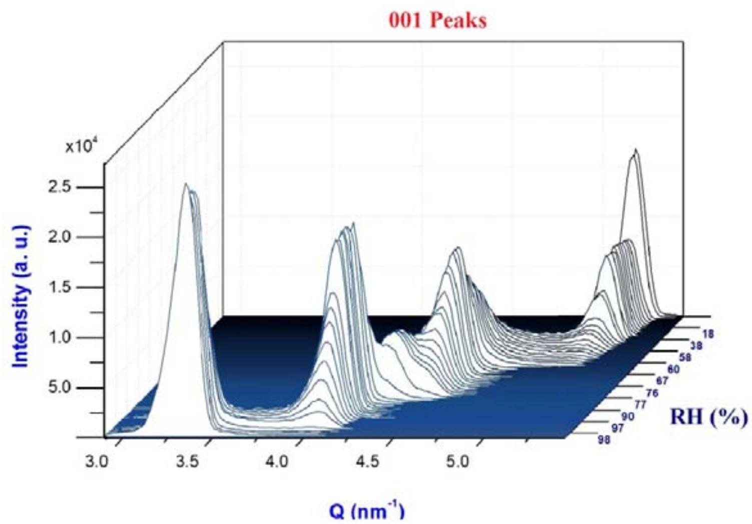

Figure: XRD pattern of Li-Fh as function of relative humidity (RH) and the scattering vector (Q).

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Experimental study of a two-phase flow in a quasi-two-dimensional porous medium

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We have performed an experimental study of the invasion of an air phase in artificial quasi-two-dimensional porous media, initially filled with a viscous fluid. Two separate series of experiments will be discussed here. In the first one, we have used a transparent rectangular porous medium to analyze a pressure-driven drainage process. The pressure was measured in the outlet and we have correlated the real-time pressure measurements with images of the air front invasion. In the second experiment we made use of a circular cell to study how the morphology of the invading phase (air) evolves as we change the confining properties of the system. In this case, the air is pumped into the system at a constant rate. This experiment is still on an early stage, but some interesting aspects are already noticeable.

Actin cytoskeleton of chemotactic amoebae operates close to the onset of oscillations

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The rapid reorganization of the actin cytoskeleton in response to external stimuli is an essential property of many motile eukaryotic cells. Here, we report evidence that the actin machinery of chemotactic Dictyostelium cells operates close to an oscillatory instability. When averaging the actin response of many cells to a short pulse of the chemoattractant cAMP, we observed a transient accumulation of cortical actin reminiscent of a damped oscillation. At the single-cell level, however, the response dynamics ranged from short, strongly damped responses to slowly decaying, weakly damped oscillations. Furthermore, in a small subpopulation, we observed self-sustained oscillations in the cortical F-actin concentration. To substantiate that an oscillatory mechanism governs the actin dynamics in these cells, we systematically exposed a large number of cells to periodic pulse trains of different frequencies. Our results indicate a resonance peak at a stimulation period of around 20 s. We propose a delayed feedback model that explains our experimental findings based on a time-delay in the regulatory network of the actin system. To test the model,weperformed stimulation experiments with cells that express GFP-tagged fusion proteins of Coronin and actin-interacting protein 1, as well as knockoutmutants that lack Coronin and actin-interacting protein 1. These actin-binding proteins enhance the disassembly of
actin filaments and thus allow us to estimate the delay time in the regulatory feedback loop. Based on this independent estimate, our model predicts an intrinsic period of 20 s, which agrees with the resonance observed in our periodic stimulation experiments.

Reference: C. Westendorf et al. (2013) Actin cytoskeleton of chemotactic amoebae operates close to the onset of oscillations. Proc Natl Acad Sci USA (Accepted for publication)

Non-Gaussian fluctuations of complex liquids and confined systems: properties and applications

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Experimental and theoretical studies of the properties of non-Gaussian fluctuations near the critical points of fluids are important for the developing the fluctuation theory of phase transitions [1, 2], for using the unique properties of the critical fluid in novel technologies (supercritical extraction, supercritical fluid chromatography, alternative methods of treatment, creation of nanomaterials and "smart materials" with desired properties), as well as for modeling of biological and social processes.

The extended equations of state of various condensed systems along the coexistence curve have been studied [3-6]. On the basis of these studies the properties of non-Gaussian fluctuations of the thermodynamic magnitudes have been analyzed in the fluctuation area of the liquid-gas and liquid-liquid critical points for molecular and ion-electron liquids, molecular and ionic solutions, condensed systems under the influence of an external field [7] and confined condensed systems.

