



ORDER, ROBUSTNESS AND
INSTABILITIES IN
COMPLEX SYSTEMS.
GEILO ADVANCED
STUDY INSTITUTE.
GEILO, NORWAY,
23 MARCH – 2 APRIL 2009:
POSTER ABSTRACTS



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Report number IFE/KR/E-2009/002			Date 2009-05-27			
Report title and subtitle Order, Robustness and Instabilities in Complex Systems.			Number of pages 47			
Project/Contract no. and name "Geiloskolen"			ISSN 0333-2039			
Client/Sponsor Organisation and reference IFE - Institute for Energy Technology Niels Bohr Institute (Denmark). PGP – Physics of Geological Processes (Norway)			ISBN 978-82-7017- 787-5 (printed) 978-82-7017- 788-2 (electronic)			
Abstract <p>Interdisciplinary scientific collaboration offers an effective method to develop new paradigms to address major societal challenges. One particularly urgent challenge involves analyzing, understanding and responding to the inherent competition between order, robustness and instabilities in complex systems involving many interdependent living or inanimate components. Many societal problems and their solutions are complex and evolve over time as the global and local environments change. The goal is to achieve predictable and robust responses while understanding the nature of instability and breakdown within the complex systems.</p>						
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1 Introduction

Interdisciplinary scientific collaboration offers an effective method to develop new paradigms to address major societal challenges. One particularly urgent challenge involves analyzing, understanding and responding to the inherent competition between order, robustness and instabilities in complex systems involving many interdependent living or inanimate components. Many societal problems and their solutions are complex and evolve over time as the global and local environments change. The goal is to achieve predictable and robust responses while understanding the nature of instability and breakdown within the complex systems. Many leading scientists believe that these problems can be addressed by “learning from nature”. In the course of the evolutionary process, nature has - over millions of years - developed numerous solutions for robustness and adaptability, including sophisticated mobility and self-healing mechanisms, highly selective sensors, and complex information storage and communication systems. This ASI will bring together physicists, biophysicists, biologists and social scientists with related interests and background in the fields of complexity, networks, and social dynamics. This will provide a scientific forum for discussion and learning of the interdisciplinary material and underpin successful development of an understanding of how various threats (such as pandemic diseases, disruption of energy/water distribution and communications and networks) evolve in time. Such an understanding is a prerequisite for designing counter measures.

2 Programme

Program Geilo School 2009, March 23 - April 2

Theme: Order, Robustness and Instabilities in Complex Systems

1st Day Monday March 23		
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	
21.30-22.00	Arne T. Skjeltorp	Opening
2nd Day Tuesday March 24		
08:30-11:30	Mogens Hoegh Jensen	Keynote address: Introduction and perspectives
11:30-15:30	Outdoor activities and lunch	
15:30-17:30	Raymond Goldstein	Evolution of Biological Complexity
17:30-18:30	Mogens Hoegh Jensen Raymond Goldstein	Tutorial group meetings and informal discussions with lecturers
3rd Day Wednesday March 25		
08:30-09:30	Raymond Goldstein	Evolution of Biological Complexity (ctd.)
09:30-11.30	Iva Tolic-Norrelykke	Spatial order in the cell
11:30-15:30	Outdoor activities and lunch	
15:30-16:30	Iva Tolic-Norrelykke	Spatial order in the cell (ctd.)
16:30-17:30	Nils Baas	Hyperstructures – a new way to deal with higher order complexity
17:30-18:30	Iva Tolic-Norrelykke	Tutorial group meetings and informal discussions with lecturers
4th Day Thursday March 26		
08:30-09:30	Nils Baas	Hyperstructures – a new way to deal with higher order complexity (ctd.)

09:30- 11:30	Itamar Procaccia	The Formation and Deformation of Amorphous Solids: Simple Theories for Complex Systems
<i>11:30-15:30</i>	<i>Outdoor activities and lunch</i>	
15:30-16:30	Itamar Procaccia	The Formation and Deformation of Amorphous Solids: Simple Theories for Complex Systems (ctd.)
16:30-17:30	Joel Stavans	Fidelity and Target Location in a Cell: The case of Homologous Recombination
17:30-18:30	Nils Baas Itamar Procaccia	Tutorial group meetings and informal discussions with lecturers
5th Day Friday March 27		
08:30-09:30	Joel Stavans	Fidelity and Target Location in a Cell: The case of Homologous Recombination (ctd.)
09:30-11:30	Martin Rosvall	Mapping change in large networks
<i>11:30-15:30</i>	<i>Outdoor activities and lunch</i>	
15:30-16:30	Poster authors	Brief intros to the posters
16:30-18:30	Poster session	Posters left on display until Wednesday April 1
6th Day Saturday March 28		
08:30- 09:30	Amy Rowat (Seminar)	Dynamics of protein expression in lineages of cells
09:30-11:30	Roger Pynn	Neutron scattering in complex materials
<i>11:30-15:30</i>	<i>Outdoor activities and lunch</i>	
15:30-17:30	David Sherrington	Physics and Complexity
17:30-18:30	Joel Stavans Roger Pynn David Sherrington	Tutorial group meetings and informal discussions with lecturers
7th Day Sunday March 29		
<i>Free</i>	<i>Choice of excursions to nearby scenic places or various skiing events in the mountains</i>	
8th Day Monday March 30		
08:30- 10:30	Kimmo Kaski	Social Networks: Can we analyse and model them?
10:30- 11:30	Øyvind Hammer (Seminar)	Pattern formation in biological and geological systems
<i>11:30-15:30</i>	<i>Outdoor activities and lunch</i>	

15:30-16:30	Ivar Giaever (Seminar)	How to start a high-tech business
16:30-17:30	Joachim Mathiesen (Seminar)	Thermodynamics of stressed solids: the slow deformation and roughening of material interfaces
17:30-18:30	Kimmo Kaski	Tutorial group meetings and informal discussions with lecturers
9th Day Tuesday March 31		
08:30- 11:30	Elizabeth Bouchaud	Structure of fracture surfaces resulting from crack propagation through complex materials
11:30-15:30	<i>Outdoor activities and lunch</i>	
15:30-17:30	Alex Hansen	Dynamics of Wetting Films in Crevices between Grains in Porous Media
17:30-18:30	Elizabeth Bouchaud Alex Hansen	Tutorial group meetings and informal discussions with lecturers
10th Day Wednesday April 1		
08:30- 10:30	Joe McCauley	Finance market instability
10:30-11:30	Giovanni Dosi	The emergence of order in socio-economic systems
11:30-15:30	<i>Outdoor activities and lunch</i>	
15:30-16:30	Giovanni Dosi	The emergence of order in socio-economic systems (c
16:30-17:30	Joe McCauley Giovanni Dosi	Tutorial group meetings and informal discussions with lecturers
19:30	Geilo School Closing Dinner	Geilo Awards, Poster Prizes etc.
11th Day Thursday April 2		
08.30-09.15	Summary	Questions and discussions
09.30-13.30	<i>Departure</i>	<i>Communal transportation of participants to Oslo airport and Oslo</i>

