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<b>Abstract</b>	<p>Rapid detection of chemical and biological agents and weapons, and rapid diagnosis of their effects on people will require molecular recognition as well as signal discrimination, i.e. avoiding false positives and negatives, and signal transduction. It will be important to have reagentless, cheap, easily manufactured sensors that can be field deployed in large numbers. While this problem is urgent it is not yet solved. This ASI brought together researchers with various interests and background including theoretical physicists, soft condensed matter experimentalists, biological physicists, and molecular biologists to identify and discuss areas where synergism between modern physics and biology may be most fruitfully applied to the study of bioprocesses for molecular recognition, and of networks for converting molecular reactions into usable signals and appropriate responses.</p>		
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## 1 Introduction

This eighteenth ASI Geilo School in Norway since 1971 brought together researchers with various interests and background including experts in the fields of bioprocesses and networks, theoretical physicists, soft condensed matter experimentalists, biological physicists, and molecular biologists. The objective was to identify and discuss areas where synergism between modern physics and biology may be most fruitfully applied to the study of bioprocesses for molecular recognition, and of networks for converting molecular reactions into usable signals and appropriate responses, as required for rapid detection of Chemical and Biological (CB) agents and weapons, and rapid diagnosis of their effects on people

Many fields of research are confronted with networks. Genetic and metabolic networks describe how proteins, substrates and genes interact in a cell; social networks quantify the interactions between people in the society; the Internet is a complex web of computers; ecological systems are best described as a web of species. In many cases, the interacting networks manifest so-called emergent properties that are not possessed by any of the individual components. This means that the detailed knowledge of the components is insufficient to describe the whole system. Recent work has indicated that networks in nature have so-called scale-free characteristics, and the associated dynamic network modelling shows unexpected results such as an amazing robustness against accidental failures, a property that is rooted in their inhomogeneous topology. Understanding these phenomena and turning them to use in chemical and biological threat detection and response will require exploring a wide range of network structures as well. Questions related to error and attack tolerance of complex networks and their robustness in particular, and the dynamics of networks in general also have to be addressed. Modelling the signal transduction networks in bioprocesses as in living cells is a challenging interdisciplinary research area. It is now realized that the many features of molecular interaction networks within a cell are shared to a large degree by the other complex systems mentioned above, such as the Internet, computer chips and society. Thus knowledge gained from the study of complex non-biological systems can be applied to the intricate braided relationships that govern cellular functions. Bio-inspired processes provide an attractive option for sensing CB agents because nature has solved many of the problems inherent to the sense-and-respond task. For example, many biological responses such as blood clotting, gene expression and the activation of enzymes require enormous amplification of signals carried by as few as a single molecule or ion. Adaptability to local environments, atomic level control of self-assembled structures, benign processing, combinatorial synthesis and complex computation are other features of biological systems that are likely to prove useful in CB sensor development.

The starting point, and the underlying theme throughout the ASI, was a thorough discussion of general network theory. The next focus was on genetic networks and bioprocesses. Finally, focus was placed on the possible universality of network structures and how this knowledge can be combined to attack the urgent problem of rapid detection and diagnosis of CB agents.

## 2 Programme

### NATO ADVANCED STUDY INSTITUTE

#### Dynamics of Complex Interconnected Systems: Networks and Bioprocesses

Bardøla Høyfjellshotel, Geilo, Norway, 11-21 April 2005

Coffee breaks 10.15-10.30 and 16.15-16.30

Dinner at 20.00

#### Monday April 11 – Day 1

- |             |   |
|-------------|---|
| 14.30-18.00 | Assembly of participants in Oslo and communal transportation to Geilo |
| 18.30-19.30 | Registration  |
| 19.30-20.00 | Reception   |
| 20.00-21.30 | Dinner  |
| 21.30-22.00 | Opening   |

#### Tuesday April 12 – Day 2

- |             |  |
|-------------|--|
| 08.30-11.30 | Kim Sneppen: Key note<br>Communication and Structure in Complex Networks: From Biological Regulation to Social Systems |
| 15.30-17.30 | Vyacheslav B. Priezzhev: Self-organized criticality in an immune system  |
| 17.30-18.30 | Tutorial group meetings and discussions with lecturers   |

#### Wednesday April 13 – Day 3

- |             |   |
|-------------|---|
| 08.30-09.30 | Vyacheslav B. Priezzhev: Exact solution of asymmetric exclusion process (ctd.)  |
| 09.30-11.30 | Sergei Maslov: Detecting topological patterns in protein networks               |
| 15.30-16.30 | Sergei Maslov: Detecting topological patterns in protein networks (ctd.)        |
| 16.30-17.30 | Joel Stavans: The bacterial SOS response to DNA damage at the single cell level |
| 17.30-18.30 | Tutorial group meetings and discussions with lecturers                          |

#### Thursday April 14 – Day 4

- |             |   |
|-------------|---|
| 08.30-10.30 | Joel Stavans: The bacterial SOS response to DNA damage at the single cell level (ctd.)                              |
| 10.30-11.30 | David Sherrington: The Minority Game: statistical physics of adaptive cooperation of speculative agents in a market |
| 15.30-17.30 | Alex Hansen and Stephane Santucci: Fracture and fracture networks   |
| 17.30-18.30 | Tutorial group meetings and discussions with lecturers  |

**Friday April 15 – Day 5**

- 08.30-10.30 Peter Beck: Prevention of nuclear and radiation terrorism networks
- 10.30-11.30 Mogens Hoegh Jensen: Diffusion, Fragmentation and Merging Processes: Ice Crystals, alpha Helices and Scale Free Networks
- 15.30-17.30 Mikhail A. Ostrovsky: Molecular mechanisms in biosignalling: visual reception
- 17.30-18.30 Tutorial group meetings and discussions with lecturers

**Saturday April 16 – Day 6**

- 08.30-09.30 Mikhail A. Ostrovsky: Molecular mechanisms in biosignalling: visual reception (ctd.)
- 09.30-11.30 Author-attended posters
- 16.30-17.30 Author-attended posters
- 17.30-18.30 Tutorial group meetings and discussions with lecturers

**Sunday April 17 – Day 7**

- Free morning
- 17.30-19.00 Author-attended posters ctd.

**Monday April 18 – Day 8**

- 08.30-11.30 Albert-Lazlo Barabasi: Error and attack tolerance of complex electronic, social and biological networks
- 15.30-17.30 Gaute T. Einevoll: Physics in the Brain
- 17.30-18.30 Tutorial group meetings and discussions with lecturers

**Tuesday April 19 – Day 9**

- 08.30-11.30 Albert Libchaber: Principles of in-vitro gene expression; application to a vesicle bioreactor and to self-reproducing systems
- 15.30-16.30 Ivar Giaever: ECIS: An electrical Biosensor
- 16.30-17.30 Arne Skjeltorp: Braided Space-Time Particle Networks
- 17.30-18.30 Tutorial group meetings and discussions with lecturers

**Wednesday April 20 – Day 10**

- 08.30-10.30 Lene Oddershede: Organization of living matter, from the single molecule to whole cell level - an optical study
- 10.30-11.30 Seminar: Joseph McCauley; Anti-Economics.
- 15.30-16.30 Alexander V. Belushkin: Neutron scattering methods for the study of self-organising soft condensed matter
- 16:30-17:30 Seminar: Jon-Otto Fossum: Complex Interconnected Materials; Networks and Processes.
- 17:30-18.30 Group meetings and discussions with lecturers

**Thursday April 21 – Day 11**

- 08.30-10.30 Harry Thomas: Summary, questions and discussions
- 10.30-14.00 Communal transportation of participants to Oslo for departure.