The equation of the critical line with the maximum probability of the formation of non-Gaussian fluctuations has been proposed. Based on the model scaling equations of state it has been shown that confinement of size of a system leads to a shift of the maximums of the heat capacity. This fact was experimentally observed [8]. The thermodynamic inequalities for the internal energy and the entropy, which indicate the differences of the physical properties of the coexisting phases, have been proposed.

On the basis of the universality hypothesis for the second kind phase transitions the properties of non-Gaussian fluctuations and thermodynamic inequalities can be used to study the evolution of living organisms, biological populations and human communities, and to develop models of biological and social adaptation. The choice of the direction of the evolution of a thermodynamic system will depend on the competition of two mechanisms of entropy increasing: a) when system size increasing at constant number of its structural units; b) when increasing the number of structural units of the system at its spatial confinement.

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Propagation of vortices in a waveguide

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In this theoretical study we present the propagation of optical pulse beams containing deployment phase (space-time vortex) in the lattice of dielectric waveguides. We describe the approximation of weak grid connection use a linear model for the response of the waveguide effect. The attention is paid to studying the effect of the discreteness of the lattice dynamics of the waveguide propagation of dislocations in a pulsed beam. Considered vortices carry small topological charge. The differences in the distribution of the pulsed beams of different width, related to the influence of a discrete system. Thus, the propagation of an extremely narrow beam pulse is the birth of new dislocations. With the increase in the width of the vortex effect disappears, and there is a simple conversion from the dislocation of the phase to the mixed phase boundary.

Loewner equation description of the interaction between viscous fingers in a pore network micromodel

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We report the results of viscous fingering experiments in a rectangular network of microfluidic channels, an analogue system for porous media. Depending on the geometry of the grid, we observe different types of dendrite-like structures spontaneously forming in the system: either wide dendrites, spanning many pore diameters or thin, pore-wide, needle-like fingers. As they grow, the dendrites interact with each other, competing for the available flow.

Next, we develop an upscaled description of this system in which only the dendrites are tracked and the effective interactions between them are introduced, mediated through the evolving pressure field. Due to the quasi-2d geometry of the system, this is conveniently accomplished using conformal mapping techniques. A complex two-phase flow problem is thus reduced to a much simpler task of tracking evolving shapes in a 2d complex plane. This description, although simplified, turns out to capture all the key features of the system's dynamics and allows for the effective prediction of the resulting growth patterns**.**

Sedimentation of Knotted Polymers

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We investigate the sedimentation of knotted polymers by means of stochastic rotation dynamics, a molecular dynamics algorithm that takes hydrodynamics fully into account. We show that the sedimentation coefficient s, related to the terminal velocity of the knotted polymers, increases linearly with the average crossing number n_c of the corresponding ideal knot. This provides direct computational confirmation of this relation, postulated on the basis of sedimentation experiments by Rybenkov et al. [J. Mol. Biol. 267 299 (1997)]. Such a relation was previously shown to hold with simulations for knot electrophoresis.

We also show that there is an accurate linear dependence of s on the inverse of the radius of gyration R_g^−1, more specifically with the inverse of the R_g component that is perpendicular to the direction along which the polymer sediments. When the polymer sediments in a slab, the walls affect the results appreciably. However, R_g^−1 remains to a good precision linearly dependent on n_c. Therefore, R_g^−1 is a good measure of a knot's complexity.

Effective diffusivity of passive scalars in rotating turbulence

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Phys. Rev. E 87, 023018 (2013)
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We use direct numerical simulations to compute turbulent transport coefficients for passive scalars in turbulent rotating flows. Effective diffusion coefficients in the directions parallel and perpendicular to the rotations axis are obtained by studying the diffusion of an imposed initial profile for the passive scalar, and calculated by measuring the scalar average concentration and average spatial flux as a function of time. The Rossby and Schmidt numbers are varied to quantify their effect on the effective diffusion. It is find that rotation reduces scalar diffusivity in the perpendicular direction. The perpendicular diffusion can be estimated from mixing length arguments using the characteristic velocities and lengths perpendicular to the rotation axis. Deviations are observed for small Schmidt numbers, for which turbulent transport decreases and molecular diffusion becomes more significant.