- Each lecture hour will last for about 50 min including questions + ~ 10 min break
- Coffee breaks approximately 10:00-10:15 and 16:15-16:30

3 Poster Abstracts

GC-MS and Molecular-Statistical Identification and Estimation of Physiological Activity of Unsymmetrical Dimethylhydrazine Transformation Products

Yu. P. Adamtseva, A.V. Ul'yanov, A.K. Buryak

A.N. Frumkin Institute of Physical Chemistry and Electrochemistry of Russian Academy of Sciences

ABSTRACT

Unsymmetrical dimethylhydrazine (UDMH) is often used as a component of [hypergolic rocket fuel](#). It is very toxic, reactive and water-soluble. Therefore due to UDMH spills toxic water solutions of the transformation products of UDMH can form. At that time many of the transformation products aren't reliable identified.

By means of gas chromatography-mass spectrometry (GC-MS) some of UDMH transformation products were identified. The retention times and mass spectra for them were obtained.

To increase reliability of identification the thermodynamic parameters of adsorption such as Henry constants for the transformation products were calculated on the basis of semiempirical molecular-statistical theory of adsorption.

Then on the basis of molecular structure, different types of physiological activity of UDMH transformation products, including human toxicity, were estimated using software PASS&CT.

Thus reliable identification and estimation of human toxicity of several UDMH transformation products were made.

Analysis of the bistable genetic switch of the temperate bacteriophage TP901-1.

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ABSTRACT

Center for Models of Life, Niels Bohr Institute, University of Copenhagen.

The genetic switch of the temperate lactococcal phage TP901-1 is fundamentally different from the classical switch found in *E. coli* phage lambda. In the lambda switch two oppositely oriented promoters are regulated by a double negative feedback mechanism where the two transcriptional regulators directly repress expression of the other repressor. In the genetic switch of phage TP901-1, the two oppositely oriented promoters, PR and PL, are regulated by a mixed double negative feedback mechanism since repression of one of the promoters requires collaboration of both of the two regulator proteins. We have constructed two mathematical models describing a simplified bistable system modified from the switch of phage TP901-1. The fold of PL and PR repression between the two stable states of this system have previously been determined from *in vivo* experiments and we use these data to limit the

number of parameters that result in a correct bistable behaviour. We show that two stable states are easily obtained if the transcriptional regulators, CI and MOR, interact in solution before binding to DNA whereas two stable states are hard to obtain if the MOR:CI complex is formed only on DNA. Our simplified system has been largely modified compared to the original switch of TP901-1. It is thus notable that the system still maintains its bistable behaviour and displays the titration of phage repressor by formation of a heteromer-complex, which in itself repress one of its components, as a remarkably robust design for a genetic switch.

The work presented was done in collaboration with:

Hiizu Nakanishi, Department of Physics, Kyushu University, Japan.

Kim Sneppen and Margit Pedersen, Center for Models of Life, Niels

Bohr Institute, University of Copenhagen, Denmark.

Sustainable Development of the Urbanecosystem like Complex Systems

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ABSTRACT

Keywords: environmental quality, water resources, complex monitoring, heavy metals, waste water

The basic idea of my presentation is global and regional sustainable development.

The principle of sustainable development is ensuring a rational growth of welfare that at least does not inhibit, and rather enhances the environmental quality in Ukraine. It is aimed at a rational use of resources, protection of nature, improving environmental factors related to human health.

From the wide range of international environmental issues, the freshwater resources are generally felt to deserve utmost priority in Ukraine.

The largest river system in this country is the Dnepr drainage basin. At least 35 million people and 45% of the industry of Ukraine depend on its water. The state of the Dnepr is a matter of major concern in Ukraine, and considered to be a matter of high priority. The total volume of water resources in the Dnepropetrovsk region is 53.3 km³ (including 0.3 km³ of underground water resources). Water resources are used intensively: the agricultural sector takes up 36% and the industrial sector uses 22% of the total input amount. Close to 50% of total wastewater volume of the region was municipal sewage. Another main source of wastewater is the mining industry. It releases a large amount of groundwater, and as the mines become deeper due to continued exploitation, the volume of water as well as its salinity increases. A considerable amount of untreated water is still discharged into the rivers, because the facilities are overloaded (e.g. 55% of all water discharged into the Dnepr river is untreated). Impacts by industry on the aquatic environment arise mainly from the discharge of process effluents to watercourses, estuaries and the sea. Most synthetic organic chemical pollution is from industrial sources, including chemical and petrochemical plants, refineries, iron and steel plants, wood processing, pulp and paper manufacture and food processing.

Objectives:

to improve availability of data and increase understanding of the amounts of various emissions to air, water and soil, and their impacts, of different industrial sectors in relation to overall emissions; to define measures to reduce ongoing pollution in as short a timeframe and as cost-effective as possible, including methods for monitoring future emissions and enforcing agreed targets;

assessment of the contribution of sewage and wastewater treatment plants to total emissions;

to improve the performance of waste water treatment plants leading to better standards of discharged water;

to improve the treatment and discharge of sewage sludge.

We implemented the detailed analysis of chemical composition of rain and snow, surface and river water of Zaporozhie reservoir, which is adjacent to the territory of Dnepropetrovsk City. High incidence of organic pollutants, namely oil products, and heavy metals in the samples of rain, snow, and wastewater shows that lubricating oil and emissions of diesel engines make the significant contribution to the contamination. The quality of the rivers has decreased over the last decades and has resulted in a sharp drop in the variety of aquatic organisms. The main pollutants are oil products, phenols, heavy metals, ammonium and nitrite. The main sources are agricultural activities and a variety of industrial activities, especially waste water discharges. Furthermore, drainage from polluted areas and erosion of soil contribute to the pollution of the rivers.

A systematic monitoring of organic pollutants and heavy metals in the lower part of the Dnepr River has been focused on Zaporozhskoe water reservoir.

In order to obtain the necessary data, the samples of the river water for analysis have been taken at the relevant places during different seasons of the year. The following parameters have been determined: petroleum products, phenols, detergents, pesticides, and biological absorption of oxygen (BAO), lead and zinc.