**Organising committee:**

Arne T. Skjeltorp, IFE, Kjeller, Norway - director  
 Alexander V. Belushkin, JINR, Dubna, Russia - co-director  
 Trine Løkseth, IFE, Kjeller, Norway - secretary  
 Geir Helgesen, IFE, Kjeller, Norway - technical assistan

### 3 Poster abstracts

#### **The use of vegetal bioindicators for monitoring heavy metal environmental pollution in Dambovita county**

Simona Apostol, Claudia Stih

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#### **ABSTRACT**

The basic objective of our work are to evaluate the impact of heavy metals and other trace elements, on the vegetal samples (moss and higher plants), soil, water and aerosols in order to assess the information on the levels of pollution with specific elements Dambovita county;

The main sources of these pollutants in the atmosphere are industrial processes, thermal power stations, domestic heating systems and motor vehicles. All these sources are present on the territory of the Dambovita County. The main polluting regional industries are coal mining and oil exploitation, cement and related materials production, glass and special lamps manufacturing, machine production and ferrous metallurgy. The most polluted towns are Fieni, Berevoiesti, Doicesti, Laculete, Moreni, Gaiesti and Targoviste in decreasing order regarding to pollution with sedimentable powders. Fieni was mentioned many years as the third town in top of the most polluted localities of Romania because here is a Cement Factory (Romanian Statistical Yearbook – 2001: National Institute of Statistics).

Within the MWFE network (Ministry of Waters, Forest and Environment Protection, Dambovita filial) the air quality in Romania is followed up by the impact pollution monitoring including a supervising network of performing routine measurements of sulphur dioxide, nitrogen dioxide and ammonia, and suspended matter. On the other side, the up mentioned industries are a very important source of pollutants as Special Steel Complex Machel Trading, Cement Factory, Oil Extraction Trading, Arctic Complex.

The present study is going to generate a new sampling network, enough dense to offer integrated information for the whole surface of the county. A combination of analytical methods will be used for determination of element concentrations, including neutron activation analysis (NAA), Inductively Coupled Plasma (ICP) spectrometry, or Particle Induced X ray emission (PIXE) spectrometry. . The neutron activation analysis (NAA) technics that allow to determine about 37 elements Al, Ag, As, Au, Ba, Br, Ca, Ce, Cl, Co, Cr, Cs, Fe, Gd, Hf, I, K, La, Lu, Mg, Mn, Mo, Na, Ni, Sb, Sc, Se, Sm, Ta, Tb, Th, U, V, W, Yb, Zn, and Zr. The determination of Pb, Cu and Cd will be carried out using the Inductively Coupled Plasma (ICP) spectrometry using Baird ICP2070 - Sequential Plasma Spectrometer with Argon and the a radio frequency generator at 40.68 MHz. The spatial deposition patterns will be revealed as GIS maps.

## Polymer-Surfactant Interactions: Adiabatic Calorimetry Study

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### ABSTRACT

Over the past years compositions based on hydrophilic polymers and surfactant systems have attracted interest due to their ability of reversible response to the small changing of the external field (pH, temperature, presence of the specific substances, lighting, electric or magnetic field). As a typical example, one of the peculiarities of such systems is the high sensitivity of conformational properties to the negligible changing of the temperature. Similar materials are perspective for application in medicine (controlled segregation of medicinal substance), electronics engineering (sensors, transducers), for a solution of ecological problems.

In the this work the investigation of the phase states of aqueous solutions triblock copolymers and sodium dodecylsulphate mixtures with taking into account of system microstructure, and the behavior of the specific heat are presented. This type of the copolymers poly(polyethylene oxide)-poly(propylene oxide)-poly(ethylene oxide) (PEO-PPO-PEO) has a macromolecular surfactant properties and manufactured by chemical concern BASF (Germany). While investigation of specific heat dependence on the temperature above mentioned polymer-surfactant systems demonstrated sharp transitions within the temperature range 20-60 °C. Differences with heat capacity dependence of pure copolymer aqueous solution were observed, which presumably were attributed to changing in a system microstructure with additives presence and with increasing of temperature. The possible physical mechanisms of the observed phenomena are discussed.



## **Inhomogenous sand pile model: Crossover of the multifractal scaling to the finite size scaling**

Jozef Černák

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### **ABSTRACT**

We study an inhomogeneous sand pile model in which two different toppling rules are defined. For any site only one rule is applied corresponding to either Bak, Tang and Wiesenfeld model or Manna two state sand pile model. The new parameter  $c$  is introduced which describes a concentration of sites where the Manna rule is applied. The results show a crossover of the multifractal scaling observed in the Bak, Tang and Wiesenfeld model ( $c = 0\%$ ) to the finite size scaling of the Manna model ( $c = 100\%$ ).

## Aggregation Dynamics of Magnetic Holes

Jozef Černák<sup>1</sup>, Geir Helgesen<sup>2</sup>, Arne T. Skjeltop<sup>2</sup>

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### ABSTRACT

Nonmagnetic microspheres confined in a ferrofluid layer are denoted magnetic holes. They form aggregates due to dipolar interactions when an external magnetic field is applied. Their cluster aggregation growth was studied for both constant and in layer rotating magnetic field. The results for smaller particles in constant magnetic field are in agreement with standard dynamic scaling theory, however for larger particles when Brownian motion is not so important, the scaling exponents  $z$  from average cluster length  $S(t) \sim t^z$  strongly depend on the magnetic field strength. In rotating magnetic field a non-equilibrium growth process was observed which has some features of the cluster-cluster aggregation.

## Structure-function self-organization in biomolecules (intramolecular synergetics)

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<sup>b</sup> *Frantsevich Institute for Problems of Materials Science, NAS Ukraine, Kiev*

### ABSTRACT

The ability of macromolecules to co-ordinate fast reaction events in their active centers with slow re-arrangements of their structure is focused upon. Under real conditions of many sequential reaction turnovers of the macromolecule the structural shifts caused by single turnovers can be of cumulative character. This, in turn, leads to drastic threshold-like changes of the reaction cycle. In that way the creative role of dynamical substrate-conformation interactions in forming of the functional regimes of the biomacromolecule is consistently uncovered for the first time. With this, isolated data on the “complex behaviour” of macromolecules (non-exponential relaxation, memory of reaction cycles, folding peculiarities, non-Michaelis kinetics and non-Langmuir saturation, cooperativity of non-oligomeric or non-allosteric enzymes, etc) turn out to be a manifestation of the unified effect of dynamical intramolecular self-organization as one of the basic principles of molecular machines at work.

The consideration is based on the development of modern stochastic theory of non-equilibrium phase transitions [1] extended to the level of single molecules [2] and comprises analytical and computer modeling of the generic reaction schemes of charge transfer and ligand binding, design and simulation of decisive experiments as well as the proofs of realization of the mentioned mechanisms and effects in specific biomolecular processes (photosynthetic charge separation, reactions of single enzymes and others).