Phase diagrams and peculiarities of fluctuations of confined systems near the critical point for biology problems

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The peculiarities of substance under critical condition are characterized by the long-scale fluctuations of the order parameter and the disorder parameter [1]. Spatial confinement of the systems [2] impacts on the behavior of their singular characteristics [3, 4].

Using the experimental data the comprehensive method for design and analysis of phase diagrams near the critical point for homogeneous infinite systems, spatial macro-inhomogeneous systems under gravity and small confined systems has been developed on the basis of a system of parametric equations of state [5]. Order field, disorder field, and the "field of geometry," determined by the spatial confinement of the system, have been used as the critical fields. It has been shown that the physical meaning of the "geometry field" is connected with the surface tension of the system.

Three-dimensional phase diagrams for infinite and confined critical fluid have been constructed for various thermodynamic responses to thermal, mechanical impacts and impacts, which change the activity of the system near the critical point. The comparative thermodynamic analysis [3, 4, 6, 7] has been made for them. The properties of the various thermodynamic potentials near the critical point have been also studied.

The shape of the phase diagrams of physical systems gave possibility to analyze the sensitive biological systems. The close vicinity of the critical point is associated with an area of high sensitivity of the biological system to external impacts. The healthy and disturbed states of the living organisms are related to the thermodynamic states of coexisting phases on the phase diagram, separated by an energy barrier.

The strategies for treatment and prevention of certain diseases have been suggested. In particular, the using of drugs that regulate the surface tension of the internal environment of organisms and the influence of external impacts on the value of entropy production and the change of the Gibbs potential of biological system are discussed.

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Geometrical frustration of chiral ordering in cholesteric droplets

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Con_ned chiral liquid crystals possess interesting optical properties that could be used as possible mechanisms to envisage soft matter optic and photonic elements in all-photonic circuits. The examples include spherical Bragg resonators [1] - cholesteric liquid crystal droplets which are characterised by tunable periodic modulations of refractive index.

Here, we studied systems of cholesteric liquid crystal droplets [2], where the relation between the confinement via the spherical surface of the droplet and the chiral twisting of the liquid crystalline orientational order is specifically expressed. We demonstrated multiple anisotropic optical profiles, emerging as a result of geometrical confinement. Detailed analysis of the droplet structure has shown presence of both cholesteric singular ±½ and non-singular λ±½ disclinations in either a double-helix like structure, rings or spanned diametrically. Changing the intrinsic twisting of the molecular optical axes induces remarkable changes in the droplet structure and stability, modifying optical and photonic properties of the droplets.

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Bacterial biofilms: toward a multicellular physiology

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Bacterial biofilms are organized communities of cells living in association with surfaces. The hallmark of biofilm formation is a well defined spatio-temporal pattern of gene expression, leading to differentiation and a complex morphology. While this process resembles the development of a multicellular organism, biofilms are only transiently multicellular. More importantly the functions associated to the biofilm phenotype are largely unknown. We first discuss aspects of biofilm physiology connected to biofilm expansion on surfaces in the soil bacterium Bacillus subtilis. We then describe a framework to probe the origin of the observed gene expression patterns, a first step to understand the basis for cell decision-making in a biofilm.

Supercritical CO_2 in aerogels and clay materials studied by small angle neutron scattering

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Keywords: supercritical CO_2, aerogel, synthetic clay, neutron scattering, SANS

Geological storage of CO_2 in deep sedimentary rocks is widely proposed to reduce CO_2 content in the air and prevent the greenhouse effect. [1,2] To implement an effective and safe CO_2 injection on a larger scale, evaluation of the aquifer and overlying caprock by determination of their trapping capacity is needed. For this evaluation small angle neutron scattering (SANS) has been used. The relevant geological structures may show large variations in composition (sandstone in a sedimentary basin, caprock, clays). CO_2 trapped in porous materials relies on different mechanisms of confinement that act on different time scales. Some important factors to consider are: 1) an impermeable caprock that keeps the fluid underground (*supercritical* CO_2 fluid); 2) the solubility of the CO_2 in the water; 3) adsorption into clay nanopores and intercalation into clay structure; 4) chemical reactions that bind the carbon in mineral form to the rock.

In order to study CO_2 in different nanomaterials we use a CO_2 cell specially designated for SANS measurements. This cell allows studying materials at different pressure and temperature conditions, including the *sub-critical* and *supercritical* (sc) state of CO_2, up to 150 °C and CO_2 pressures up to 415 bar.