The concentrations of above mentioned ingredients had a tendency to increase downstream and depended on sites, season and quantity of annual river flow.

It has been studied retrospective data regarding to organic pollutants and heavy metals of the Dnepr River in administrative framework of the Dnepropetrovsk Region to know the dynamic of it changes. Relevant databases have been created. The graphics of many years fluctuations of different contaminants have been created.

Unfortunately, we did not see tendency to reduction of contamination of aquatic ecosystem of Zaporozhskoe water reservoir.

The quantity and composition of industrial waste waters of different companies have been studied in order to provide with data concerning the specific situation with organic pollutants and heavy metals.

The main industries, which form a lot of wastes are mining, metallurgical, chemical, energetic companies. During last years more than 10 mln m³ of industrial wastes were formed and transported to storage sites and landfills that occupied about 40 ha.

Enormous amounts of different organic substances and heavy metals come to Dnepr River annually. An inventory of the industrial sources of organic pollutants has been made and main sources have been determined. The sites and parameters for systematic monitoring have been selected.

Approach:

to start an investigation to assess the composition and contribution of industrial emissions;

introduction in the industrial sector of responsible and environmental care systems, good housekeeping measures, hazardous waste management systems;

use of water resources (including water conservation) through planning (including spatial planning), the recycling of waste water and the utilization of storm water collected in a separate drainage system (such methods make it possible to achieve water savings and also energy);

to reduce the supply of sewage, discussions should be started together with the drinking water suppliers to reach consensus on the ways in which water savings, and thus reduction of amounts of waste water.

References

Gritsan N.P., Shmatkov G.G., Shapar A.G. Methodical Approaches to the Selection of Sustainable Development of Territory / under edition of Prof. Shapar A.G. - Dnepropetrovsk, 1997. - 332 p.

Percolation on hyperbolic lattices

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ABSTRACT

The percolation transitions on hyperbolic lattices are investigated numerically using finite-size scaling methods. The existence of two distinct percolation thresholds is verified. At the lower threshold, an unbounded cluster appears and reaches from the middle to the boundary.

This transition is of the same type and has the same finite-size scaling properties as the corresponding transition for the Cayley tree. At the upper threshold, on the other hand, a single unbounded cluster forms which overwhelms all the others and occupies a finite fraction of the volume as well as of the boundary connections. The finite-size scaling properties for this upper threshold are different from those of the Cayley tree and two of the critical exponents are obtained. The results suggest that the percolation transition for the hyperbolic lattices forms a universality class of its own.

Phase transitions in populations of coupled phase oscillators

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ABSTRACT

Coupled phase oscillators are used widely in describing cooperative phenomena in physics, biology, chemistry, engineering, and so on. We study the models of Winfree and Kuramoto of synchronization of phase oscillators. Both models show that for typical distribution of natural frequencies a synchronous behaviour emerges when coupling intensity between oscillators exceeds certain value. A coherence is suitably described with an order parameter. The order parameter attains non-zero value for couplings stronger than the critical, thus making the onset of synchronization a phase transition. For the Kuramoto model the phase transition is of first or second order depending on the type of distribution function of the natural frequencies of the oscillators. The transition is of first order when the distribution has a plateau where the seed of the synchronized cluster is formed. The exponents characterizing the dependence of the order parameter on the coupling increase in vicinity of the critical point are derived analytically for both first- and second-order phase transitions.

We also consider an analytically solvable version of the Winfree model of synchronization of phase oscillators [proposed by J. Ariaratnam and S. Strogatz, *Phys. Rev. Lett.* 86, 4278 (2001)]. It is obtained that the transition from incoherence to partial death state is characterized by third or even higher order phase transitions according to Ehrenfest classification. The order depends on the type of distribution function of natural frequencies of the oscillators. The corresponding critical exponents are found analytically.

Analytical results for the critical exponents are supported with numerical integration of equations of motion.

PACS numbers: 05.45.Xt

Extracting intermolecular forces in protein-DNA complexes from structural data

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ABSTRACT

It is a standard exercise in mechanical engineering to infer external forces acting on a body, when given its shape and elastic properties. We apply this kind of analysis to distorted double-helical DNA in complexes with proteins, and extract the local mean forces and torques acting on each base-pair of bound DNA from high-resolution complex structures.

The results reveal the complex nano-mechanical patterns of interaction between proteins and DNA. An application of this idea to 146bp and 147bp crystal structures of the nucleosome core particle reveals a characteristic force pattern at the well-known DNA contact sites, and leads to an explanation of twist defect placement in the irregular 146bp structure.

Flow improvement caused by traffic-rule ignorers.

Sebastian Bernhardson

Umeå university, Sweden

ABSTRACT

A system of agents moving along a road in both directions is studied numerically within a cellular automata formulation. An agent yields to the right with probability ' q ' or to the left with ' $1-q$ ', when encountering other agents. Our model is restricted to two agents types, traffic-rule abiders

(' $q=1$ ') and traffic-rule ignorers (' $q=1/2$ '), and the traffic flow, resulting from the interaction between these two types of agents, are obtained as a function of density and relative fraction. The risk for jamming at a fixed density, when starting from a disordered situation, is smaller when every agent abides by a traffic rule than when all agents ignore the rule. Nevertheless, the absolute minimum occurs when a small fraction of ignorers are present within a majority of abiders. The characteristic features for the spatial structure of the flow pattern are obtained and discussed.

Non-Abelian self organized criticality model with one stochastic site in each avalanche shows multifractal scaling.

Jozef Cernak

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ABSTRACT

A non-Abelian and stochastic self organized criticality model has been proposed in which each avalanche contains one stochastic site and all remaining sites in the avalanche are deterministic. Studies of avalanche structures, waves and size moments showed the shell-like avalanche structures, correlated waves within avalanches and complex size moments. We may assert that the model shows multifractal scaling like the Abelian and deterministic BTW model.

AFM investigation of DNA adsorption onto the self-assembled octadecylamine monolayer

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ABSTRACT

In this work we used octadecylamine (ODA) modified highly oriented pyrolytic graphite (HOPG) as the surface for immobilization of DNA. ODA molecules on HOPG form domains of nanostructured surface, which were characterized with low-current scanning tunneling microscopy (STM). Peculiarities of DNA adsorption on these surfaces were investigated with atomic force microscopy (AFM) both in air and in liquid, and in different salt conditions. AFM images of DNA molecules immobilized on octadecylamine modified HOPG reveal segmented shape of biopolymers: it constitutes straight segments with sharp turns at angles 120° (about 90% cases) or 60° (about 10% cases) between them, reflecting the symmetry of underlying pattern. We consider this alignment as the consequence of electrostatic interaction between DNA backbone and the rows of amine groups of modifier, which cross at specific angles at the boundaries of domains. The obtained results show potential application of HOPG modified surface for alignment of biological molecules. This molecular layer is an interesting candidate for suitable immobilization of DNA for STM studies, where one has to deal with stronger electric fields.