[1] L. Christophorov *et al*, Chem. Phys. 256, 45 (2000)

[2] L. Christophorov *et al*, Ukr. J. Phys. 48, 672 (2003); Chem. Phys. (2005, *in press*)

## **SANS and SAXS investigations of synthetic clays dispersions doped with ferrofluid**

Fábio Luís de Oliveira Paula<sup>1</sup>, Jérôme Depeyrot<sup>1</sup>, Geraldo José da Silva<sup>1</sup>, Francisco Augusto Tourinho<sup>2</sup>, Luciano Ribeiro dos Santos<sup>2</sup>, Rosângela Itri<sup>3</sup>, Jon O. Fossum<sup>4</sup>, Kenneth D. Knudsen<sup>5</sup>

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### **ABSTRACT**

Recently, a new way to probe the microscopic structure of laponite dispersions has been proposed. Maghemite magnetic nanoparticles are incorporated into the clay dispersions in order to characterize their spatial repartition and microrheological behavior [1]. In this work, we investigate the structure of clay dispersion doped with magnetic fluid using small angle scattering experiments. A clay laponite dispersion (0.1wt%) in the isotropic liquid phase is doped with citrated ferrofluid based on cobalt ferrite nanoparticles at several concentration values. Small angle scattering experiment using neutrons (SANS) were collected at IFE-Norway and X-rays (SAXS) were done at USP-Brazil. The sample texture is investigated using an optical microscope before all measurements. All samples show phase separation, with a supernatant, diluted in magnetic nanoparticles and a more concentrated phase in the lower part of the cell. The scattering experiment is done for each sample concentration and for both liquid phases. The analysis of our experimental data is performed using the unified global equation [2]. This equation incorporates the Porod's and Guinier limits and allows to obtain information about parameters such as radius of gyration, log-normal polydispersity index and the exponent associated with the power-law scattering interfacial regime. Assuming that the contribution to the scattering signal is mainly due to the ferrofluid particles, the physical information obtained from the fitted parameters shows that there does exist a strong interaction between the laponite and the magnetic particles. The scattering object presents a diffuse interface and its size does not depend on the concentration of the dopant.

[1] F. Cousin, V. Cabuil and P. Levitz, *Langmuir* 18, 1466 (2002).

[2] G. Beaucage, *J. Appl. Cryst.* 28, 717-728, (1995).

## **Magnetic and structural characterization of ferrofluids based on spinel ferrite nanoparticles: A combined XRD synchrotron, EXAFS and magnetization study**

Jérôme Depeyrot, Juliano de Andrade Gomes, Geraldo José da Silva

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Francisco Augusto Tourinho, Marcelo Henrique Sousa  
Complex Fluids Group, Instituto de Química - Universidade de Brasília*

### **ABSTRACT**

Magnetic nanoparticles based on spinel ferrites offer some attractive possibilities in biomedicine such as in cancer diagnosis and treatment. Differently from the bulk, when this kind of material decreases to the nanometric scale the lack of coordination for surface ions does induce a large number of broken exchange bond for surface atoms, which can therefore results in frustration and spin disorder. On the other hand, the size reduction can induce cation redistribution in the particle structure different from that of the ideal spinel ferrite. Both, surface effects and degree of inversion confer special characteristics and properties to this type of compounds, particularly in the magnetic behavior. In this way, it is necessary to study the local structure of the nanograins, mainly the surface, before binding biological molecules to functionalize and to make the particles interact with a biological entity.

In this work, the nanoparticles are obtained by hydrothermal synthesis and a control of the synthesis conditions permits a modulation of the particle diameter from 3 to 12 nm. A core/surface strategy is adopted to chemically stabilize the nanoferrites which are coated by an iron-rich shell whose thickness is of the order of the spinel unit cell. These nanoparticles, which bear a surface charge density, are individually peptized in aqueous media by a careful control of the electrostatic repulsion between the particles.

To characterize and to model the structure of the spinel ferrites nanoparticles, Rietveld structure refinement of Synchrotron x-ray powder diffraction data is used to determine the structural parameters and the cation distribution of the nanostructures, indicating the existence of a mixed spinel and a magnetic structure different from that of the bulk. On the other hand, parameters such as inter-atomic distances and coordination numbers are obtained by probing the local environment of copper and iron ions using EXAFS measurements. Furthermore, these results are compared with those obtained by Mössbauer spectroscopy measurements (at 5K) in the presence of an applied magnetic field and with those deduced from magnetization curves at room temperature.

Low temperature magnetic measurements show that the structure of the nanograins is composed of a monodomain ordered core and a surface shell of disordered spins which can fluctuate at high temperatures. The hysteretic properties of the magnetization permit to estimate the anisotropy energy and the anisotropy field of the particles. Its size dependence shows that magnetic anisotropy energy of the nanoparticles comes also from surface effects.

## Possibilities of simulation of interconnected systems with no constraints

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### ABSTRACT

We consider hybrid systems of both rigid and elastic bodies coupled into united structures using joints of various kinds. The most common way to simulate them is using differential-algebraic equations (DAE) that introduce additional difficulties into numerical investigations. However it is possible in many cases to avoid DAE.

Equations of motion of a rigid body are Newton-Euler equations that use any appropriate triplet of orientation angles.

Elastic bodies are simulated using any finite-element (FE) formulation (allowing large displacements), which can employ different sets of nodal coordinates, such as: rotation angles in large rotation vector formulation; finite slopes in absolute nodal coordinate formulation (ANCF).

In the first approach, generalized coordinates for both rigid and elastic bodies are compatible and if we apply the well-known assembling procedure, we will obtain ODE only.

In the current paper we pay the main attention to the latter quite new approach.

When a rigid body is connected to an ANCF finite element without restrictions for relative angular orientation (revolute joint in planar case or spherical joint in spatial case), we can still apply the assembling procedure to obtain ODE.

If there are such restrictions (e.g. the body is rigidly attached to FE), we have two possibilities: 1) we implement constraint equations for the body and the FE and obtain DAE; 2) we develop new rigid-body elements that employ ANCF nodal slopes instead of rotation angles as generalized coordinates and further we can apply the assembling procedure again and obtain ODE.

The research was carried out under the projects of Russian Foundation for Basic Research (05-01-00756-A) as well as of National Research Laboratory at the Ministry of Science and Technology of Korea (M1-0203-00-0017).

