IFE/KR/E-2011/002

Cooperative Phenomena in Flows Geilo Advanced Study Institute. Geilo, Norway, 4 – 14 April 2011: Poster Abstracts

Institute for Energy Technology

Institute for Energy Technology

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Report number	Date
IFE/KR/E-2011/002	2011-05-27

Report title and subtitle

Cooperative Phenomena in Flows

Number of pages: 60

Project/Contract no. and name: "Geiloskolen"

ISSN: 0333-2039

Client/Sponsor Organisation and reference
- IFE - Institute for Energy Technology
- Research Council of Norway

ISBN: 978-82-7017-837-7 (printed) 978-82-7017-838-4 (electronic)

Abstract

The objective of this "Geilo School" was to bring 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 *Cooperative phenomena in flows.*

There were altogether 21 lecturers at the School with about 80 participants from 19 countries. This was the 21st Geilo School held biannually since the first one in 1971. Reference to the earlier Geilo Schools 1971-2009 may be found here:

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

Most of the lectures are collected in a CD attached to this report.

Keywords:

	Name	Date	Signature
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Introduction

Cooperative phenomena in flows in the context of the present School relate to liquid, particle/granular flow, flow in and of organic/living systems, turbulence and vortex flow. Special emphasis was placed on studies of fluid (gas, liquid) flow around and inside micro- and nanoscale systems. Since biological systems have evolved in water and are mostly composed of water, uncovering the secrets of biomolecular flows is crucial in understanding origins of life. Nanofluidics is a key technology for designing engineering devices for biological applications, such as biomedical devices and has over the past few years experienced a rapid development. They find applications in a range of areas such as microelectronics cooling, e-paper, micro-reaction devices, Lab-on-a-chip systems etc. Among the challenges in nanofluidics are topics like: Fluid transport - Hydrophobic / Hydrophilic forces - Diffusion, dispersion and sample mixing - Particle and molecular transport - Electroosmosis/Electrophoresis - Adhesion, flow boundary conditions - Nanopumps. In order to solve these challenges both experimental and modelling/ simulation approaches are needed. In particular, the reduced system dimensionality and the reduced number of degrees of freedom have to be handled properly. Breakthroughs in this field will have great impact in industrial fields such as: Pharmaceutics, biotech, medical diagnostics, health care, semiconductors, and chemicals processing.

Program

Program Geilo School 2011, 4 - 14 April
Theme: Cooperative Phenomena in Flows

1st Day Monday April 4		
14.30-18.00	*Arrival*	*Communal transportation from Oslo airport and Oslo to Geilo*
18.30-19.30	*Registration*	
19.30-20.00	*Reception*	
20.00-21.30	*Dinner*	
21.45-22.00	Arne T. Skjeltorp	Opening
2nd Day Tuesday April 5		
08:30-11:30	**L. Mahadevan**	**Keynote address: Introductory overview of various phenomena in flowing systems**
11:30-15:30	*Outdoor activities and lunch*	
15:30-17:30	**Suzanne Fielding**	**Non-equilibrium dynamics and rheology of complex fluids**
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
3rd Day Wednesday April 6		
08:30-09:30	**Suzanne Fielding**	**Non-equilibrium dynamics and rheology of complex fluids (ctd.)**
09:30- 11:30	**Tiina Roose**	**Flow in biological branching structures**
11:30-15:30	*Outdoor activities and lunch*	
15:30-16:30	**Tiina Roose**	**Flow in biological branching structures (ctd.)**
16:30-17:30	**Elisabeth Bouchaud (Seminar)**	**Stress corrosion cracking in glass**
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
4th Day Thursday April 7		

08:30-11:30	**Amber T. Krummel**	**Multiphase flow**
11:30-15:30	*Outdoor activities and lunch*	
15:30- 16:30	**Namiko Mitarai (Seminar)**	**Granular flow**
16:30-17:30	**Jon Otto Fossum (Seminar)**	**Flow of clays**
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
5th Day Friday April 8		
08:30-11:30	**Roberto Benzi**	**Flow at High Reynolds Numbers**
11:30-15:30	*Outdoor activities and lunch*	
15:30-16:30	Poster authors	Brief intros to the posters
16:30-18:30	**Poster session**	**Posters left on display until Wednesday April 13**
6th Day Saturday April 9		
08:30- 10:30	**Lene Oddershede**	**Flow and diffusion inside living cells**
10:30- 11:30	**Amy Rowat (Seminar)**	**Probing single cell deformability by flow**
11:30-15:30	*Outdoor activities and lunch*	
15:30-17:30	**Mogens H. Jensen**	**Complex Patterns in Networks, Tissues and Populations**
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
7th Day Sunday April 10		
Free	***Choice of excursions to nearby scenic places or various skiing events in the mountains***	
8th Day Monday April 11		
08:30- 10:30	**Tom Henning Johansen**	**Vortex flow**
10:30- 11:30	**Yves Couder**	**Turbulence complex matter**
11:30-15:30	*Outdoor activities and lunch*	
15:30-16:30	**Yves Couder**	**Turbulence complex matter (ctd.)**
16:30-17:30	**Joel Stavans (Seminar)**	**Fluctuations of Fluctuations**

17:30-18:30		Tutorial group meetings and informal discussions with lecturers
9th Day Tuesday April 12		
08:30- 11:30	**Albert Libchaber**	**Temperature Gradient at the Molecular Scale: Soret Effect, Osmotic Pressure, Depletion Force**
11:30-15:30	*Outdoor activities and lunch*	
15:30-16:30	**Joseph L. McCauley**	**Stochastic Processes that seem Markovian but aren't *Memory of a past state***
16:30-17:30	**Ivar Giaever (Seminar)**	**The strange case of global warming**
17:30-18:30		Tutorial group meetings and informal discussions with lecturers
10th Day Wednesday April 13		
08:30- 10:30	**Renaud Toussaint**	**Patterns and flow in granular fluid system**
10:30- 11:30	**Gemunu Gunaratne**	**Effective Models for Gene Networks**
11:30-15:30	*Outdoor activities and lunch*	
15:30-16:45	**Arne T. Skjeltorp (Chair)** **Jens Feder** **Roger Pynn** **David Sherrington** **Joseph L. McCauley**	**Flashback earlier Geilo Schools and the legacy of Harry Thomas**
16:45-17:00	**Arne T. Skjeltorp**	**Closing**
17:00-18:00		Tutorial group meetings and informal discussions with lecturers
19:30	**Geilo School Closing Dinner**	**Geilo Awards, Poster Prizes etc.**
11th Day Thursday April 14		
09:30-13:30	*Departure*	*Communal transportation of participants to Oslo airport and Oslo*

- **Each lecture hour will last for about 50 min including questions + ~ 10 min break**
- **Coffee breaks approximately 10:15-10:30 and 16:15-16:30**

Poster Abstracts

Mean-field Generated Herding Behaviour in Financial Markets

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ABSTRACT

An agent-based financial market model with single asset is proposed. The agents are assumed to have strategy of technical analysts that determine their trading activity upon analysis of the recent price history. The price serves as a mean field promoting the herding behaviour of the agents. The adjustment of the asset price depends on the difference of the demand and supply and also on their sum. With an appropriate choice of the fitting parameters this model can reproduce the heavy tails of the distributions of the log returns that span one order of magnitude.