Parallell instability in two-phase flow through porous media

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ABSTRACT

Parallell flow of two immiscible fluids through a porous medium is considered. The mixing region is diffusive when only viscous forces are present. When capillary forces are important a non-trivial mixing front develops. A foam layer forms on the surface of the non-wetting fluid. Its characteristics are affected by the relative viscosity of the two fluids, the magnitude of capillary forces relative to viscous forces, and the degree of disorder in the porous medium. If capillary forces are sufficiently large the foam layer freezes, preventing flow normal to the dominant flow direction. If the foam layer is mobilized, it is found to move with constant width and velocity, eating into the non-wetting fluid. Configuration space is probed using a computer simulation on a two-dimensional network.

Why are Window-Glasses Sensitive to Magnetic Fields at Low Temperatures?

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ABSTRACT

Recent experiments on the thermal and dielectric properties of multicomponent silicate glasses at low temperatures (< 1 K) have revealed an unusual response in some thick-film glass sensors to an applied magnetic field. The heat capacity, which should be linear with temperature, has a non-monotonic response to the field, the dielectric constant has both an enhancement peaking around 1000 Gauss and a suppression beginning around 2000 Gauss. Theories proposed so far, based on a mesoscopic coherent tunneling state or on a nuclear dipole/quadrupole coupling mechanism, have been unable to explain qualitatively most of the experimental findings. A statistical-mechanics theory will be presented which explains quantitatively all of these puzzling experimental findings. The theory is based on an extension of the standard tunneling model for structural low-temperature glasses in which the tunneling particles are assumed to move in a multi-welled local potential. The theory does explain the thermomagnetic enhancement as well as both the magnetocapacitance enhancement and subsequent suppression. It turns out that a small cluster of coherently tunneling charged particles is involved in what are basically multicomponent, multiphase complex materials.

- [1] P. Strehlow et al, Phys. Rev. Lett. **84**, 1938 (2000)
- [2] G. Jug, Phil. Mag. **84**, 3599 (2004)
- [3] G. Jug, submitted to Phys. Rev. Lett. (2008)

Dynamics Of Concentration Fluctuations In Lipid Bilayers Near A Critical Point.

Aurelia R. Honerkamp-Smith, Sarah L. Keller.

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ABSTRACT

Abstract: Membranes produced from appropriate mixtures of lipids separate into coexisting liquid phases. I previously presented correlation lengths and line tensions for liquid domains in membranes near a miscibility critical point. I found that the static critical exponents for correlation length and order parameter were consistent with the universality class of the two-dimensional Ising model [1]. By applying scaling laws, I predicted the size distribution of composition fluctuations in model membranes above their critical temperature. Here I analyze the dynamics governing the lifetimes of these composition fluctuations. Fits of the dynamic structure function to a theoretical model are relevant to predictions of how long fluctuations of a certain size persist in the membrane. This information is important for thinking about how distributions of membrane proteins may be affected by the dynamic heterogeneity of lipids.

[1] A.R. Honerkamp-Smith et al., Biophys J. 2008 95(1): 236-46.

Nanoparticles and Nanostructures as New and Unpredictable Civilizational Threat

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ABSTRACT

The recent opening of the completely new world – nanoworld, undoubtedly, is connected to detection and creation essentially of new carriers of properties - nanostructures and nanoparticles. The main and unique feature of these nanoobjects is that their behavior and the properties essentially differ from nowadays known substances. These results are received in the field of chemistry and physics however they essentially have changed all our representations about potential opportunities of human reason. The opportunity has appeared to manipulate by nanosized objects and in the long term, at a molecular level, to create nanocars, nanorobots and also it is essential to raise quality and duration of life. The epoch of nanominiturizing (occurrence nanochemistry, nanotechnology, nanomedicine ...), epoch of formation of new area of knowledge – nanology as sciences about nanoworld began. Now nanotechnology are considered by panacea for the decision of many global problems, however of researches devoted to study of influence of nanoparticles on health of the people, is carried out too little. Therefore even the experts - nanologists practically nothing know about problems of ecological character of objects, to which they constantly contact. The study of influence these new untraditional for microsystems of properties on an environment and, first of all, on health of the man is represented extremely important

The high penetrating ability of nanoparticles in organism of the man is connected to their size, morphology and extreme aggressiveness. Nanoobjects are capable to penetrate in organism of the man by all possible routes: through bodies of breath and digestion, and also skin. The evolution has not created yet not natural mechanisms of protection from essentially new carriers of properties, the obtaining and which application is carried out already in huge amount. Nanoparticles are capable easily to overcome biological barriers of the man organism, to change physiological and biochemical mechanisms and to cause various pathologies. The penetration of nanoparticles in biosphere is fraught with many consequences and problems connected to generically modified products and radiation, can seem thus simply «flower». So inhaled nanoparticles of radioactive iridium, getting in easy are distributed on all organisms and after 24 hours are found out even in a head brain. Carbon nanotubes on toxicity do not concede to such known cancerogen as benzopyrene

Original classification of nanoobjects, their chemical and nanotoxicological features here will be submitted.

Financial Instability in Social and Economic Systems Under World Economic Crisis

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ABSTRACT

Social and economic system of every state is a complex system that involves many interdependent human, financial, ecological components. Analyzing, understanding and responding to the global competition under instabilities and threats of world economic crises is a complex matter that evolves over time as the global and local environments change. The goal is to research the complexity, network and socioeconomic dynamic of the state as a separate component of the global socio-economic network.

One main point of the research is the adaptation and stability of usage of Kondrat'ev waves for the current world situation.

Globalization of world economy bringing to valuate activity of international investment processes that can show high robustness under economic crises.

Despite on the scientific importance of existent researches, there are a lot of non resolved problems, related to foreign direct investing. There is not enough attention to the complex analysis of correlation between foreign investors' interests and national economy, to the development of the mechanism of FDI effectively involving under terms of global economic threats. The complex analysis is held for: as the state potential for FDI attraction, ways of such attraction influences, as the influence of attracted invest-resource on level of the socioeconomic dynamic of the state-recipient.