## Piezoelectric based biosensor for biomedical use

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### ABSTRACT

In this study, we have prepared several biosensors based on piezoelectric (PZ) quartz crystal microbalance (QCM) system for different applications. PZ crystal surfaces were first treated in a glow-discharge apparatus with ethylene diamine (EDA) plasma to create amino groups on the crystal surfaces. Then, the amino groups on the crystal surfaces were converted to aldehyde groups by reacting with glutaraldehyde (GA) at different conditions. The ligands were then immobilized covalently to aldehyde groups on the surface through their amino groups. The following five different sensors were developed by using this surface modification technique: (i) the crystals carrying the antisiphilis antibody molecules were immobilized crystals to detect the antigen (i.e., cardiolipin). After incubation, the frequency shifts and the mass were measured as  $2306 \pm 334 \text{ Hz}$  and  $15.42 \mu\text{g}$ . (ii) an antibody against Hepatitis-B antigen was immobilized onto PZ quartz crystals to determine the antigen molecules in aqueous media having antigen with 3 different concentrations. There is almost a linear correlation between the antigen concentration of 0.010 to 0.056 IU/ml and frequency shift of  $50 \pm 19$  to  $200 \pm 32 \text{ Hz}$ , relatively. (iii) an anti-HSA antibody molecules were immobilized on PZ crystals for the detection of HSA molecules in aqueous media. Four different HSA concentrations (16, 32, 64,  $128 \mu\text{g/ml}$ ) used to observe frequency shifts ( $53 \pm 12$ ,  $78 \pm 25$ ,  $196 \pm 17$ ,  $227 \pm 21 \text{ Hz}$ ) during the interaction of the probe carrying antibody immobilized PZ crystals with the HSA. (iv) a metallothionein (MT) oligopeptide were immobilized on crystals to follow the interaction of this MT with Zn(II) and Cd(II) ions. The highest Cd(II) binding capacity of the MT (frequency shift  $507 \pm 33 \text{ Hz}$ ) was achieved at pH 7.4. The sensitivities ( $\Delta f/\Delta C$ ) of the sensors for Cd(II) and Zn(II) ions appears to be higher for Cd(II) than Zn(II) for adsorption from a single-metal solution in the range of 1.25 to 10 ppm. (v) a double strand oligonucleotide, having one extra base on 5'-end of one of the complementary strands (P2) was immobilized through the amino groups of this base onto the GA-modified crystals. The covalently bound strand was used in the hybridization experiments. The frequency shifts observed during the interaction of the probe with the P2 in the solution. Equilibrium is achieved in about 5 min and the frequency shifts ( $200 \pm 47$ - $90 \pm 21 \text{ Hz}$ ) measured is related to the concentration (1.0-0.5  $\mu\text{g/ml}$ ) of the target strand in the medium.

## **Neural Networks (NN) Based Sensor Fusion for Autonomous Robot Navigation**

Huseyin Goksu

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Isparta, Turkey*

### **ABSTRACT**

We investigate a modular NN based sensor fusion system which first fuses individual sensor networks and then fuses the networks into control outputs. Fused information is used for the autonomous navigation of a robotic system. Major sensor systems are stereoscopic vision cameras and ultrasonic sensor networks where both systems report overlapping events. Performance of the system is tested on computer simulation and a real world system.



## **Molecular Interaction Model for the C1B Domain of Protein Kinase C Isoforms in the Complex with its Activator PMA and Inhibitor Hypericin in Water Solution and Lipid Bilayer**

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### **ABSTRACT**

Protein kinase C (PKC) isoforms constitute a family of closely related isoforms, which are involved in the regulation of several processes that are deregulated in cancer cells. These include proliferation, apoptosis, differentiation, and migration. It is conceivable that each isoform has a specific role in one or several of these processes. Moreover, activation of some isoforms of PKC modulates proapoptotic and activation of other isoforms antiapoptotic signaling pathways in cell. This fact is extremely important for the strategy of antitumoral treatment.

My research is focused on understanding of molecular mechanism of activation and inhibition of PKC. The results dealing with activation of PKC were published two weeks ago in *J. Med. Chem.* [1], where we have presented detailed molecular models of free C1B domain (regulatory domain) of PKC and the C1B domain with its activator PMA in water solution and in the presence of dipalmitoylphosphatidylcholine (DPPC) bilayer. The reason why we have investigated C1B-PMA-DPPC complex is that PKC is activated by its translocation to cellular membranes, which is mediated by the embedment of regulatory domains C1 (composed of C1A and C1B) and C2 on the membrane, providing the energy to release an autoinhibitory pseudosubstrate sequence from the active site of PKC [2].

One of important results of our study is improved structural basis of C1B domain of PKC, which we use for creating of molecular model of complex of potent antitumoral drug-hypericin targeting C1B domain of PKC. One of antitumoral mechanisms of hypericin is inhibition of PKC and in our project we investigate its influence on the C1B domains of different PKC isoforms. These results will shed light on the effect of activation/inhibition of different PKC isoforms in various cell processes that are deregulated in cancer and also provide information on how to influence these processes by modulating the activity of specific PKC isoforms. Because PKC is one of key proteins in cell signaling pathways, our study can also contribute to the better understanding of the role of other members (proteins, ligands, membranes surfaces) of this essential protein network in the cell.

[1] Hritz, J.; Ulicny, J.; Laaksonen, A.; Jancura, D.; Miskovsky, P. (2004) Molecular Interaction Model for the C1B Domain of Protein Kinase C- in the Complex with Its Activator Phorbol-12-Myristate-13-acetate in Water Solution and Lipid Bilayer. *J. Med. Chem.* 47, 6547-6555.

[2] Newton, A. C.; Johnson, J. E. (1998) Regulation of Protein Kinase C by Two Membrane-Targeting Domains. *Biochim. Biophys. Acta Biomembranes*, 1376, 155-172.

## **A real-time hazardous wastes recognition and on-line transmission**

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### **ABSTRACT**

Hazardous wastes effect human and the other alive badly. So it needs to recognize and transmit them very fast. This study proposes an efficient real-time recognition system of some hazardous wastes by using arrays of odour sensors and artificial neural networks. This proposed system has transmitting of these odour's information by point to point network systems.

## Crystallisation singularities of fullerenes macromolecules from various organic solvents

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### ABSTRACT

Fullerenes are, probably, only first and most simple representatives of a new type of frame, in particular spherical, inorganic molecules. As against organic macromolecules spatial molecules because of the exclusive structure and high degree of an aromaticity can be characterized (as well as fullerenes) high conjugation of chemical bond and, as a consequence, extremely high electronic deficiency. The variety of the forms of existence of frame molecules is supposed owing to an opportunity of a variation of composition and structure of molecules on the basis of geometrical principles of their spatial construction from identical or similar elements of structure. The uniqueness of electronscarce molecules of carbon consists in their extremely high ability to ionize metals and to absorb (to accept inside of a carbon skeleton) a plenty of molecules, free radicals, turning, thus, in steadier radicals, polyions or various ionic complexes. As even it is a lot of less electronscarce organic macromolecules have the increased biochemical activity, the interest to research in this respect the fullerenes continuously grows. If the size, composition and structure of spatial molecules of carbon depend basically on a method of synthesis, their reactionary ability in many respects is determined also by chemical nature of the solvent. Electrondonor molecules of the solvent such as benzene, toluol and other aromatic molecules are capable to lower (to extinguish) oxidizing ability of fullerenes molecules due to formation of donor-acceptor complexes. At the same time, at crystallization of fullerenes a molecule of the solvent take root into huge cavities of formed molecular crystals, forming so-called clatratric crystals.

In the given communication the results on research of singularities of fullerenes crystallization, extracted by means of the various organic solvents will be submitted. In research the fullerene-containing soot received at pyrolysis also various (saturated, olefin, acetylene and aromatic) hydrocarbons is used. The products of salting-out and deposition are investigated by means of crystalloptical and X-ray analysis, and also with the help the SEM and TEM.