The studies were divided in two parts. In the first part, the porous Vycor glass and aerogel served as standard samples and synthetic clays (sodium fluorohectorite and Laponite RD) were measured afterwards. In contact with sub-critical and supercritical CO_2 porous Vycor glass (porosity ~28%) and aerogel (porosity ~96%) demonstrate two-phase and three-phase systems, respectively. A characteristic maximum, "Vycor" peak[3], appears at $q_{max} \sim 0.02$ Å^{-1}. The dependence of $I_{max}^{1/2}$ vs. ρ_{CO2} and near linear behavior show that the porous Vycor glass saturated with $scCO_2$ represents a two-phase system with no extra adsorbed phase present.

In case of the aerogel, and unlike the Vycor + $scCO_2$ system, the change of I(q) vs. CO_2 pressure reaches a maximum and decreases at higher pressures. The plotted values of $I(0)^{1/2}$ for different CO_2 pressures vs. ρ_{CO2} show "positive" deviation from a straight line (two-phase system). This behavior indicates the presence of a third "phase" – CO_2 of high density adsorbed to the surface of the nanopores, in line with what has been observed earlier by Melnichenko et al. [3]

The synthetic clays: sodium fluorohectorite NaFH and Laponite RD behave similar to the Vycor glass + $scCO_2$ system. NaFH represents a two-phase system, although showing small "positive" deviation from linear dependence. Laponite also represents two-phase system.

In the second part the studied NaFH clay was surface modified using the organic long chained cation, CTAB, where the CTAB replaces the inorganic cations between the clay platelets, forming 4CEC LiFH. After modification the d_{001} spacing between the clay sheets increased from 1.2 up to 3.1 nm. These studies allowed us to check the intercalation ability of the clay.

The SANS from 4CEC LiFH dehydrated and hydrated (one water layer) clays were measured at 35 °C as a function of fluid density. With increasing CO_2 density the peak maximum shifts to lower q values. This effect corresponds to enlarging the *d* value of the clay structure. The *d* values are increasing up to ~80 bar and slightly decreasing at higher pressures. The change of *d* value between pressures of 1 and 110 bar is ~0.45 nm and between 1 and 80 bar is ~0.47 nm regardless of whether the clay sample is hydrated or not. This enlargement of the interlayer distance suggests intercalation of CO_2 into the clay structure.

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Dynamic Light Scattering measurements of clay materials in liquid CO_2: Preliminary results

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Keywords: supercritical CO_2, DLS, synthetic clay, laponite

Dynamic Light Scattering, also known as Photon Correlation Spectroscopy or Quasi-Elastic Light Scattering, is a useful technique for measuring the size of particle in the sub-micron range [1].

In the present study we have employed a CO_2 cell primarily designated for small angle neutron scattering (SANS) measurements to perform DLS measurements. The design of the CO_2 cell allowed us to apply DLS in backscattering mode (140° - 175°). The CO_2 cell allows studying materials at different pressure and temperature conditions, including *sub-critical* and *supercritical* state of CO_2, up to 150 °C and CO_2 pressures up to 415 bar.

Our present research focuses on physical processes that are of importance for the understanding of CO_2 transport into the ground (CCS technology) where CO_2 trapped in porous materials relies on different mechanisms of confinement that act on different time scales. The DLS method implemented with the cell could help to understand the thermodynamic behavior of clay particles interacting with liquid CO_2.

Aqueous PS suspension. To validate the application of the CO_2 cell for the DLS measurements, polystyrene spheres [2] (PS) suspensions (100 nm and 200 nm in diameter) were placed in a quartz cuvette both inside and outside the CO_2 cell, keeping the rest of the DLS setup unchanged. The results showed good agreement between the diameter calculated from DLS and the nominal value.

Aqueous Laponite clay suspension. The DLS measurements were performed with a 2 minute waiting period between data collections. The results showed that the correlation function signal drops (after 4 minutes) and then becomes more “noisy” (after 6 minutes). Nevertheless, the calculated diameter values are in the same order of magnitude as for PS beads (~150 nm).

Modified Laponite clay in *sub-critical* CO_2. For the measurements in *sub-critical* CO_2, the samples were placed directly in the CO_2 cell, omitting cuvettes. These measurements were more difficult to perform because of the following reasons: i) Laponite particles do not swell and exfoliate in CO_2 solution (large aggregates that sediment to some extent), and ii) CO_2 viscosity is two orders of magnitude lower then water. Therefore, we decided to use instead organically modified Laponite SCPX2849. The results obtained from probing clay particles in the *sub-critical* state of CO_2 indicate formation of large clay aggregates and the calculated diameter values were enlarging with time (112 bar, 24 °C).