A goal of the research is to apply new special methods for working out a complex approach to raise the investment efficiency under financial instability, in particularly that of FDI. The object of the research is the investment potential of a state, influence of FDI on the socioeconomic dynamic and robustness of a state-recipient. The subject of the research is economic–mathematical and econometric methods of analysis, monitoring and modeling of investment potential and its influence on economy, ecological and social system.

The focus is on the overall effect of FDI on macroeconomic growth and other welfare-enhancing processes of state-recipient, and on the channels through which these benefits take effect, on threats that increase on the way of capital networks under world economic crisis. For the first time it was proposed to use complex surveys investigations for modelling, estimation and forecasting the investment potential. The box of econometric models of the evaluating of the inter-state changing in its impact on FDI inflows and the impact of FDI on the economic welfare of a state-recipient is created.

For investigation of the heterogeneity of investment space on regional and industrial level Herfindal-Hirshmann index of concentration is proposed to use.

Proposed and used the author's method for the estimation of investment attraction on the level of regions, economic activities, and industries.

Strain Fluctuations During Primary Creep

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ABSTRACT

Fracture of paper is studied during creep experiment. Paper, as a composite material, exhibits all the typical phases of creep fracture, Andrade or primary, secondary and tertiary creep (see e.g. [1]). The experiment consists on 30 x 100 mm paper sheet, which is stressed with constant load. The strain of the sample is measured using digital image correlation technique [2] on image time series.

The outcome is a vector field describing the deformation rate in paper plane. The strain y-component parallel to stress is much larger than the horizontal x and z-components due to a small Poisson ratio and geometry.

The y-strain is evaluated in a grid producing a strain rate distribution. In primary creep the mean of the distribution exhibits Andrade scaling ($t^{-0.7}$) and the width, i.e. strain fluctuations, scale as $t^{-0.5}$. This indicates that the role of fluctuations increases during primary creep. Similar phenomena can be seen in crystal plasticity simulations [3]. In the simulations the creep rate is calculated as an average movement of dislocations in a box, similar to experimental evaluation of strain rate.

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Chaos in atoms confined in billiard geometries.

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ABSTRACT

An atom confined in a spherical box was proposed as an approximation by Michels et al to represent a pressurized atom in 1937. This model has been used widely in many fields to analyse the effect of pressure on the energy levels, polarizabilities and ionization potential of atoms. At present, the great attention to confined atoms caused by advanced techniques and investigations over large classes of nanostructure systems such as quantum dots, quantum wells, quantum wires and artificial atoms. We consider classical and quantum dynamics of one-electron atoms confined in 2D billiards of different shapes. Atoms are localized not in the center of billiard. Studying the energy level statistic it has found that in comparing to central-symmetric case, shifted one has a new feature such as transition from regular dynamics to chaotic one. Classical counterparts were analyzed by plotting Poincare surface of section which has a good agreement with quantum problems.

Sensors and Systems for Monitoring the Environment

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ABSTRACT

The paper is a study of a distributed system for monitoring important physical and chemical quantities of the environment, including meteorological information. The monitoring system consists of: measurement stations with sensors, communication interface, and system controller with data acquisition, data processing, storage and presentation. From a technical point of view, it is necessary to know the dynamics of the whole monitoring system and its reliability. The sensors measure air and water quality and other parameters like water levels. Monitoring of infrastructure (road, power and communications networks, sewage systems) is as important as natural environment monitoring for population security. It is assumed that dynamics of environment processes is rather slow if we compare it with performances of high speed communication system. But more accurate calculations shown that a monitoring system with many measurement field points has its limit. The dynamics of a monitoring system depends not only on the number of field points but on number of sensors at each point as well. The dynamics depends on the transmission speed in communication system.

There are used different communication interfaces in monitoring system: the public switched telephone network (PSTN), a cellular telecommunication system (GSM) and a communication with radiomodems. GSM has many advantages as the interface in systems for monitoring of environment. GSM system offers following digital data transmission services:

- Short Message Service (SMS) and Multimedia Messaging Service (MMS) are the store-to-forward transmissions of text, graphic and sound files. Typical message delivery time is a few seconds (5 s in our measurements) from the moment of sending. However, delivery delays can be much longer.
- Circuit Switched Data (CSD) transmission, which is the switched transmission of digital data with speeds up to 9.6 kbps via traffic channel.
- General Packet Radio Service (GPRS), a packet data transmission mode. Each packet, or set of data transferred, is an integrated whole, and can be transmitted independently of the other packets. A great advantage of GPRS is high data transfer speeds – up to 115.2 kbps.

The security of the environment create both parameters of the natural environment (the quantity and the quality of water, the quality of air and soils, the weather conditions), as and the artificial environment (the technical infrastructure). So in the care for the safety the monitoring of several quantities is necessary, e.g. the air pollution, the approaching flood or the hurricane, and the road traffic as well. Monitoring environmental systems are vital for environmental security.

Some problems of solution of large systems of equations in structural mechanics

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ABSTRACT

Large systems of linear equations are typical in structural mechanics when the finite element method is used. The relaxation method and conjugate gradients method may be used for solution if the problem requires iterative solution. If a problem leads to the systems with millions (or even billions) of DOFs, solution of such a system may be not a trivial problem from technical point of view. At first, sparse matrices are usual and require cost-effective ways of storing and operating. At second, the problem of storing a large volume of data in memory arises. And, finally, in large physically non-linear problems (such as contact problem) convergence rate becomes pressing and sometimes not predictable. Several ways of improving of strength of casualty, optimizing of data exchange and cost-effective data storing which are applied in solving of such problems are discussed.

Choosing of Order Parameters for Complex Liquid System with large Fluctuations near the Critical Point

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ABSTRACT

One of the important tasks for the adequate description of the properties of the complex system is correct choosing of the order parameter. The cooperative phenomena appear in the system near the critical point, the order parameter has the significant fluctuations. The characteristic size of the system is correlation length R_c , which considerably exceeds the average distance between the particles.

The spatially inhomogeneous liquid system with dispersed fluctuations in the critical region is the good practicable model for studying of the complex systems. The equations of state for such one- and multi-component systems is adequately described by the equations of the fluctuation theory of phase transitions [1], taking into account Van der Waals ideas [2]. The model takes into account the own volume ($v_f = 4/3\pi R_c^3$) of the fluctuations of the order parameter, interaction forces between the fluctuations at distances $r > R_c$ and the presence of quasiassociations of fluctuations.