## **New unusual morphology carbon nanostructures: toroids in the form of rings and polyhedrons**

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### **ABSTRACT**

Now the unique representatives of the new spatial form of existence of a matter are the molecules with a spherical surface. The general and distinctive attribute of spatial nanostructures such as fullerenes, fullerene-like and glandular nanostructures is that they are characterized only by positive curvature of a framed surface. A new morphology of carbon nanostructures as toroids, which alongside with positive have as well negative curvature of a surface, will be submitted in the given report. The negative curvature of a surface of a toroid can be achieved at the expense of a combination in monolayer carbon sheet not only pentagons and hexagons, as in fullerenes and nanotubes, but heptagons as well. Earlier it was supposed, that carbon toroids as the least stable framed structures of carbon can be received only at short circuit in a solution carbon nanotubes with the open ends. The unusual carbon morphology as rings and polyhedrons (4 -, 5- and 6 -hedrons) of a different diameter were found out by us in products of pyrolysis (at temperatures below 1000oÑ) hydrocarbons (benzene, toluol) at the presence of catalytic Fe/SiO<sub>2</sub> system. The feature of given catalytic system is that highly active nanoparticles of metal as the centers of growth of carbon nanostructures are received by mechanoactivating of a silica powder in a high-speed planetary mill with metal spheres and drums. We assume that the iron is distributed not only on a surface of silica particles, but also is introduced into structure of amorphous SiO<sub>2</sub>. It is established, that alongside with toroids the product of hydrocarbon transformation contains carbon nanotubes, at which tops, however, are absent metalcontaining particle. As we are first in synthesizing of carbon toroids, so the principle new mechanism of nucleation and growth of framed nanostructures of carbon will be considered also in the given report. The stages both decomposition of hydrocarbon up to carbon and formation of low temperature eutectic are not considered as intermediate ones. On the contrary, the formation of new Ñ-Ñ bonds at growth carbon nanostructures is carried out owing to dehydrogenated polymerization between molecules of an initial hydrocarbon. As against a destruction process of a molecule hydrocarbon the reaction of dehydro-polymerization, in particular, benzene is highly exothermal, that promotes significant increase of temperature of the local centre of growth carbon nanotubes and, as a consequence, melting of metal.

## Influence Cu (II) Ions on the blue-green micro alga *Spirulina platensis* in the growth dynamic.

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### ABSTRACT

On one hand, copper is an essential element both for human, animals and plants, but on the other hand in concentrations above physiologic ones it exerts strong toxic effect.

Different organisms differ by their resistance to toxic concentrations of Cu. *Protozoa* die at Cu concentration of 0.5 mg/L, unicellular marine algae perish at  $1-2 \times 10^{-2}$  mg/L, where as cyanobacteria die at  $10^{-6} - 10^{-7}$  mol/L .

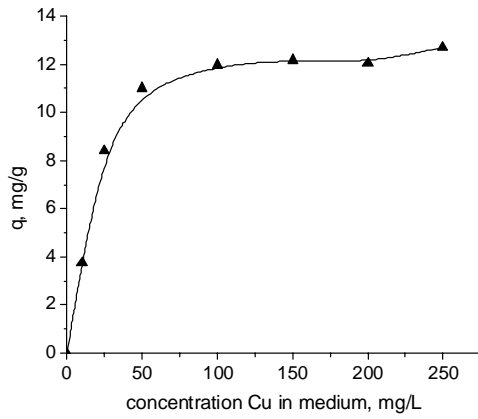
Different micro algae, (*Spirulina platensis*) *S. platensis* included, are used both as living and dry biomass for treatment of waste waters and sea and ocean waters to remove heavy metals.

Furthermore experiments on studies of dynamics of  $\text{Cu}^{2+}$  adsorption by *S. platensis* cells were carried out in the time interval 5-120 minutes.  $\text{Cu}^{2+}$  in concentration 100mg/L was added to the cell suspension 7.5 g/L dense. Agitation was performed by continuous air bubbling at the temperature 22-24°C. Biomass sampling was carried out by filtration through special filters. After filtrate sampling for Cu determination, cells were thoroughly washed with bi-distilled water. Washed biomass was freeze-dried for Cu determination.

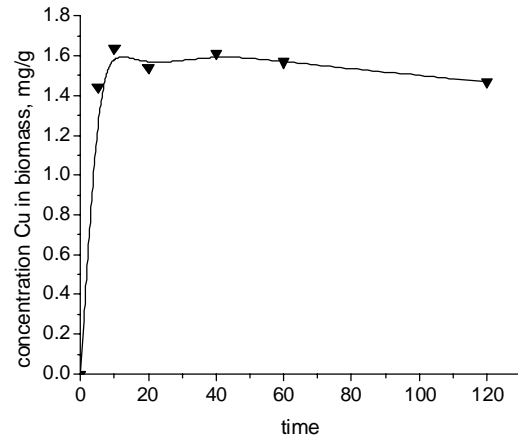
To determine the maximal value of  $\text{Cu}^{2+}$  adsorption by certain amount of biomass for given time interval, the experiments were carried out where *S. platensis* suspension 1.8 g/L dense was exposed to  $\text{Cu}^{2+}$  load (10, 25, 50, 100, 150, 200 and 250 mg/L) for 30 minutes. The experiment conditions and sampling of biomass and filtrate for Cu determination were the same as in the experiments described above. The mathematical treatment of the data was performed by the Langmure method.

It has been shown in studies of  $\text{Cu}^{2+}$  adsorption by *S. platensis* cells that maximal value of adsorption is  $q_{\max} = 12.14 \text{ mg/g}$ . The data are represented as the Langmure isotherm (Fig. 1), where Cu concentration in the nutrient is laid off as the abscissa and  $q$  – adsorption of Cu by algae biomass (mg/g) is laid off as the ordinate. According to literature data, more intensive adsorption on the cell surface is observed in case of Cd load of the nutrient and for *S. platensis*  $q_{\max} = 98.04 \text{ mg/g}$  where as for *S. maxima* strain  $q_{\max} = 47.63 \text{ mg/g}$ .

Data on dynamics of  $\text{Cu}^{2+}$  adsorption by *S. platensis* cells over the time interval 5-120 min are given in Fig. 2. According to our earlier data on binding of such toxic metals as Zn and Cd, binding of copper occurs during the first 15-20 minutes and then cell content of Cu remains unchangeable.



**Fig. 1.** The Langmuire isotherm for suspension of *S. platensis* cells at different  $\text{Cu}^{2+}$  loads.



**Fig. 2.** Dynamics of  $\text{Cu}^{2+}$  adsorption by *S. platensis* cells during 120 min

*S. platensis* biomass both living and dead, the last chiefly, is a promising adsorbent for treatment of waste and industrial waters for cadmium removal. We have shown that adsorption level for copper is less than that for cadmium and living *S. platensis* biomass does not seem to be promising for application in industrial and waste waters as copper adsorbent.

## **Role of Free Radicals in Low Energy Laser Irradiation (LELI) Induced Photobiological Effects**

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### **ABSTRACT**

A hypothesis of free radical mechanisms of stimulatory and inhibitory actions of low energy laser irradiation (LELI), used for therapy of a variety of inflammatory diseases, is formulated. Light absorption induces the production of initiating radicals that are involved in subsequent free radical reactions and subsequent leukocytes stimulation of the greater production of prooxidants and other biologically active products. These products include nitric oxide intermediates (NOI), reactive oxygen intermediates (ROI), which dependent on their induced concentrations, can alter expression (increase or decrease) of proteins involved in multiple signal transduction pathways and induce the expression of inducible proteins, whose genes are highly influenced by external stimuli. Some of these proteins represent protective mechanisms against external stresses, while others amplify adaptation to the induced redox effect. Activation of Mitogen Protein Kinase pathway (MPKP) via cell membrane receptor is suggested.