Density Fluctuations in Vibrating Granular Monolayers

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ABSTRACT

This study aims to quantify density fluctuations in a fluidized quasi-two-dimensional granular system close to a solid-liquid-like transition. This transition is reached above an acceleration threshold and at sufficiently high density. The system is a shallow square cell built with two square ITO coated glass plates. The cell is filled with
approximately 10000 spherical 1 mm stainless steel particles and the filling density is about 85%. Due to the dissipative nature of grain contacts, energy is injected in the system by vertical vibrations. To characterize the system we measure its Static
Structure Factor as well as dynamical correlation functions.

Viscous fingering patterns in rectangular grid geometry

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ABSTRACT

Viscous fingering experiments were performed by injecting a less viscous liquid to displace a more viscous one in a regular, rectangular network of channels. This geometry promotes the formation of anisotropic, dendrite-like structures, which then compete with each other for the available flow. This may lead to the appearance of ascale-free, hierarchical growth pattern. Combining experiments and numerical simulations, we analyze different growth regimes in this system, depending on the network characteristics and fluid miscibility.

Electric field induced rotation of Clay particles

Rene Castberg

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ABSTRACT

The electric field induced structuring of Sodium Flourohectorite clay particles suspended in silicone oil have been studied using WAXS and a high speed camera. This allows us to study the behavior from the microsecond regime to severals minutes. The WAXS experiments give us information of the distribution of particle orientation during the chain formation. Using a simple model and the data from the Highspeed camera gives some insight into the effect of the electric field, shape of the particles and viscosity of the oil on the rotation rate of the particles.

Toxin-Antitoxin Battle in Bacteria

Ilaria Cataudella

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ABSTRACT

Toxin-Antitoxin (TA) pairs can be found in many single organisms as a mechanism to respond to starvation induced stress. One of the most well studied example is RelE-RelB pair in Escherichia Coli . RelE-RelB pair is expressed by the same operon, but antitoxin proteins have very short half-life and compensate it by having much higher translation rate than toxins. In ordinary situations the total amount of the antitoxin is around 10 fold higher than the toxin.
The antitoxin RelB can form tight complexes with the toxin, inhibiting this way the toxic activity. The toxin RelE is an mRNA interferase that cleaves mRNA at the empty ribosomal A site. When the cell is in a healthy state all the toxin is sequestered in complexes with the antitoxin and no toxic activity is performed. Toxin-Antitoxin complexes have also been shown to autoregulate the TA operon by means of a mechanism involving cooperativity.
When the cell faces amino-acid starvation the lower overall translation rate results in the concentration of the toxin to get higher than the concentration of the antitoxin.
To test this current experimental scenario, we built a stochastic model involving a feedback mechanism working both at a transcriptional and translational level and simulate the stress response against starvation.
By comparison with a deterministic model, we found out that stochasticity is necessary for the cell to switch, under starvation, to a state in which the total amount of toxin is higher than the antitoxin. Furthermore, cooperativity in the operator repression mechanism is found to be required for the system to get a fast recovery when amino-acid starvation is over.

Digital Nomenclature Code (*dncm*) for Description of Topology and Kinematics of Finite Elements used in Fluid Dynamics

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Keywords: finite elements, kinematics, topology, digital nomenclature code, classification

ABSTRACT

There are wide varieties of finite elements that have been developed in different physical areas such as structural analysis, fluid mechanics, electromagnetism, and coupled-field elements. This development work has been conducted by a large number of researchers, many working in FEA code development within the commercial sector. Given this commercial emphasis for much of the development, it is understandable that a conventional system of identification or numeration of finite elements does not exist. Because of the missing system of identification, authors usually describe finite elements in their papers with words such as ‘constant-strain triangle’, or ‘drilling triangle’. This approach is acceptable if a single element or a few of them are discussed. However, if one needs to deal with many elements simultaneously and to describe their common features or interrelationships, the need for a short element designation becomes obvious.

A good example is the recent paper [1], where an attempt has been made to discover relationships between the absolute nodal coordinate formulation (ANCF) and conventional finite elements (FEM). It was found that ANCF elements can be formally constructed from existing FEM elements using an operation called vectorization, which can be characterized by a vectorization multiplier *m*, an integer, such that informally it looks like FEM × *m* = ANCF.

The latter formula led to the idea of devising a system of identification to describe FEM elements with a few integers. Finite-element notations that have been employed in the literature are as follows:

– by abbreviations, *e.g.* CFT, CST, LST, PLANE3, MIT123 *etc.*; this notation does not contain any information about nodes or coordinates that allows reconstructing the element;

– by number of nodes, *e.g.* quadrilaterals Q4, Q6, Q8, Q9, bricks B8, B20; the disadvantage of this approach is that there is no information about kinematics and nodal coordinates;

– by number of degrees of freedom, *e.g.* B4, B8 (beams), ANCF-B30, ANCF-B48; the problem arising here is that different elements can have exactly the same number of d.o.f.

In a recent research [2], a new classification called digital nomenclature code in the form *dnc* has been proposed for a systematic classification of conventional elements: *d* is the dimension; *n* is the number of nodes, and *c* is the number of coordinates (derivatives) per node. Further, it has been found the kinematics of a great number of widely used elements is described in the form *dncm*.

In the current research, more complicated elements are incorporated into this classification. They can employ nodal coordinates X that formally correspond to some digital code *dncm*; however, their kinematics requires an auxiliary element ($d\eta\varsigma\mu$) to be created with different topology η and kinematics ς, μ having a different set of nodal coordinates $\tilde{X}$. Then, a transformation T towards coordinates X leads to an element, which can be systematically denoted by code $dncm(d\eta\varsigma\mu)\{\tilde{X} = T(X)\}$ called the

extended digital nomenclature code.

References

[1] Dmitrochenko O., Mikkola A., 'A formal procedure and invariants of a transition from conventional finite elements to the absolute nodal coordinate formulation', *Multibody System Dynamics* 22, 2009, 323–339.

[2] Dmitrochenko O., Mikkola A., 'Digital Nomenclature Code for Topology and Kinematics of Finite Elements based on the Absolute Nodal Coordinate Formulation', *Proceedings of the Institution of Mechanical Engineers, Part K, Journal of Multi-body Dynamics*, accepted in September 2010, 26 pages.

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Fractal Avalanche Ruptures in Biological Membranes

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ABSTRACT

Lipid membranes envelope cells as well as organelles, and constitute the most ubiquitous building material in cell architecture. Cell membrane rupture is an important biological process, substantial rupture rates are found in skeletal and cardiac muscle cells under mechanical load, and active cell membrane repair mechanisms are therefore essential to preserve cell integrity.
Pore formation in cell membranes is also at the heart of many biomedical applications, such as in drug delivery. According to common understanding, cell membranes rupture by formation of circular pores, and several studies consistently report circular pore rupture in lipid vesicles under strain.

We observed a very different rupture mechanics in bilayer membranes and cell membranes spreading on solid supports: the rupture proceeded in a series of rapid avalanches causing fractal membrane fragmentation. The intermittent character of rupture evolution and the broad distribution in avalanche sizes is consistent with so called crackling-noise dynamics, which is characteristic to earth-quakes, fracture of solid disordered materials, dislocation avalanches in plastic deformations, and domain wall magnetization avalanches. Adhesion is widespread in biological cells, which suggest that the newly discovered rupture mechanism could be commonly occurring in cell biology.