The equation of state was found on the basis of the fluctuation part of the free energy of a system F_f . On the basis of this equation the temperature dependences of the concentrations $c_i(T)$ for some mixtures were analyzed in the work. The parameters of the equation of state have been calculated on the basis of the experimental data. The transfer equations from some order parameter to another one [3] were used in this work.

Universality in the behavior of systems near the singularity regions (critical points, points of phase transitions, etc.) can give possibility to use the results for the prediction of the behavior of different complex systems (physical, biological, social etc.). The singular behavior of these systems can be described by identical equations by using the appropriate isomorphous parameters.

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The study of surface instabilities using iterated conformal maps

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ABSTRACT

Nature confronts us with a wide variety of complex, disorderly patterns. Many of them are formed by moving-boundary processes, in which an interface moves due to internal fluxes of e.g. mass and heat, and eventually evolves into a complex, rough structure. A simple and well studied family of moving-boundary problems in two dimensions is where the interface velocity is controlled by a Laplacian field, i.e. by diffusion transport. Under these circumstances, the growth can be modeled in several different ways.

Various growth models are presented with a main focus on chordal fingered growth, which can be studied using the Loewner differential equation. A competition between fingers will occur in the models and allow for a simple comparison with experimental results.

A Wnt Oscillator Model for Somitogenesis

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ABSTRACT

We propose a model for the segmentation clock in vertebrate somitogenesis, based on the Wnt signalling pathway. The model produces oscillatory states of the involved constituents with typical time periods of a few hours (ultradian oscillations).

The oscillations arise from a combination of two features: (1) A core negative feedback loop: a high concentration of free β -catenin promotes high concentrations of Axin2 mRNA and protein, which promotes the forming of a destruction complex composed of Axin2 and GSK3 β . This complex degrades β -catenin by phosphorylation, leading to a lower concentration of Axin2 and so on. (2) Binding of Axin2 at the LRP5/6 co-receptor that enables the degradation of Axin2. This results in an effective time delay, which is required to make a negative feedback loop oscillate.

Essential for oscillations is the degradation of Axin2 in its binding to the LRP5/6 co-receptor at the membrane. The oscillations are robust to changes in parameter values, and are often spiky, where low concentration values of β -catenin are interrupted by sharp peaks.

Somite formation in chick and mouse embryos is controlled by a spatial Wnt gradient which we introduce in the model through a time dependent decrease in Wnt3a ligand level. We find that the oscillations disappear as the ligand concentration decreases, in agreement with observations on embryos.

Fingered growth in channel geometry: A Loewner equation approach

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ABSTRACT

A variety of natural growth processes, including viscous fingering, electrodeposition, or solidification can be modeled in terms of Laplacian growth. Laplacian growth patterns are formed when the boundary of a domain moves with a velocity proportional to the gradient of a harmonic field, which satisfies the Laplace equation outside of the domain. A simple model of Laplacian growth is considered, in which the growth takes place only at the tips of long, thin fingers. Following Carleson and Makarov (J. Anal. Math. 87, 103, 2002), the evolution of the fingers is studied with use of the deterministic Loewner equation. The method is then extended to study the growth in a linear channel with reflecting sidewalls. One- and two-finger solutions are found and analyzed. It turns out that the presence of the walls has a significant influence on the shapes of the fingers and the dynamics of the screening process, in which longer fingers suppress the growth of the shorter ones.

Linear and nonlinear quantum transport in tetrahedron graphs

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ABSTRACT

We investigate quantum transport properties of quantum tetra-hedron graphs describing their as a network of quantum dots. Linear transport was explored by solving discrete Schrödinger equation and applying Landauer formalism. Role of boundary conditions also was studied. The conditions to have a stable soliton in Bose-Einstein condensation in such a network and its propagation through such graphs are explored. Surprisingly, it was found that transport properties based on the soliton picture obeying the nonlinear Schrödinger equation and those obtained by Landauer formula applied to (linear) Schrödinger equation are identical.

Non-equilibrium dynamics in two-dimensional Ising model with small dipolar interaction

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ABSTRACT

Thin magnetic materials have gathered a lot of attention recently due to the possible applications and new experimental techniques. In these materials the interplay between short-range exchange interaction and long-range dipolar interaction emerges. In general, especially in non-equilibrium, the effects of long-range interactions, which one can not reduce to effective short-range interactions is poorly known. Domain wall dynamics in two-dimensional Ising model with small long-range dipolar interaction, model to describe magnetic thin films with strong perpendicular anisotropy, with and without short-range impurities is studied using Monte Carlo method. Our main attention is focused to domain switching dynamics, starting from magnetically saturated state, in small temperatures, with small external magnetic field values.

Influence of the water molecules near surface of viral protein on virus activation process.

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ABSTRACT

Electrostatic forces play the crucial role in protein interactions in an aqueous media.

Presenting work is based on widespread model of behavior of protein molecules mainly contacting with water. Protein in water is a carrier of electrostatic charges, which are result of oxidation-reduction reaction. The values of these charges depend on a medium pH value and isoelectric point of amino acid residues, which bear charges. Because of difference of isoelectric points of amino acid residues the alteration of pH value change not only electrostatic intensity, but also the geometry of the field. This protein property is used by many viruses to infect the cell by metabolic pathway. This pathway of infection is used by such dangerous viruses as tick-born encephalitis, influenza viruses.

Thorough consideration of the model brings to light that the geometry of electrostatic field is also affected by relief surface of protein molecule. Curve boundaries of different dielectrics, protein and water, distort electrostatic field with so called polarization effects.

These effects play an important role in the interactions of contacting protein molecules or molecular domains.

Since almost all functional protein, including virus envelope ones, have domain structure the polarization effects make a significant contribution to their interactions and transformations. Such influence of the protein molecule form on the electrostatic forces can explain the surprising fact that the replacement of amino acid residue in the protein structure, which don't alter neither charge nor hydrophilic value, dramatically alter biological property of viruses, strengthening or attenuating their activities.

At the moment the physical theory is capable to describe polarization effects. However, since their characteristic sizes are commensurable with atom there is a difficulty to calculate them. This is boundary value disjunctive the adaptabilities of atomic description of biological macromolecules and their description as continuum objects.

But on the other hand this fact can give an advantage consisting in that there is possibility to describe with two different models verifying one another. Their combination gives the most precise description of experiment.

These theoretical concepts underlay a procedure for modeling and calculation of protein interaction, which was realized in the original computer program.