Modified Laponite clay in *supercritical* CO_2. The measurements performed in *supercritical* state of CO_2 showed a better stability of the clay/CO_2 suspension. The diameter values obtained were still high but more consistent. As in the *sub-critical* state of CO_2, clay particles also form aggregates. However, better stability was achieved due to the 10 times higher viscosity of the *supercritical* CO_2 compared to that of the *sub-critical* state.

Summary. Results obtained from polystyrene spheres suspension in water showed good agreement with data provided by the producer of this material. The hydrodynamic diameter values gained from DLS measurements of the Laponite and the organically modified Laponite clays in *sub-* and *supercritical* state of CO_2 showed that in both cases clay particles form aggregates which are difficult to disrupt. The measured diameter values were significantly higher than the values obtained from probing Laponite clay in water suspension.

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Untying a protein knot - translocation of knotted proteins through a pore

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Proteins need to be unfolded when translocated through the pores in mitochondrial and other cellular membranes. Knotted proteins, however, might get stuck during this process since the diameter of the pore is smaller than the size of maximally tightened knot. We report the result of computer simulations of knotted protein translocation, which show how the protein can avoid the topological traps and untie its knot during the translocation

Real time observation of λ phage integration in *E. coli*

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Bacteriophages, which infect bacteria, are the most abundant viruses on earth. Bacteriophage λ, which targets *E. coli* cells, is a well-studied model system. When a λ phage infects an *E. coli* cell, there are two possible outcomes:

1. In the lytic response, the λ DNA is replicated multiple times resulting in the lysis of the host bacterial cell and the release of progeny phages to the environment.
2. In the lysogenic response, the λ DNA integrates in a unique site along the bacterial chromosome and stays in a dormant state, replicating together with the bacterial genome.

The infection of the *E. coli* cell by the λ phage begins with the binding of the phage to one of the bacterial maltose pores, which are located primarily at the cell poles, followed by the injection of the ~50 Kbp λ chromosome into the bacterial cell, and the lysogeny/lysis decision.

In this work we are concerned with the question of how λ DNA locates the unique site of integration along the bacterial chromosome during the lysogenic response. Phage integration requires a specific site of ~240 bases on the phage chromosome to find a site of ~15 bases on the 5 Mbp bacterial chromosome. To shed light on this question, we labeled the integration sites of the phage and the bacteria with different fluorescent markers using the ParB/ParS system, enabling us to follow in real time the position of both the bacterial and phage integration sites during the infection process. We found that the λ DNA does not diffuse freely inside the bacterial cell, but remains confined to a radius of ~120 nm around the infection point up to the moment of integration, possibly anchored on the cell membrane near the cell pole. The bacterial integration site, typically located around mid-cell just after cell division, is pushed towards the pole by the replication machinery, facilitating the encounter of the integration sites along the λ and bacterial DNAs. Infection by λ phage does not affect the motion of the bacterial integration site, precluding the existence of a phage-induced active mechanism of search. We suggest that instead of performing a diffusion-driven search of the bacterial chromosome on large lengthscales, the λ DNA remains at the cell poles taking advantage of DNA replication to push the bacterial integration site to the pole.

Influence of shear flow and hydrodynamic interactions on particle aggregation

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A number of experimental and theoretical studies show that the aggregation processes are significantly influenced by the presence of a shear flow, however a full understanding of this phenomenon is still elusive. We present the results of Brownian dynamics simulations of aggregating spheres in the shear flow, with and without hydrodynamic interactions using the Rotne-Prager-Yamakawa approximation. The dependence of the aggregation rate on the shear flow is determined in a wide range of flow velocities and the results are compared with those of other studies.

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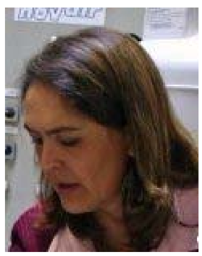
Bordallo, Heloisa		Niels Bohr Institute, University of Copenhagen Denmark bordallo@nbi.ku.dk
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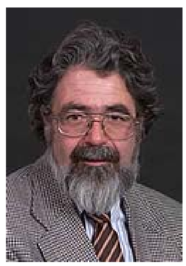

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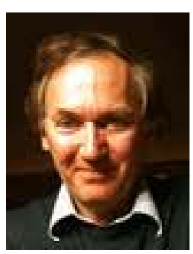

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