Nature Materials **9** , 11 908-912 (2010)

Effect of hydrodynamic flow on the alignment of biological molecules on the substrate

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ABSTRACT

Alignment of biological polymers on the substrate is the important task in surface science and biotechnological applications. The use of hydrodynamic flow represents an effective example of "top-down" approach for aligning and stretching polymeric molecules. Here we investigate the effect of hydrodynamic flow on the alignment of long DNA molecules and viral particles on the solid substrate. We should assume that electrostatic interaction often accompanies hydrodynamic flow and we observe their mutual effect.

Acknowledgements. This work is supported by the Program of Grants of the President of Russian Federation" (MK-5121.2010.2)

Computational Fluid Dynamics simulations of flow and concentration polarization in forward osmosis membrane systems

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ABSTRACT

Forward osmosis is an osmotically driven membrane separation process that relies on the utilization of a large osmotic pressure differential generated across a semi-permeable membrane. In recent years forward osmosis have shown great promise in the areas of wastewater treatment, seawater/brackish water desalination, and power generation. Previous analytical investigations have demonstrated how characteristics of typical asymmetric membranes, especially a porous support layer, influence the water flux performance in osmotically driven systems. In order to advance the understanding of membrane systems, models are required that can accurately encapsulate all significant physical processes occurring in the systems. The present study demonstrates a computational fluid dynamics (CFD) model developed within the open source framework OpenFOAM capable of simulating forward osmosis systems. The model is inspired by a previously published CFD model for pressure-driven systems developed using commercial CFD software and the general analytical theory for flux modeling in asymmetric membranes. Simulations are carried out with simple two-dimensional geometries as well as with complex three-dimensional representations of real membrane chambers. Simulations reveal a non-negligible external concentration polarization on the porous support, even when accounting for high cross-flow velocity and slip velocity at the porous surface. This means that the common assumption of insignificant external concentration polarization on the porous surface of asymmetric membranes used in current semi-analytical approaches may not be generally valid. Our implementation furthermore demonstrates the ease with which efficient and complex custom-built CFD models can be developed using the OpenFOAM toolbox.

Falling sand in a narrow pipe: spontaneous discretization of plug velocities

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ABSTRACT

It is known that grains falling through a narrow pipe may form plugs - regions of high density moving at a low velocity. A grain falling onto a plugfrom above will move within the plug for some time before it escapes andaccelerates into the void beneath the plug. Within the plug, grains collidewith each other and with the walls of the pipe.

Recently, a much simplified one-dimensional model with two coefficients of restitution has been used to explore this phenomenon [1]. Inelastic collisions between the grains and the static wall slow the grains down, balancing the gravitational acceleration such that the grains reach a finite terminal mean velocity. The steady-state properties of the system can then be studied for different values of the two coefficients of restitution. The effects of arching, interstitial air and static friction is not included in the model.

We find that discrete collision modes form spontaneously in this model, yielding a discrete set of characteristic plug velocities. Each velocity is deter-mined by a ricocheting motion of grains within the plug. Also, we find that a plug can alternate between two characteristic velocities in an unpredictable manner.

References

[1] S. °A. Ellingsen, K. S. Gjerden, M. Grøva, and A. Hansen,

Density waves in gravity-driven granular pipe flow,

Phys. Rev. E 81, 061302 (2010)

A model for the bacterial CRISPR system and phage diversity

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ABSTRACT

"Stimulated by the recent discovery of the targeted bacterial phage resistance system clustered, regularly interspaced, short palindromic repeat (CRISPR) we investigate phage-bacterial coexistence and evolution with and without bacterial immunity to phage invasion.
We propose a simple two-dimensional lattice model for the evolution of bacteria and bacteriophage species and their interaction.
In particular, we explore this ecosystem under evolutionary pressure of more than one competing phage strain. The model explicitly incorporates the effect of space and population densities are given with respect to two parameters, namely the phage replication speed w and the ratio of phage species present n_p and bacterial resistancies n_{res}. The results suggest that space plays a crucial role in enabling phage coexistence and cooperation. We find that coexistence is a consequence of the very presence of many interdependent species. We contrast our results with a well-mixed lab system. "

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A Life on the Edge: Virulent Phage Bacteria Coexistence on the Boundary of Self-organized Refuges

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ABSTRACT

Abstract: "Bacteriophage are voracious predators of bacteria and a major determinant in shaping bacterial life strategies. Many phage species are virulent, meaning that infection leads to certain death of host and immediate release of a large batch of phage progeny. Despite the apparent voraciousness of their phage predators, bacteria have stably coexisted with virulent phages for eons. This coexistence is not well understood and is therefore worth exploring in-silico. Here we suggest that coexistence is robustly obtained on the edge between two habitats, one of which is a bacterial refuge with conditions hostile to phage while the other is phage-friendly. We show how bacterial density dependent, or quorum sensing, mechanisms such as the formation of biofilm can naturally produce such refuges and edges. Coexistence on these edges exhibits the following properties, all of which are observed in real phage-bacteria ecosystems but are hard to explain without bacterial refuges and a phage "life on the edge": (i) highly efficient virulent phage with long lifetimes, high infection rates and large burst sizes, (ii) large, stable and high density populations of phage and bacteria, (iii) a fast turnover of both phage and bacteria, and (iv) stability over evolutionary timescales despite imbalances in the rates of phage vs. bacterial evolution. Our work suggests that virulent phage may have evolved to thrive on the edges of bacterial refuges such as biofilms."

Carbon cones – a special class of nanocarbon materials

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ABSTRACT

Large-scale production of perfect conical carbon nanostructures that are fundamentally different from the other nanocarbon materials, such as buckyballs and nanotubes, can be made using the so-called Kvaerner Carbon Black & Hydrogen Process. This involves pyrolysis of hydrocarbons using a proprietary plasma torch process. The carbon cones (CC) that occur appear in five distinctly different forms. In addition, disk-shaped particles may be produced. The carbon cones consist of curved graphite sheets formed as open cones with one to five carbon pentagons at the tip with successively smaller and discrete cone angles, respectively.

Carbon cones are an unconventional material. They are not crystals, but molecules too large to be modeled accurately atom by atom. They are not periodic like graphene, yet they possess a high degree of regularity.

Although advanced theoretical work has been done on the atomic structure and electronic properties of carbon cones, equally vital aspects are still largely unexplored. The nucleation and growth mechanisms, for example, are poorly understood, thus making it very difficult to reproducibly grow cones in the laboratory. Outside the laboratory, there is no evidence that carbon cones have ever occurred. Except from a few types of seashells, Nature does not seem to produce hollow cones by herself. Another feature of the cones that is not understood yet is their extraordinary ability to store hydrogen gas reversibly at ambient temperatures. To pursue this and other suggested applications, substantial progress must be made on synthesis and separation.