The program showed a high efficiency on application in experimental exploration of the influenza virus activation process. A gist of the process is a transformation of the virus envelope protein, which occur mainly through interaction with water molecule. At the first step the electrostatic forces in protein changed by the decreasing of pH value performed by the target cell. This change results in the separation of molecular domains creating a cavity. At the second step the water molecules fill this cavity hydrating inner amino acid residues. Because of contact with water they acquire charges and alter the electrostatic field. This alteration results in the almost total damping of inner domains, which have such structure that the contact with water causes the formation a long helix. At the third step this helix grows and attaches to the cell membrane hydrophobic part of the virus envelope protein. The hydrophobic part roots into the cell membrane causing the fusion virus and cell membrane that results in penetration the virus genetic material into the cell cytoplasm.

SELF-ORGANIZATION IN NETWORK GLASS-FORMING SYSTEMS: on some controversies in the adaptability concept

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ABSTRACT

Covalent-bonded glasses have been in a sphere of tight interests for scientists because they exhibit a large variety of possible useful device applications. In general, these disordered solids possess many glass-forming compositions in dependence on their connectivity defined in mean coordination number Z taken as average number of covalent bonds per one atom of structural unit. Within Phillips-Thorpe mean-field rigidity theory [1,2], the covalent-bonded networks proper to such glasses reveal three distinct phases in dependence on Z – floppy, intermediate and rigid. The networks having less than 3 Lagrangian constrains per atom are under-constrained ones (floppy phase), while those having more than 3 constrains per atom are over-constrained and enthalpically-stressed ones (stressed-rigid phase). The onset from floppy to stressed-rigid networks predicted to be solitary one [1,2], but it split into two points with accepting that bonds are not distributed randomly revealing a tendency to self-organization [3]. Thus the second-order transition occurs from floppy to unstressed-rigid phase and first-order transition occurs from unstressed-rigid to stressed-rigid phase. So the stressed-free intermediate phase having just 3 Lagrangian constrains per atom appears so as to avoid stress, forming a so-called reversibility window. In device application, the self-organized intermediate-phase glasses are most attractive since they reveal unique non-aging ability under natural conditions. In contrast, the under-constrained glasses exhibit pronounced drift in their properties caused by thermodynamically-driven forces to achieve a more favorable energetic state, this effect being known as physical ageing. The over-constrained glasses can be affected by ageing too but at higher temperatures. Compositional boundaries of reversibility windows for different glass-forming systems were determined experimentally previously [4].

We try to examine the idea on adaptability of glassy network owing to computational cluster-modeling approach justifying energetically the validity for previously-reported boundaries of reversibility windows in binary Ge-S/Se system.

Quantum mechanical calculations were performed using *HyperChem* program, *ab initio* calculations with RHF/6-311G* basis set being used to determine the total energies of $\text{Ge}_m\text{S}(\text{Se})_n$ clusters. All boundary S atoms belonging to two clusters were terminated by H atoms to be two-fold coordinated. Only half-part contributions from these atoms were considered after subtraction both energies of H atoms and $-\text{S}(\text{Se})\text{-H}$ bonds from total cluster energy. This value was taken as a measure for cluster formation probability.

The performed calculations showed that directly linked edge- and corner-shared $\text{GeS}(\text{Se})_{4/2}$ tetrahedrons are basic glass-forming blocks in the studied glasses, the former being more energetically preferential. These overconstrained tetrahedrons are specifically interconnected in a space within more extended structural blocks forming a so-called outrigger raft structural motive [1]. Despite overconstrained nature of constituting blocks, they are specifically distributed in a glassy network via optimally-constrained intercation linking elements. In such a way, the pseudo-reversibility window appears in glass compositions between Z ranging from 2.4 to 2.5.

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SELF-ORGANIZATION IN NETWORK GLASS-FORMING SYSTEMS: the adaptability concept probed for binary As-Se glasses

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ABSTRACT

In respect to Phillips-Thorpe mean-field rigidity theory [1,2], the covalent-bonded networks like to chalcogenide vitreous semiconductors (ChVS) can form the stressed-free intermediate phase having just 3 Lagrangian constraints per atom, which appears so as to avoid stress. In general, these disordered solids possess many glass-forming compositions in dependence on their connectivity defined in mean coordination number Z taken as average number of covalent bonds per one atom of structural unit. In such a way so-called reversibility window in ChVS compositions appears possessing their unique non-ageing ability.

In the present report, we shall try to examine this idea for binary As-S/Se glass-forming system using computational cluster-modeling approach for different two-cation As_nSe_m clusters ranging from $Z=2.0$ to $Z=2.50$. Our approach, namely CINCA – the cation-interlinking network cluster approach, – was developed to simulate glass-forming tendencies at the ground of the *HyperChem* program package (the RHF/6-311G* basis set) being used to determine the total energies of $Ge_mS(Se)_n$ clusters. The probabilities of different glass-forming structural fragments both two- and three-cations are estimated via cluster-forming energy in mean per-atom determination.

The performed calculations showed that corner-shared $AsS(Se)_{3/2}$ structural blocks (pyramids) with $Z=2.4$ within binary As-S(Se) network are more energetically favorable than edge-shared ones. Thus, the self-organized phase in the case of As-S(Se) glasses should be formed only by corner-shared $AsS(Se)_{3/2}$ pyramids having 3 Lagrangian constraints per atom in obvious contrast to previous results [3], where compositionally-dependent reversibility window was predicted to be in this system from $Z=2.285$ to $Z=2.38$. The optimally-constrained quasi-tetrahedral $S(Se)=AsS(Se)_3$ structural units ($Z=2.285$) is energetically impossible in this system. So the lower limit of previously reported reversibility window in this system near $Z=2.285$ is impossible.

To examine the idea on possible upper limit in the reversibility window, we recalculate the numerical values of forming energies for some three-cation network clusters in this system. It is shown that this limit can be stretched to $Z=2.46$, provided $As_3Se_{3.5}$ structural blocks possessing one homopolar As-As chemical bond will be formed. This process is partly compensated by another one connected with $As_2Se_{4/2}$ clusters ($Z=2.50$) having one simple homopolar As-As covalent bond.

Additional precise measurements with differential scanning calorimetric technique used in *direct real-time chronology* with ChVS samples above stoichiometric As_2Se_3 composition ($Z=2.40$) should be performed to check this idea experimentally.

The authors acknowledge support from Science and Technology Center in Ukraine under Project No 3745.