## Simulation of random packing of binary sphere mixtures by mechanical contraction

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<sup>2</sup>*Physics Department, Institute for Energy Technology, NO-2027 Kjeller, Norway.*

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### ABSTRACT

The mechanical contraction simulation for random dense packings is extended to binary mixture of spheres. The volume packing density as function of sphere composition follows a characteristic triangular shape and resembles previous experiments on length scales from colloidal particles to metal shots. An excluded volume argument, which qualitatively explains trends in random packing densities of monodisperse particles, is insufficient to account for this triangular shape. The coordination number, or the average number of contacts on a sphere, shows a remarkable dip from 6 to 4 at the crossover from many small spheres to many large spheres, which has not been reported earlier.

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## **Investigation of microwave irradiation of croton bug hydrobionits**

Michael Lunika

### **ABSTRACT**

The influence of microwave irradiation on some hydrobionits of croton bug origin was investigated. The cumulative effect of the microwave radiation of the decimeter range was not observed

## Intercalation-enhanced electric polarization and chain formation of nano-layered particles

Yves Méheust<sup>1</sup>, Kanak P.S. Parmar<sup>1</sup>, Jon O. Fossum<sup>1</sup>, Kenneth D. Knudsen<sup>2</sup>, Knut J. Måløy<sup>3</sup> and David M. Fonseca<sup>1</sup>

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### ABSTRACT

Microscopy and X-ray scattering experiments demonstrate that suspensions of synthetic and natural nano-layered smectite clay particles submitted to a strong external electric field undergo a fast and extended structuring typical of electro-rheological fluids. Comparison to the electro-rheological response of similar suspensions of a non-welling clay indicates that ions and water molecules intercalated inside the smectite particles are essential for the particle polarization process that results in the suspensions' electro-rheology. The particles' orientational distributions, as measured from the scattering experiments, are consistent with such a hypothesis. The macroscopic properties of our smectite suspensions may be tuned by controlling the nature and quantity of the intercalated species, at the nanoscale.

## **On the reaction coordinate in protein folding**

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### **ABSTRACT**

In my thesis I have investigated the folding pathways of various small proteins via a Mean First Passage Time approach. This analysis also enabled me to investigate how well the reaction coordinate: "numbered of folded residues" describes protein folding. As it turned out this reaction coordinate can, in spite of its very coarse grained nature, be used quite successfully for certain classes of small proteins.

## Electrical conductance quantization in nanostructures

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### ABSTRACT

Costa-Kramer et al. showed [1] that quantization of electrical conductance occurs in a nano-wire formed between two macroscopic wires. Conductance quantization in a conductor with nanometer size has been theoretically described by Landauer [2]. The transport of electrons is ballistic when the length of the narrow part of a conductor is less than the mean free path  $L < \lambda$ . Quantum of the conductance  $G_j$  and the total conductance can be determined as  $G = \sum_j G_j = \frac{2e^2}{h} \sum_j T_j$ , where  $G_0 = 2e^2/h \cong 77.5 \times 10^{-6}$  A/V. For the ideal case of the ballistic electron transport the probability  $T_j$  is equal to one. In such a case the conductance  $G_0$  of a single transport channel is exclusively determined with fundamental physical constants.

The object of the experiment was a circuit with a parallel LC circuit and a pair of metallic wires – Fig. 1. The process of quantization of electrical conductance is occurring in the junctions of a relay. We have measured transient states of a current  $I(t)$ . Transient states in a LCR circuit depend on the parameters  $L$ ,  $C$  and  $R$  (or conductance  $G$ ). Transients in the mechanical switch circuit may have oscillatory or non-oscillatory property, depending on the current value of conductance  $G(t)$  in this circuit. In a transient state the current in the circuit is described with using a Laplace transform, as follows.

$$I(s) = \frac{V_s (s^2 LC + 1)G}{s (s^2 LC + sLG + 1)}$$

From circuit theory it is known that the form of the transient signal in a circuit is characterized by the determinant  $\Delta$  of the quadratic equation  $M(s)$  in the denominator of the formula.

$$M(s) = s^2 LC + sLG + 1, \quad \Delta = (LG)^2 - 4LC.$$

Output function (current in the circuit) has oscillatory character when  $\Delta < 0$ . Consequently, for the oscillating circuit, the limit value of conductance  $G = G_{lim}$  when  $\Delta = 0$  is given by the relation:  $G_{lim} = 2\sqrt{C/L}$ .

In a transient state, for the conductance less than the limiting value  $G_{lim}$  the current in the circuit exhibits an oscillatory character. For example, for the circuit parameters  $L = 4$  mH and  $C = 30$  pF, the limit conductivity  $G_{lim}$  amounts to  $10^{-4}$  A/V. It means that in a transient process of quantization the electric current in the circuit is of oscillating form for the first quantization level  $G_0 \cong 77.5 \times 10^{-6}$  A/V. For the second it is  $G(2) = 2G_0$ , the third  $G(3) = 3G_0$ , and the remaining quantization levels has non-oscillatory property. We have measured a quantization at contacts made from cobalt wires and copper wires.

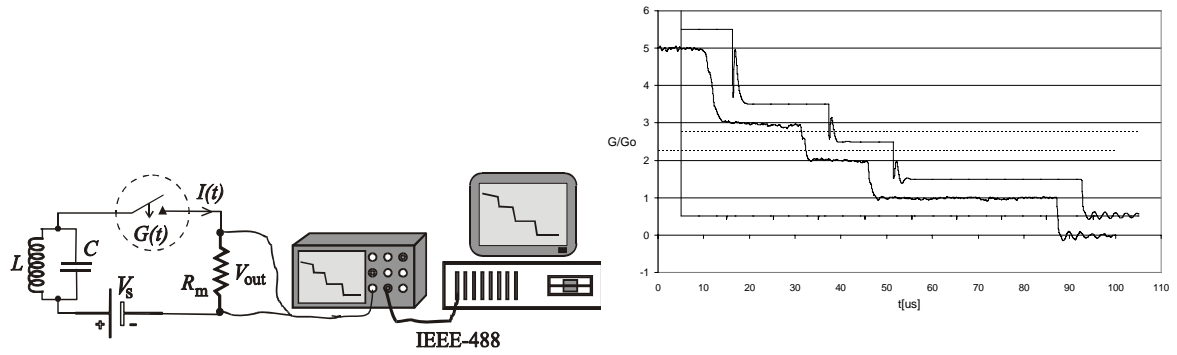


Fig. 1. Setup for the measurement of the conductance quantization in LC circuit (left) and the conductance ratio proportional to transient  $I(t)$  in the circuit (right): the simulation curve and below the measured curve.

## Structure and dynamics of virtual social networks

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### ABSTRACT

Objects of our study were the basic features of virtual social networks' dynamics and structure formation. We analysed a particular discussion topic in a forum hosted at a Hungarian magazine's website. A field survey was carried out among the forum participants to determine the tie strengths. Community structure was discovered by applying the Markov clustering algorithm on the community's graph representation.