Reference

[1] H. Heiberg-Andersen, G.S. Walker, A.T. Skjeltorp and S. Nalum Naess, *Graphene Cones*, in Handbook of Nanophysics, Ed. K.D. Sattler, CRC Press 2010 ISBN-10: 1420075381, ISBN-13: 978-1420075380

Hybrid photovoltaic devices using a carboxyl-poly(3-hexyl thiophene) derivative

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ABSTRACT

Organic/inorganic nanostructured semiconductors have been applied as active materials in optoelectronic devices with emphasis on photovoltaics (PV). They exhibit several technological advantages as low cost, chemical stability and easy processing. Furthermore, the control of film morphology on nanometric scale is its more interesting advantage, since this makes possible increasing the effective contact area of the devices [1]. In particular, porous, nanostructured titanium dioxide/poly(3-hexyl thiophene) (TiO2/P3HT) hybrid systems have received special attention due to promissory results obtained recently, although it has been shown power conversion efficiency is limited by polymer infiltration degree within the porous in TiO2 films [2]. In this work is proposed the utilization of a carboxyl-poly(3-hexyl thiophene) in hybrid TiO2/polymer hybrid solar cells in order to study pore filling of the oxide matrix by the polymer. Results show pore filling as well as long-term stability may be enhanced when the carboxylated derivative of P3HT is used. [1] B. O'Reagan, M. Grätzel, Nature 353 (1991) 737. [2] G. P. Bartholomew, A. J. Heeger, Adv. Func. Mat 5 (2005) 677.

Memristive effects in ionic capillary flow

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ABSTRACT

Using a simple and general model we show that ionic flow in small scale capillaries, subject to a periodically varying electric field, may behave as memristive systems. Memristive systems are generalizations of the memristor concept predicted theoretically by Chua in 1971 [1], but not described as a physical component until recently [2]. The memristor, basically acting as a resistor with some memory of its electrical history, is an elementary circuit component, complementing resistors, capacitors and inductors. We show that the memristor as well as the more general memristive systems are promising in describing ionic flow in various small scale systems exhibiting pores such as biological membranes, solid state materials and potentially in sequencing of the DNA. Such kind of flow is a prerequisite for living cells as well as for many other biological systems. The memristive effects of these systems are shown to increase rapidly as the systems grow smaller and are therefore interesting also for nano systems [3]. As the memristor cannot be represented by any combination of passive resistive, capacitive or inductive elements, it is promising with respect to a more correct description of the underlying physics of phenomena that are yet not fully understood.

References:

1. Chua LO, 1971 IEEE Trans Circuit Theory 18(5) 507.

2. Strukov DB et al, 2008 Nature 453 80

3. Johnsen GK et al, 2011 Phys Rev E (accepted).

Magnetic Effect(s) in the Dipole Echo in Non-Magnetic Cold Glasses: the Solution of a Riddle

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ABSTRACT

Startling magnetic effects have been reported, in the last decade or so, when structural glasses (multi-silicates, but also amorphous glycerol) are studied at low and ultra-low (mK) temperatures. The heat capacity and dielectric constant of glasses, dominated by tunneling systems at these temperatures, ought to display universal features and to be oblivious to the magnetic field. Instead, small non-monotonic deviations have been observed in the dielectric constant (real part and loss) when the glasses are immersed in weak magnetic fields (10 mT up to 1 T). But significant deviations have been reported for the heat capacity and also for the amplitude of the dipole or polarization echo. We have developed a theory to explain quantitatively the magnetic effects in the heat capacity, and present our best results for the dielectric constant and loss in a magnetic field. Also, we have solved the problem of the astonishing magnetic effects reported on

the echo amplitude, and using the very same model. We present our explanation - for

ALL of the magnetic effects - in terms of special tunneling systems coupled orbitally to the magnetic field and residing in ``crystal embrios'' (nanocrystals or smaller) within the otherwise homogeneously-disordered solid. This theory shows that the glass transition is more associated to the formation of crystal droplets around Tg than to development of frustration, as in the spin-glasses case. The ``magnetic'' tunneling systems become therefore viable probes to reveal these crystal embryos when other spectroscopies would fail.

Crystal structure and thermal properties of novel mixed-metal and anion-substituted borohydrides

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ABSTRACT

The mechanochemical reaction between $LiBH_4$ and $CeCl_3$ in a molar ratio of (3:1) led to the formation of $LiCe(BH_4)_3Cl$ instead of the lanthanide borohydride $Ce(BH_4)_3$, in contrast to previously published results. This compound is a rare example of a mixed-metal and anion-substituted borohydride. Its structure has been solved by a combined refinement with high-resolution synchrotron radiation powder X-ray diffraction (HR-SR-PXD) and powder neutron diffraction (PND). DFT-calculations are in excellent agreement with experimentally obtained structural data.

$LiCe(BH_4)_3Cl$ crystallizes in the cubic space group *I-43m* (*Z*=8) with lattice constant a = 11.5950(2) Å. Its thermal properties have been studied by thermogravimetric and calorimetric methods (TGA-DSC) as well as by in-situ SR-PXD. The material starts to decompose below 250 ^oC and shows partial reversibility: 15% of the initial hydrogen content could be reabsorbed at 340^oC under 80 bar of hydrogen.

The crystal chemistry and thermal properties of other mixed-metal and anion-substituted transition metal borohydrides will be presented as well.

Filament velocity scaling in SOL plasmas

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ABSTRACT

In the edge region of magnetically confined plasmas one observes inter- mittent transport of plasma by filaments elongated along the magnetic field lines. These filaments carry excess plasma particles and heat and are referred to as blobs. Blobs are created behind the LCFS and move radially outwards through the SOL, contributing significantly to parti- cle and heat loss as well as wall erosion. Recent experimental progress shows a broad range of blob velocities with regimes where the blobs ac- celerate and regimes where it presents a constant velocity in the range of the acoustic velocity.
This work presents the blob velocity scaling for a electrostatic in- terchange model. Numerical simulations show the blob velocity scaling depending on sheath parallel currents. We identify regimes blob accel- eration behaviour and a velocity scaling depending on the size of the structure.

One-Particle Correlation Function in Evanescentwave Dynamic Light Scattering - Effect of Hydrodynamic Internactions

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ABSTRACT

In Evanescent Wave Dynamic Light Scattering (EWDLS) experiments in colloidal suspensions one measures the scattered electric field time correlation function, which is connected to diffusive properties of the system. This technique allows to probe areas close to an interface but also introduces exponentially decaying illumination profile. The resulting decay of the correlation function results from an interplay between the nonuniform illumination and hydrodynamic interactions with a planar surface.

A theoretical prediction is crucial for interpretation of new experimental data. We consider a dilute system, where effectively we have a one-particle problem. Hydrodynamic interactions with a surface result in strong modification of particle's mobility when approaching it. We describe the effect of this change on the dynamics and relate it to the electric field correlation function decay rate. Comparing this to a case with no hydrodynamic interactions, we identify the influence of the penetration depth and the scattering vector.

Even for a dilute suspension the interactions are complex and it is not possible to have an analytic solution. We have employed a Brownian Dynamics simulation with a very precise numerical implementation of mobility matrix elements, which allows us to predict the shape of the electric field correlation function for given values of experimental parameters. We compare the results with recent experimental developments.