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Two Regimes at Time Scales of the Single-chain Polymer Dynamics and Mobility of the Polymer Chain Themselves

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ABSTRACT

The computer simulations of single-chain motion in semidilute polymer solutions show Zimm-like behaviour of the dynamic structure factor for short time-scales up to the crossover time and Rouse-like behaviour for large time-scales due to time-dependent screening of hydrodynamic interactions. This work presents a phenomenological theory for the single-chain dynamics in semidilute and concentrated polymer solutions and allows to describe the crossover from Zimm to Rouse-like behavior both in time domain and in spatial domain. The polymer solution is described by submerged in the incompressible fluid a set of oscillators, fixed in space. It is shown that the coupled equations of motion of such a polymer system give rise to the time dependence of the Oseen-like tensor and, as a consequence, the time-dependent hydrodynamic screening length. Monomer mean square displacements and the single-chain dynamic structure factor are calculated. Zimm-like behaviour for short times and Rouse-like one for large times are obtained.

The comparative analysis of the presented model and models [1,2] is discussed. It is shown all these models, based on the consideration of the polymer chain as a mobile chain themselves, give close results for monomer mean square displacements and for the single-chain dynamic structure factor at the same design conditions.

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A dynamic network model for imbibition in porous media.

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ABSTRACT

We present a dynamic network model, based on the governing equations describing two phase flow in porous media.

The swelling of wetting films is incorporated, and is driven by the non-equilibrium in the capillary pressure.

This give rise to the complex interplay of frontal displacements, film swelling and snap-off which is observed in experiments.

The flow simulations are performed on realistic networks of sandstone.

Saturation profiles are compared with experiments for different capillary numbers. For spontaneous imbibition we find that the position of the wetting saturation front shows a behavior proportional to the square root of time.

Population Number Control for Ixode Ticks In an Ecosystem

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ABSTRACT

The presence of an undesired species in an ecosystem is usually a result of action of various biotic and abiotic factors. Elimination of one or several of these factors may lead to removal of the undesired species, while the entire ecosystem remains unaffected. This is a possible approach to the socially important program on targeted elimination of ticks (the major carrier of encephalitis, borreliosis and other diseases) from the Eurasian ecosystems by controlling the population density of the mouse-like rodents. This approach, takes advantage of a weak link in the interaction between warm-blooded animals and ticks: at early stages of tick growth, the blood of small rodents plays the main role in tick nutrition.

A tick female is known to lay about 2000 eggs in to the litter of an ecosystem at a probability of η_1 ($0 \leq \eta_1 \leq 1$). The eggs develop into larvae at a probability of η_2 ($0 \leq \eta_2 \leq 1$). Transition to the next stage (nymphs) is possible when larvae become saturated with animal blood, mostly with that of small rodents. The probability of this transition is $\beta(n)$, where n is the population density of rodents in the ecosystem, which is calculated as the number of rodents per unit area of the ecosystem ($0 \leq \beta(n) \leq 1$). The nymphs climb up the plant stems to a height of several centimeters to attach to an animal body and become saturated with animal blood; afterwards, the nymphs go back to the litter and, after wintering, develop into the next stage (imago) at a probability $\eta_i(n)$ ($0 \leq \eta_i(n) \leq 1$), where i is 4 or 5, depending on the ecological conditions of the locality. At the last i th stage, the nymphs are transformed into imagoes; part of them are females, which are especially dangerous when the causative agents of encephalitis, Lyme disease, etc. are present in the ecosystem. Adult ticks may climb up plant stems as high as 0,5 m to attack large mammals, including humans. A tick attaches to the mammalian body to feed on blood for many hours, and then it lays N eggs into the litter. The presence or absence of ticks in the ecosystem is defined

by the coefficient of reproduction $K = \frac{x_{j+1}}{x_j}$. When $x \rightarrow 0$ $K \rightarrow \alpha$, where α – Malthusian parameter of reproduction:

$$\alpha = \varphi(n, y_1, y_2, \dots, y_r), \quad (1)$$

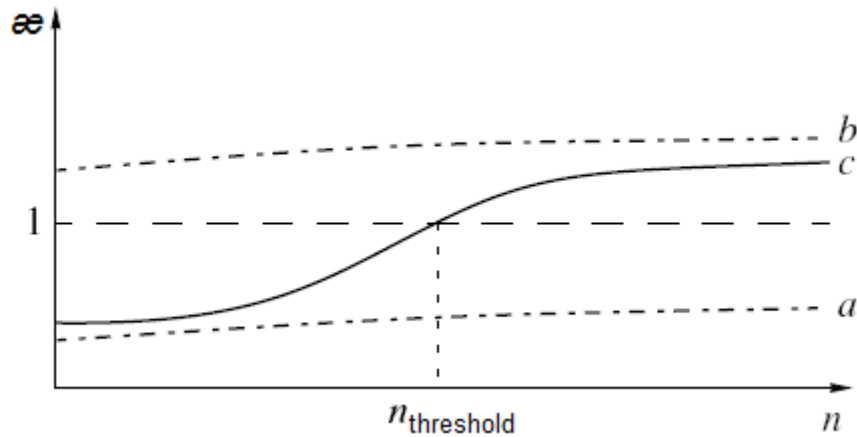


Fig.1. The Malthusian parameter of tick reproduction versus the population density of mouse-like rodents in the ecosystem. The X axis, rodent population density; the Y axis, Malthusian parameter of tick reproduction.

By virtue of Eq. (1), the dependence of the Malthusian parameter α on the mouse population density n can be expressed as the curves shown in Fig. 1. As evidenced from Fig. 1, if the tick reproduction Malthusian parameter curve has the form a , there is no need for using the proposed method; if the solution takes the form of curve b , the method of tick elimination by controlling the population density of mice is unfeasible; curve c corresponds to the case when our approach yields positive results; i.e., an almost complete disappearance of the tick population: it is sufficient to shift the population density of mice in the ecosystem to the region left of $n_{\text{threshold}}$. If $n < n_{\text{threshold}}$, then $\alpha < 1$, and ticks are eliminated from the ecosystem.

Real-time simulation of complex mechanical systems

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ABSTRACT

Real-time numerical simulation of dynamics of complex mechanical systems such as robots, railway vehicles, and automobiles is considered. The example of computer simulation of remote control robots operating in danger zones (accidents in an ammunition depot, radioactive contaminations, chemical pollutions, etc) is given. As a rule these robots equipped with radiation detectors and range-finding sensors are used to detect and neutralize radiation sources. The main purpose of the research is creation of training simulator for robot operators.

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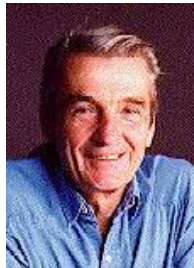
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