We created a model which is capable of calculating quantitative tie strengths in the function of time by analysing message frequencies and lengths between participants. The same clustering algorithm was evaluated on the simulated community graph.

Our results indicate strong relation of the virtual community structure and the communication patterns within it. Our model was also able to predict most of the strong ties, where success rate is based on the comparison with the self-reported tie strengths. This supports the idea of tracing the information flow within the network, based on its structural properties and the communication patterns.

## **Relaxation phenomena in Biological Active nanostructure Substances evidence from: low frequency spectra**

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### **ABSTRACT**

The glycyrrhizinic acid is wide use as chemical composition of drugs. Biological specificity glycyrrhizinic acid and its derivative are rather wide. They have antiviral activity, antitumour, antidiabetic and other useful properties.

Glycyrrhizinic acid and its some derivative can form chemical compound with various medicinal substances. This ability has open wide opportunities to create of drugs of the directed action. At the same time glycyrrhizinic acid and its derivative in the certain conditions can form micelles. As against clatrat of complexes, micelles are forming irregular associat, with unessential by a "correct" arrangement of molecules each other. It is large multimolecular weak -mobile complexes with possible essential dynamics of supramolecular structures. Study GL physical - chemical methods therefore are necessary.

One of advantages of ultrasound methods is a possibility of simultaneously measuring static and dynamic properties of systems near critical points. Measurements of low frequency sound wave velocity make it possible to obtain exact information on equilibrium parameters of the system. At the same time acoustic methods make it possible to study in depth influence of temperature, pressure and external fields on the matter properties. Data on absorption of ultrasound can give direct knowledge of dynamic properties of liquid systems.

Study the kinetics of relaxation processes of aqueous solutions mono-ammonium glycyrrhizinate (monoammonium salt Glycyrrhizinic acid, glycyrrhizin) using ultrasonic relaxation method. The ultrasonic relaxation spectra of glycyrrhizin were determined in the concentration range 0.01-0.4%. The ultrasonic attenuation measurements in the frequency range 0.5-110 MHz showed the existence of excess absorption with respect to water, occurring at concentrations above the CMC of the glycyrrhizin solutions investigated. In investigated solutions were discovered two relaxation processes. First relaxation the process can be referred to an exchange of monomeasures - micell, the second process found out on high frequencies can be connected with intermolecular by processes.

Using given received from acoustic experiment the energy Gibbs,  $G = 10,4$  kJ/mol was calculated; and change Molar volume,  $\Delta V = \pm 122,436 \text{ sm}^3/\text{mol}$

## Trying to predict avalanches

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<sup>2</sup> *“Henri Poincaré” Group of Complex Systems, University of Havana, Cuba*

### ABSTRACT

We explore the possibilities of avalanche prediction in a Self Organized Critical system. In a quasi-2D granular pile experiment the structural network suffers, in average, a continuous disorder increase before a large avalanche happening. Current simulation and experiments are performing trying to correlate the structure and avalanche sequence in earthquake-like systems.



## **Navigation in Cities: A Limited Information Perspective**

Martin Rosvall

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### **ABSTRACT**

Cities are a fundamental part of human organization and we daily face the problem of navigation in cities. As a newcomer in a city, we in principle must ask a citizen to find our way to the target.

We analyze this problem by mapping city street-maps to information counterparts where streets are identified as nodes and intersections between the streets are identified as links between the nodes. The networks show the broad degree distribution found in many other complex networks. The mapping to information city networks makes it possible to quantify the information associated with locating specific addresses. We compare different cities and find that modern planned cities are easier to navigate than old historical cities with a complicated past of cut and paste construction.

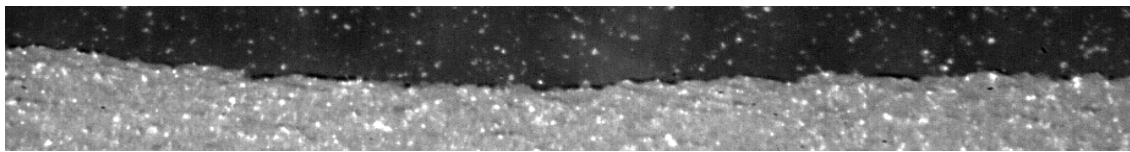
## Slow crack growth and crack pinning in heterogeneous media

### Dynamics and structure of interfacial crack front

Stéphane Santucci, Knut Jørgen Måløy, Renaud Toussaint and Jean Schmittbuhl

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#### ABSTRACT



We have performed an experimental study of the slow crack front propagation through a weak plane of a transparent Plexiglas block using a high speed and high resolution camera. We have observed that the dynamics of the fracture front is controlled by local and irregular avalanches with very large velocity fluctuations. We have focused our study on the dynamics and the structure of the local bursts which lead to the rough fracture front line. In particular, the local front velocity distribution follows a power law for velocities larger than the average crack speed. The burst size distribution exhibits also a power law behavior. Moreover the burst size scales differently in the direction parallel and normal to the fracture front with an exponent consistent with the roughness exponent of the fracture front  $\zeta \approx 0.6$ .



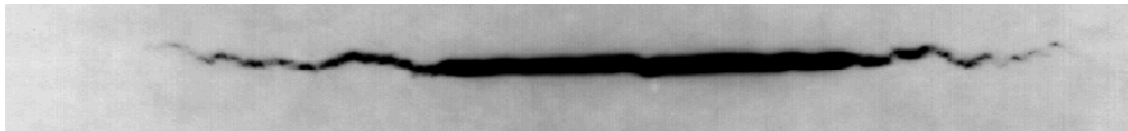
## Slow crack growth and crack pinning in heterogeneous media

### Thermal activation in creep rupture of fibrous materials: experiments and model

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#### ABSTRACT



We have studied experimentally and theoretically the slow growth mechanisms of a single crack under stress in a bi-dimensional geometry. We have performed traction experiments (creep tests) of heterogeneous fibrous materials (paper samples) with an initial macroscopic defect (mode 1). We have observed that the slow crack growth is actually progressing by steps. The average dynamics of the crack growth from an initial length  $L_i$  to a critical length  $L_C$ , where the fracture is rapid, shows an exponential law for the crack growth defined by 2 parameters: the rupture time  $\tau$  and a characteristic growth length  $\zeta$ . A measure of the surface energy needed to open the crack permits to distinguish the Griffith length  $L_G$  and the critical length of rupture  $L_C$ . A statistical study of the step size during the damaging process reveals that the step size distribution follows a power law truncated by an exponential, which is typical of a critical point approach in a sub-critical process. This complex dynamics can be predicted quantitatively describing the slow crack growth in a pure bi-dimensional elastic system in terms of an activation process, where the statistical stress fluctuations allow to overcome a breaking threshold through a series of irreversible steps. Our theoretical approach based on a numerical model (a 2d spring network describing a bi-dimensional elastic "discrete" system) shows the importance of the irreversibility of the rupture process and the crucial role of heterogeneities, which appear only in our model as a characteristic mesoscopic length scale.

## Intermittency, aging and extremal fluctuations

P.Sibani

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### ABSTRACT

Extremal fluctuations are able to trigger irreversible changes in metastable systems, e.g. water level extrema can damage a dam. We argue that a qualitatively similar mechanism can explain key statistical properties of an aging glassy system.