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Cluster Model Study of CO2 adsorption on ZnO Surfaces

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ABSTRACT

The interaction of CO/CO2/H2 molecules on ZnO(0001) and (10 0) surfaces has an important application in catalytic methanol formation. Therefore, the Hartree-Fock and Density Functional calculations were performed at the 3-21G basis set level in order to study the methanol formation. Cluster models are used in order to model the surface, the point charge model is used to embed the cluster and avoid finite size. The size of cluster used was (ZnO)16 in a array of 660 point charge. We have optimized the charge used and a molecular dynamics was performed in order to have conformations of adsorbed molecules. The geometry parameters of suggested intermediates for the methanol formation we re optimized at ab initio and Density Functional levels. The structures energy, orbital SCF energies, DOS, and Mulliken population were analyzed.

Simultaneous XRD and EXAFS Measurement of Water Diffusion in Synthetic Ni – Fluorhectorite

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ABSTRACT

Extended X-Ray Absorption Fine Structure (EXAFS) is a highly sensitive and extremely useful technique to study the local structure around a selected probe element. In our case the Ni2+ cation was utilized as a probe to study the process of water intercalation and diffusion in the synthetic clay Ni-Fluorhectorite. Ni-FHT can absorb or lose water causing variations of the distances between the platelets as the temperature and humidity change. In this work the X-ray scattering technique (XRD) was done simultaneously with EXAFS. The data was collected at the pre-absorption edge of Ni (8.26 keV) at Brazilian Synchrotron (LNLS, Campinas-SP, Brazil). The XRD results show the connection between the hydration states and the coordination spheres behavior given by EXAFS Fourier Transform analysis procedure.

Stationary configurations of point vortices in classical and quantum fluids past a cylinder

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ABSTRACT

The problem of finding stationary configurations of point vortices in an ideal fluid past a circular cylinder is studied analytically. The classical solution for a pair of vortices behind a cylinder due to Föppl (1913) is revisited. It is shown that Föppl's linear stability analysis is in error, and the correct results are presented. Also the case of stationary configurations with two pairs of vortices, one in front and the other behind the cylinder, is considered and novel solutions are reported. A similar arrangement consisting of four vortices was recently observed by Zhang and Sciver (Nature Physics 1, 36, 2005) in superfluid helium flow past a cylinder. Since such a configuration has not been observed in classical fluids, it was suggested by those authors that it originates from the complex interaction between the two fluid components of He II. In view of our 4-vortex solution, which is obtained entirely in the context of classical fluid mechanics, we argue that it is not necessary to invoke the two-fluid model to explain the existence of the multi-vortex configuration observed in the experiment.

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How do crystals melt: the role of dislocations and grain boundaries

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ABSTRACT

Melting of crystals is a ubiquitous phenomenon in nature, e.g. ice melting, and a fascinating example of a phase transition, where the small-scale details for crystal breakdown brings up challenging problems. Whilst 3D heated crystals generally melt through a first order phase change associated with a latent heat release, it is more problematic to characterize the melting transition from the microscopic breakdown in thin-film (2D) crystals. The common theoretical approach to describe 2D melting is based on a dislocation-induced melting mechanism with two competing scenarios: i) the collective effects of dislocation dipoles leads to the formation of a gas of free dislocations and a universal jump in the elastic properties at the critical point, or ii) a proliferation of dislocations piling up in strings forming grain boundaries. The former scenario, also known as Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) theory, is associated with a sequence of two continuous phase transitions, while the later, i.e. grain boundary melting, leads to a discontinuous transition.

In contrast to traditional theoretical approaches based on atomistic simulations, such as molecular dynamics or Monte Carlo methods, we propose to study melting using a phase field crystal model. This approach allows us to study the long-time dynamics of a quenched crystal phase, that is described by periodic modulations of the time-averaged particle density field. The diffusive dynamics of the density field is controlled by a suitable free energy which allows for ordering in periodic structures. Deviations from a perfect crystal ordering are associated with defects, such as dislocations and grain boundaries. Here we present a numerical investigation to further characterize the dynamics of dislocations and the eventual formation of grain boundaries during various heating protocols, such as by a shear flow or by a temperature gradient.

Non-Darcian effects in a rough fracture using lattice-Bolztmann methods

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ABSTRACT

Some natural fractures may be considered, at first order, as flat. However, looking at the influence of the fracture morphology in a geothermal background, it was shown that the complexity of the fracture topography changes the hydro-thermal flows which occurs when a cold fluid is injected into a hot fractured bedrock [1]. This was shown under lubrication approximations, which assumes that the fracture morphology varies in a smooth way, by solving Stokes equation and a bidimensional (integrated over the thickness) advection-diffusion equation. However, some features which are observed in nature, like fluid recirculation, and time-dependent temperature at the pumping well, cannot be explained with this model.

We therefore wish to go beyond this lubrication assumption and be able to observe non Darcy effects, which may happen due to highly variable morphology of the fluid-rock interface.

Lattice-Boltzmann methods appear to be very suitable to implement this problem. Indeed, as the algorithms require only local operations, they can handle very well complex boundaries. We develop an algorithm which is based on two coupled lattice Boltzmann methods, allowing us to solve both the advective mass transport and the conducto-advective heat transport. No term are discarded in this solving: Navier-Stokes and the full advection-diffusion equations are solved in three dimensions in fluid and solid. This allows us to observe how both the velocity and the temperature evolves with time and space, also possibly under a time variable pressure gradient. We investigate the effect of recirculation around sharp asperities and wedges along the fracture over the mass and heat transport. We observe that the velocity profile is far from a quadratic profile in the surrounding of sharp asperities: cold fluid may be first trapped into such zones showing a low velocity, and released later.

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Hydro-thermal flows in a self-affine rough fracture.
Physical Review E, 82, 036317.

Simulation of large rotations in multibody system dynamics using absolute coordinate formulation of finite element method

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For the last decades a number of researches are contributed to the problems of multibody system dynamics that combine rigid body motion with large elastic deformations. One of the efficient approaches in solving such problems is using absolute nodal coordinate formulation (ANCF) of finite element method. One of the distinctive features of the ANCF is that no local systems of reference are used in element kinematics. This leads to constant mass matrix and highly nonlinear vector of elastic forces appearing in equation of motion that can be solved using standard methods. Elements using ANCF can be successfully used both in flexible multibody dynamics and coupled problems, for example, for simulating a motion of flexible structures in liquid media. We proposed several new types of finite elements using positions of nodes and coordinate of slopes as nodal coordinates. A number of numerical examples illustrate efficiency and accuracy of the elements.

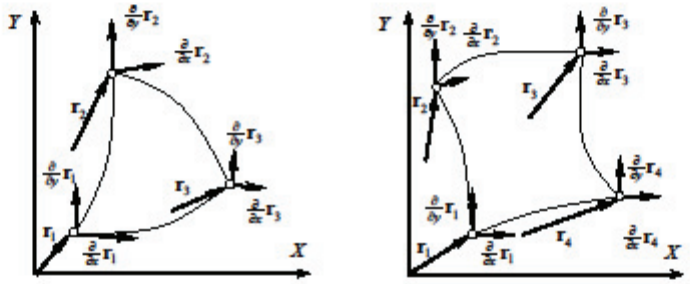

Figure 1. Two-dimensional plane elements with 18 and 24 degrees of freedom.

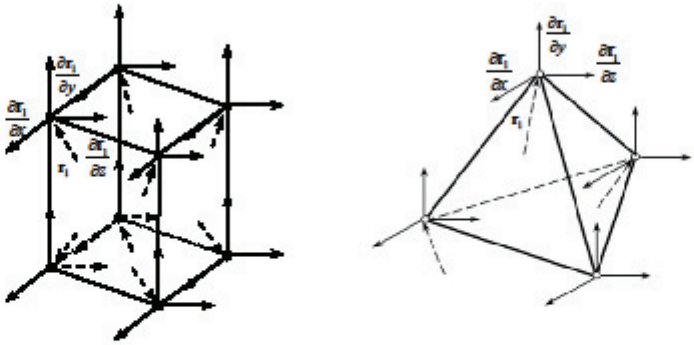

Figure 2. Three-dimensional solid elements with 96 and 48 degrees of freedom.

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INHOMOGENEITIES AND FLOW OF LIQUID SYSTEMS NEAR THE CRITICAL POINT

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ABSTRACT

Study of the kinetic properties of liquids and liquid solutions near the critical point (CP) are the topical question of the soft matter physics. The correlation length R_c of the fluctuations of a system grows near the critical point according to the fluctuation theory of phase transition [1]. Many singular properties of substance (anomalous increase of the heat capacity and the susceptibility of system, a significant increase of the light and neutrons scattering, diffusion slowing, anomalous increase of thermal conductivity, etc.) appear in a system.

The flow of the methanol-hexane binary solution through the capillary has been studied in the work in the wide temperature range near the consolute CP. The time of flow was measured and then the temperature dependence of the shear viscosity was obtained. It has been found the exponential temperature dependence of the viscosity far from the CP. As the critical point is approached the temperature dependence deviates from the exponential due to grows of fluctuations of the substance.

The data near the CP have been analyzed on the basis of the equation of the viscosity of the dynamic theory of critical phenomena [2] $\eta_f=\eta_r(qR_c)^Z$ and equations for viscosity [3], which takes into account its spatial dispersion in system near the critical temperature [4].

On the basis of the studies the conclusions have been made as follows: 1) Equation of viscosity [2], obtained on the assumption of conditions $qR_c>>1$, $\eta_f/\eta_r >> 1$, can be used in the temperature range $\theta=(T-T_c)/T_c\approx10^{-5}\div10^{-4}$. It is necessary to use a crossover term [5] in the region $\theta>10^{-4}\div10^{-3}$; 2) The equation of the fluctuation part of the viscosity [3], based on the work [4], adequately describes the experimental data of the solution viscosity $\eta(\theta)$ in whole investigated temperature range $\theta=10^{-2}\div10^{-5}$ and gives finite value of viscosity at $\theta=0$.

Study the influence of inhomogeneities on flow in methanol-hexane solution under gravity [6] near the critical temperature T_c has been also carried out. It has been revealed a whole set of peculiarities in the behavior of inhomogeneous liquids, which are not observed for homogeneous systems. A nonmonotonic temperature dependence at temperatures $T > T_c$ has been detected for the first time for the equilibration time $t_e(\Delta T=(T-T_c))$ of the inhomogeneous substance under gravity [7, 8]. A nonmonotonic height dependence of the relaxation time $\tau(z)$ has also been obtained at temperatures $T > T_c$ for the inhomogeneous liquid under gravity. Maximum values of the relaxation time of concentration gradient dc/dz correspond not to the level of the critical isoconcentrate ($z = 0$) but to the heights $z \sim \Delta T^{\beta\delta}$. It has also been detected that the relaxation properties of the inhomogeneous liquid at a certain height z are determined not by a single relaxation time, but by the spectrum of these times $\Sigma\tau_i(z_j)$, which characterizes the entire inhomogeneous solution under gravity. A dynamic nonequilibrium equation has been proposed on the basis of the fluctuation theory of phase transitions

for the binary solution under gravity near the critical point.

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Optical pulses in nonlinear media

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ABSTRACT

We present novel effects for few-cycle pulses propagation and interaction in cubic nonlinear media with the dispersion. A theory of compression of a few-cycle pulse with quadratic phase modulation has been developed within the SVP (slowly varying profile) method. The equation for the electric field was numerically solved varying the quadratic phase modulation index, number of oscillations, and input pulse width. The optimal modulation index was found, at which a pulse can be compressed to one oscillation period and the fundamental limits are shown. When the modulation index exceeds the optimal value, the width at the compression point increases. The theory of a chirped pulse compression up to one-period optical oscillations is advanced. The optimum value of the phase modulation index for the maximal compression achievement is found. Also in the report the process of self-compression of few-cycle ultrashort femtosecond pulses (without phase modulation) is examined in cubic nonlinear medium with dispersion. The process of self-compession to one-two period pulse is simulated. And the equation for the electric field was numerically solved for different conditions (number of oscillations, input pulse width, nonlinear and dispersive indexes of medium). The process of ultra broadening of spectrum in these cases is discussed and examined. The equations for self-compression in nonlinear medium limits are found and compared to equation for linear medium.

This study was supported by the Russian Foundation for Basic Research, projects nos. 09-02-01028 and LG Chem.

Tip splitting in deterministic models of Laplacian growth

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ABSTRACT

Laplacian growth is one of the fundamental mechanisms of pattern formation, driving such natural processes like electrodeposition, dielectric breakdown or viscous fingering. All of these processes havesimilar dynamical behaviour with a strong competition between spontaneously formed dendrite-like structures, and tip-splitting effects when dendrites bifurcate into secondary branches.

Here we consider a simple, deterministic model of Laplacian growth, in which the growth takes place only at the tips of the long-and-thin fingers. The dynamics of the system can then be described by a determisitic Loewner equation [1]. We extend this approach allowing the fingers to split, which is crucial to obtain the qualitative

behaviour seen in nature and experiments. We discuss different splitting criterions and study the dynamics of the model in variety of geometries: half-plane, channel, stripe, and radial geometry.

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Studies of water intercalation and diffusion in nanosilicates by means of XAFS technique.

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ABSTRACT

We study the processes of intercalation and diffusion of water in the synthetic swelling clay Ni-Fluorohectorite (Ni-FHT) by means of experimental techniques of XRD and XAFS at LNLS, Campinas-SP, Brazil. Ni-FHT absorbs or loses water causing the distances between the platelets change. This process, which is controlled by temperature and humidity, yields stable hydration states referred to as having either 0, 1, 2 or more water layers. For some given value of humidity the temperature was taken as the controlled parameter. The results of Fourier transformed XAFS data indicates that the first coordination sphere around the nickel is oxygen whereas the second one is nickel even for a situation where the relative humidity was maintained around zero and the temperature has gone from 125 °C to 20 °C. In all situations of humidity and temperature it was observed the presence of both coordination spheres peaks being due to the presence of a stable structure like a Brucite type that emerges in the process of dialysis preparation of the sample cationic exchange.

Anomalous scaling of passive scalars in rotating flows

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ABSTRACT

We present results of direct numerical simulations of passive scalar advection and diffusion in turbulent rotating flows. Scaling laws and the development of anisotropy is studied in spectral space, and in real space using an axisymmetric decomposition of velocity and passive scalar structure functions. The passive scalar is more anisotropic than the velocity field, and its power spectrum follows a spectral law consistent with $\sim k_\perp^{-3/2}$. This scaling is explained with phenomenological arguments that consider the effect of rotation. Intermittency is characterized using scaling exponents and probability density functions of velocity and passive scalar increments. In the presence of rotation, intermittency in the velocity field decreases more noticeably than in the passive scalar. Its scaling exponents show good agreement with Kraichnan's prediction for passive scalar intermittency in two-dimensions, after correcting for the observed scaling of the second order exponent.