We consider the stochastic dynamics of a glassy system in contact with a thermal bath. The initial quench occurs at age  $t_w = 0$  and typically produces a configuration of high excess energy, subsequently released through de-facto irreversible re-arrangements ('quakes') leading from one metastable basin to another. Smaller energy fluctuations occur reversibly within each metastable basin.

If the extremal values of the energy fluctuations induce the irreversible re-arrangements, the latter are to a good approximation described by a Poisson process with a logarithmic time argument, or Log-Poisson process. In particular, the rate of the events decreases as  $1/t_w$ .

We argue that the quakes are directly observable as intermittent events in the heat exchange between a glassy system and its thermal bath, and that the underlying role of extremal fluctuations can directly be verified by small temperature shifts imposed while the system ages.

Numerical evidence from simulations of the heat exchange in a short range spin glass model is presented to support these claims.

References: Sibani P., Jensen H.J., Intermittency, aging and record fluctuations. Europhys. Lett. 2004; 69,4:563-9

Sibani P., Jensen H.J., How a spin glass remembers; memory and rejuvenation from intermittency data: an analysis of temperature shifts. J Stat 2004: P10013-30.

## **A Kinetic Model Describing the Processivity of Myosin-V**

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### **ABSTRACT**

The question of how myosin-V coordinates the biochemical reactions and mechanical motions of the two head elements of the protein to become an effective processive molecular motor is still unresolved. To achieve a better understanding of the motion of myosin-V along actin filaments, there is a need to compare the quantitative predictions of plausible models with experimental results. We have recently proposed a quantitative model which considers the main reaction path followed by the molecular motor, and also how the overall motion is influenced by the presence of futile reaction cycles and molecular detachment rates. In this way we can establish how the molecular motor can compensate for unavoidable perturbations of the main reaction path by adjusting the reaction rates.

## How a Venus flytrap snaps: a design principle for hydraulically activated movements

Jan Skotheim

### ABSTRACT

The rapid closure of the carnivorous plant Venus flytrap (*Dionaea muscipula*) is one of the fastest motions (typically 100 ms) in the plant kingdom and led Darwin (1875) to describe the plant as 'one of the most wonderful in the world'. The closure is initiated by the mechanical stimulation of trigger hairs. Previous studies have focused on the biochemical response of the trigger hairs to stimuli and quantified the propagation of an action potential in the leaves. We complement these studies by considering the post-stimulation mechanical aspects of Venus flytrap closure. Using high-speed video imaging, non-invasive microscopy techniques and a simple theoretical model we show that the fast closure of the trap results from a snap-buckling instability. Our study illuminates an ingenious solution to scaling up movements in non-muscular engines and provides a general framework for understanding nastic motions in plants and fungi. A comparative study with other rapid plant and fungal movements elucidates a general design principle, which may be useful for the engineering of soft hydraulically actuated systems.

## **Biodisponibility of drug hypericin after in vivo study**

Mariana Stan

### **ABSTRACT**

The HPLC analysis of plasma sample of hypericin extract of animals test. I obtained a pharmacokinetics profile of this antidepressive drug using a HPLC method with FLD detector for identification a concentration at more times.

## Hydrodynamic Screening In Polymer Solutions

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### ABSTRACT

The generalization of the Debye-Bueche-Brinkman equation to the dynamic permeability of the medium leads to the Oseen-like tensor with the frequency-dependent hydrodynamic screening length [1]. This phenomenological theory is used to investigate viscoelastic properties of polymer solutions. The relaxation modulus of elasticity and the static shear viscosity were calculated. Zimm-like behaviour for short times and Rouse-like one for large times are obtained.

1. Tchesskaya T.Yu. Kinetics of semidilute and dense polymer solution: the time dependence of single-chain dynamics// Journal of Molecular Liquids, in press.



## **Forced transport of molecules through the membrane by means of a nanosyringe**

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### **ABSTRACT**

Molecular dynamics simulation of a complex system, imitating a nanovehicle based on a carbon nanotube, is carried out. The system comprises a hydrated lipid bilayer, a nanotube soldered at one end, and certain molecule to be pushed through the membrane. A constant force in normal direction to membrane is applied to a molecule (in this case pentadecameric polyalanine) located in the channel of the nanotube adjoining a lipid bilayer at right angle. Under the action of the force the oligopeptide gets into the membrane. This construction can be considered as a delivery vehicle which drives the peptide to the membrane surface. Tuning the nanotube (by adding of functional groups) one may achieve the selectivity of nanotube's landing area on the cellular membrane. The pressure expelling the peptide could arise as a result of the chemical reaction which makes the reaction mixture volume increase in the soldered nanotube. The chemical agents start the reaction under the action of certain signal (for instance, a flash of light), and during the time in the order of a nanosecond the peptide finds oneself inside a cell. Different regimes of penetrations are considered in the reported simulation which is only a first step on the way to construction of such a nanomachine. It is also shown that such a nano-injection can be spontaneous according to results of longer simulations. The whole system thus is represented as a self-assembled machinery.

## Kinetics of cluster growth in fullerene solutions

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V.L.Aksenov<sup>3,4</sup>

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<sup>3</sup>*Physical Faculty, University of Rostock, Rostock, Germany*

<sup>4</sup>*Physics Department, M.V. Lomonosov Moscow State University, Moscow, Russia*

### ABSTRACT

In recent time, interest to fullerene solutions has considerably grown mainly due to their much promising medical and biological applications. Investigating any fullerene solution one encounters the problem of describing cluster formation and growth. Current theoretical description restricts itself to chemical thermodynamics or simplest phenomenological models.

In the reported work, we have first made an attempt of presenting a stage-by-stage description of the kinetics of cluster growth in fullerene solutions. The Frenkel-Zeldovich equations of the theory of nucleation (Fokker-Plank equations) are used as a basic model. Two simple models of cluster growth in solutions – the liquid drop model and the limited aggregation model for unsaturated and supersaturated solutions – are discussed. The kinetic equations for the evolution of the cluster size distribution function  $f(n,t)$  are solved in a numerical way. The time dependence of the cluster state characteristics – the mean cluster size and the concentration of clusters in the solution – has been obtained and compared with analytical estimates. According to the two models in unsaturated solutions the preferential state of fullerenes in the solution is monomers. In supersaturated (metastable) solutions, clusters form. Estimated time of cluster formation and growth in the liquid drop model is much smaller, than the time observed in experiments on fullerene solutions. As an appropriate development, the limited growth model is considered. The model introduces a phenomenological parameter, describing some kind of mechanism, that limits cluster growth. As the result, we obtain characteristic times of cluster growth, that are in agreement with experiment. The behavior of mean cluster size in metastable solutions is the following. If liquid drop model is used, the mean cluster size decreases as the solution concentration grows. In the limited aggregation model, the average size of fullerene aggregates does not depend on the initial supersaturation.

An analysis of experimental data on C<sub>60</sub> solutions in carbon disulfide, toluene and benzene including UV-vis spectroscopy, electron microscopy, small-angle neutron scattering, dynamic light scattering, positron annihilation spectroscopy, differential-scanning calorimetry is given with respect to the above developed approach. It is shown, that the model of limited growth reflects qualitatively experimentally observed behavior of fullerene clusters in these solutions. However, the question of mechanism of cluster stabilization in this case is open and requires further investigation.

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