WAXS studies of Clay/Paraffin Composites"

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ABSTRACT

The physical properties of stimuli-responsive soft materials can dramatically change when subjected to external stimuli such as temperature or electric/magnetic fields. In the present work, Li-Fluorohectorite clay particles were embedded into the paraffin-wax matrix. E-field induced particle alignment was achieved when the paraffin-wax was kept in a melted state (140-150 deg). Solid casts of ~15 x 6.5 x 1.5 mm3 were made and investigated using wide angle X-ray scattering (WAXS) in order to find the clay particle's orientational distribution, as well as the water content inside the clay galleries and its influence on the clay orientation. WAXS patterns observed are highly anisotropic and show differences compared to the patterns obtained from paraffin/clay composites in zero electric field. The clay nanolayered particles have preferential orientation in the direction of the electric field. The degree of anisotropy was found to be weakly dependent on water content inside the clay galleries. The Hendricks-Teller mixed-intercalation state was observed when sample stirred for a long time at high temperature above water boiling point. From the 3D picture it can be concluded that particles align along the E-field direction but are randomly distributed concerning the rotation along their major axis (parallel on average to the direction of the applied electric field).

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Flow of inhomogeneous liquid under gravity near the critical point at equilibrium establishment

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ABSTRACT

The aim of the work is studying of the kinetics of equilibrium establishment for inhomogeneous liquid near the liquid-vapour critical point using gravity effect data.
According to the fluctuation theory of phase transitions the kinetic properties of macro-homogeneous substance near the critical point are determined only by the correlation length R_c and correlation time τ_c [1]. At the same time under the actual conditions of physical experiment carried near the critical point in the gravity field presence really equilibrium system is the system inhomogeneous along vertical direction. Quick heating of this equilibrium system from the critical temperature T_c to various temperatures $T>T_c$, compulsory removes the system from the state of equilibrium. Such non-equilibrium macro-inhomogeneous systems are characterized by behaviour peculiarities that are not observed in spatially homogeneous systems.

The average velocity v_a of center of mass drift has been investigated by using the refractometry method for one-component inhomogeneous liquid when moving away from the T_c. It was experimentally obtained, that temperature dependence of equilibrium establishment time $t_e(\Delta T)$ is essentially non-monotonous. It was shown on the basis of $t_e(\Delta T)$-dependence and of a monotonous temperature dependence of drift of the center of mass coordinate $\Delta z(\Delta T)$ that the average velocity $v_a(\Delta T)=\Delta z/t_e$ is monotonous temperature function. In temperature region $\Delta T=T-T_c<1$ K, when substance in sample cell is strongly inhomogeneous, v_a increases very slowly and it is determined not only by dependence of v_a on diffusion coefficient $D=R_c^2/\tau_c$, but also by temperature dependence of thickness of inhomogeneous layer with near-critical density. In temperature region $\Delta T=T-T_c>1$ K, when substance in sample cell is weakly inhomogeneous, v_a sharply increases and is determined only by increasing D [1].

The behaviour of relaxation times of refraction index $n(z,T)$ and density $\rho(z,T)$ for macro-inhomogeneous liquid under gravity above critical temperature has been also investigated with the refractometry method. Using the exponential relaxation relation, the relaxation times $\tau(z)$ of density $\rho(z)$ at different heights of investigated system have been calculated at different temperatures $T>T_c$. It was drawn a conclusion that on each selected height of one-component inhomogeneous system the kinetics of the equilibrium establishment is characterized not by one relaxation time $\tau(z)$, but the spectrum of times $\Sigma\tau_i(z_i)$, that characterize whole macro-inhomogeneous system in a gravitational field.

Based on the obtained data the 3-dimension surfaces relaxation time τ – density ρ – temperature T, relaxation time τ – height z – temperature T and relaxation time τ – chemical potential $\Delta\mu(z)$ – temperature T have been constructed. The surfaces characterize the process of flow of system to equilibrium state at all heights of fluid under gravity. For the analysis of the shape of these surfaces

there were proposed the dynamic scale equations of state for spatially inhomogeneous liquid. In obtained equation the reduced equilibrium temperature is connected with time of non-equilibrium process by a scale relation.

Using obtained results for $t_e(\Delta T)$ and $dn/dz(z,T)$, on the basis of the fluctuation theory of phase transition and the theory of gravity effect, the equations for height and temperature dependences of the relaxation times of refraction index gradient dn/dz and density gradient $d\rho/dz$ $\sim dn/dz$ for inhomogeneous liquid near the critical point are obtained.

As opposed to homogeneous liquid, it is concluded, that the kinetics of equilibrium establishment for inhomogeneous liquid under gravity when moving away from the liquid-vapour critical point is characterized by increasing of relaxation times of density and density gradient and increasing of average velocity of drift of the center of mass. These results are in a qualitative agreement with the investigations of the kinetic properties of binary solutions near the consolution critical point.

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From fingering to fracture in complex fluids

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ABSTRACT

We present a novel experiment – a specific Hele-Shaw cell with mobile sides - with which both liquids and solids can be loaded with the same boundary conditions, beyond the small deformation regime. With such a system, one can examine quantitatively the response of a viscoelastic material when the loading rate is varied. On the liquid side, a bubble grows in the material and destabilizes in a Saffman-Taylor manner, forming an elongated finger, while on the solid side, a crack develops. Thus, a study of the morphologies of the pattern formed in the fluid allows for a quantitative analysis of the liquid to solid behavior. Furthermore, in our geometry, the two kinds of patterns have inverse aspect ratios. This study could hence give some new insight on liquid to solid phase transitions such as the sol-gel and the glass transition.

We present a set of experiments obtained on Newtonian fluids of different viscosities. The observed viscous fingers present several similarities with the Saffman-Taylor patterns. Furthermore, we present some analysis of the dynamical response of our various systems. Finally we also show preliminary results on viscoelastic materials and the associated perspectives.

The role of small-angle scattering in the investigation of nanoscaled hydrides in carbon scaffolds

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ABSTRACT

One of the most promising routes towards a hydrogen economy is the use of hydrogen as energy vector for vehicular and stationary applications in the form of solid storage material based on nanoscaffold hydrides. When dealing with nanoporous materials, small-angle scattering gives invaluable information that can help to develop the most suitable solid material. The successful wet or melt infiltration of hydrides into carbon scaffolds has been demonstrated by small-angle neutron scattering (SANS) performed at the JEEP II reactor at IFE.[1] Depending on the hydride and/or the scaffold used, the particle sizes range from 1 to 6 nm. Using *in situ* small-angle X-ray scattering (SAXS), it was possible to underline important differences in the morphology and surface area of the hydride particles during heating when they are nanoconfined in the porous scaffolds, compared to their values in the bulk state. The demonstrated changes in hydrogenation/dehydrogenation properties of these nanoconfined systems could be related to the differences mentioned above. SANS and SAXS, combined with wide-angle X-ray scattering, were used to investigate $Mg(BH_4)_2$, $NaAlH_4$ and MgH_2 infiltrated in carbon scaffolds. The main results will be presented.

The authors gratefully acknowledge the collaborations with Karlsruhe Institute of Technology (Germany), Demokritos (Greece) and University of Oslo. Funding under the EU project NANOHy ("Novel Nanocomposites for Hydrogen Storage Applications", contract n. 210092) is gratefully acknowledged. The skilful assistance from the Project team at the Beam Line BM26B, ESRF, Grenoble, is also gratefully acknowledged.

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Hydrodynamic dance: Stokesian dynamics of close particles

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ABSTRACT

Stokesian dynamics simulations of a three-particle cluster sedimenting in a fluid are reported. A simple periodic solution is found, with the three particles chasing each other (in the center-of-mass frame) around a butterfly-shaped curve, remaining constantly within a very short distance to each other. Most of the time, the particles are in a sliding motion relative to each other, followed by rapid changes of direction of the relative motion. The smallest gap between the particles constantly remains below 1 percent of their diameter. This is in contrast to previously reported trajectories which mostly have a scattering character, i.e., particles drift away from each other after some short-distance interaction. Permanent proximity of the particles makes the considered trajectory an ideal benchmark for comparisons of accuracy between different numerical methods.

The simultaneous flow of two phases in a porous medium

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ABSTRACT

We report on experiments of a low viscous non-wetting gas and a high viscous wetting fluid, simultaneously injected into in a quasi-two-dimensional porous medium, initially saturated with the latter phase. Sequential imaging of the flow structure at different capillary numbers, accompanied by pressure measurements, allows us to study the characteristic cluster dynamics of the non-wetting phase and its relation to the global pressure gradient.

Computer simulations of sedimenting colloidal dispersions

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ABSTRACT

The program for the investigation of sedimentation processes of colloidal dispersion by the direct numerical simulation is presented. The smoothed profile method was used for the simplification of complicated enormous calculations that arise due to the boundary conditions imposed on the surfaces of colloidal particles.

A finite differences method was used for the calculation of a viscous flow. The projection method was used for the solving of the time-dependent incompressible Navier-Stokes equations. The semi-discrete Navier-Stokes equations that resulted from the projection method were solved in a Cartesian staggered grid.

The simulation program was implemented in C language. The results obtained for the sedimentation of colloidal particles were visualized.

The decay of turbulence in rotating flows

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(Dated: November 30, 2010)

ABSTRACT

We present a parametric space study of the decay of turbulence in rotating flows combining direct numerical simulations, large eddy simulations, and phenomenological theory. Several cases are considered: (1) the effect of varying the characteristic scale of the initial conditions when compared with the size of the box, to mimic “bounded” and “unbounded” flows; (2) the effect of helicity (correlation between the velocity and vorticity); (3) the effect of Rossby and Reynolds numbers; and (4) the effect of anisotropy in the initial conditions. Initial conditions include the Taylor-Green vortex, the Arn’old-Beltrami-Childress flow, and random flows with large-scale energy spectrum proportional to k4. The decay laws obtained in the simulations for the energy, helicity, and enstrophy in each case can be explained with phenomenological arguments that separate the decay of two-dimensional from three-dimensional modes, and that take into account the role of helicity and rotation in slowing down the energy decay. The time evolution of the energy spectrum and development of anisotropies in the simulations are also discussed. Finally, the effect of rotation and helicity in the skewness and kurtosis of the flow is considered.

Viscous fingering and dynamic saturation–pressure curves in two-dimensional porous media

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ABSTRACT

We present results from primary drainage experiments in quasi-twodimensional porous models. We study the unstable displacement of a viscous liquid by air in transparent models that allow the displacement process and structure to be monitored in space and time. Primary drainage experiments are carried out under various displacement velocities.

By combining detailed information on the displacement structure with global measurements of pressure, saturation and the capillary number Ca, we obtain a scaling relation that relates pressure, saturation, system size, and capillary number. This scaling relation allows pressure–saturation curves for a wide range of capillary numbers to be collapsed on the same master curve. We also show that in the case of primary drainage, the dynamic effects in the capillary pressure–saturation relationship commonly observed on partially water-saturated soil samples can be explained by the combined effect of capillary pressure along the invasion front of the gaseous phase, and pressure changes resulting from viscous forces in the displaced wetting liquid phase.

Reference:

G. Løvoll et al., Trans. Porous Med., in press (2010)

Simulation of dendritic flux avalanches in superconducting films

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ABSTRACT

The gradual flux penetration in superconducting thin films is sometimes interrupted by dendritic flux avalanches. Such avalanches are potentially damaging for devices.

They typically last less than one microseconds and forms either fingers or large, complex, branching structures. The poster explains how the avalanches are caused by a thermomagnetic instability mechanisms and how simulations based Maxwells's equations are able to reproduce, qualitatively and quantitatively, the complex dynamics of the avalanches.

Numerical simulation of gas dynamics in pneumatic brake system of train

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ABSTRACT

The numerical simulation of gas-dynamic processes in pneumatic brake system of railway train is considered.

The pneumatic brake is a complex system which includes brake pipe with many different components such as driver's brake valve, control valves, compressors, brake cylinders, auxiliary reservoirs and others. To create the complete model of the pneumatic braking system which correctly responds to driver's operations, all these components must be simulated.

The brake pipe is a circular pipe with constant diameter which runs along the train length. The unsteady air flows in the brake pipe are modeled by one-dimensional gas equations of continuity and momentum, and the gas state equation. The brake components are modeled as volumes connected by means of valves and calibrated orifices.

The main purpose of this research is to develop the model of train brake system for train driving simulator.

Modeling the NF-κB mediated inflammatory response predicts cytokine waves in tissue.

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ABSTRACT

Waves propagating in "excitable media" is a reliable way to transmit signals in space. A fascinating example where living cells comprise such a medium is Disctiostylium D. which propagates waves of chemoattractant to attract distant cells. While neutrophils chemotax in a similar fashion as Dictyostelium D., it is unclear if chemoattractant waves exist in mammalian tissues and what mechanisms could propagate them. We propose that chemoattractant cytokine waves may naturally develop as a result of NF-κB response. Using a heuristic mathematical model of NF-κB-like circuits coupled in space we show that the known characteristics of NF-κB response favor cytokine waves. While the propagating wave of cytokines is generally beneficial for inflammation resolution, our model predicts that there exist special conditions causing chronic inflammation and re-occurrence of acute inflammatory response.

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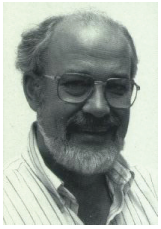
Feder, Jens		Prof. emeritus., Physics Department, University of Oslo Norway jens.feder@gmail.com
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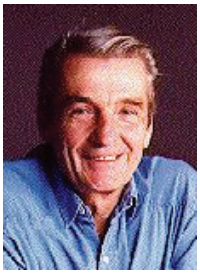

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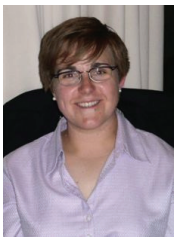

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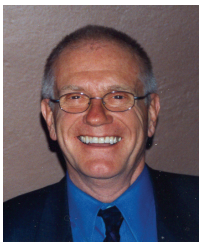

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