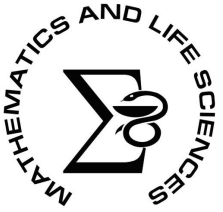

2nd EUMLS Conference

Mathematics for Life Sciences

September 05 – 10, 2013

Kyiv 2013

Information on the project:
The goal of the EUMLS project is to contribute to overcoming the historical communication and cross-disciplinary barriers that exist between the biosciences and mathematics through a comprehensive 48 month research staff exchange programme between five Ukrainian mathematical institutes and three partners in Germany, Italy, and Norway already active in different aspects of computational life sciences.

April 2012 — March 2016
Marie Curie Actions — International Research Staff Exchange Scheme (IRSES)
FP7-People-2011-IRSES Project number 295164

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Information on the workshop: The meeting is an event of the EC-funded project EU-Ukrainian Mathematicians for Life Sciences (EUMLS), yet it is open to all interested scientists with a mathematics or life science background, especially those at the early stages of their careers. The morning sessions will consist of series of tutorial lectures from a mathematical and a life science perspective and aimed at non-specialists from both fields. In the afternoon sessions all participants will have the opportunity to present their own ongoing research to the interdisciplinary audience in shorter contributed talks.

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Evgeniya Semenova

Dates: 5–10 September, 2013.

Location: Olenivka, Crimea, Ukraine.

Talks

R. GRIGONIS, D. KURMANAVICIUTE, R. BUISAS,
R. GUZULAITIS, A. ALABURDA

Effect of increased membrane conductance on response properties of spinal motoneurons

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The pattern of action potential generation in spinal motoneurons depends on synaptic input and intrinsic response properties. Synaptic activity of premotor network not only directly excites, inhibits and modulates the neuron, but it may also contribute by shunting intrinsic properties. During spinal network activity motoneurons receive massive balanced synaptic excitation and inhibition [1], therefore their membrane conductance dramatically increase [2]. This can substantially decrease an influence of intrinsic properties of motoneurons.

It is straightforward to expect that shunting inhibition will increase the rheobase of the neuron, and therefore decrease the number of spikes when stimulated with depolarising current pulse. However, it is not trivial to predict how increased membrane conductance will influence the gain of motoneuron and the threshold for action potential generation.

This issue was investigated by intracellular recordings from adult turtle spinal motoneurons. Membrane conductance was pharmacologically increased by extracellular application of muscimol, GABAA receptor agonist.

Our findings suggest that membrane conductance increased up to 50% does not affect the threshold for action potential generation and causes a subtractive rather than divisive action on the gain of motoneurons.

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L. P. BABENKO, L. M. LAZARENKO, V. V. MOKROZUB,
M. YA. SPIVAK

Antagonistic and Immunomodulatory Action of Lactobacilli and Bifidobacteria in Cases of Intravaginal Staphylococcosis

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Developing alternative treatment methods for patients with uncomplicated urinary tract infections and vaginosis, is of the utmost concern. The newest probiotics based on representatives of the non-pathogenic lactic acid bacteria, that have antagonistic effects towards infectious diseases' causative agents and the ability to balance the immune response expressed — may become such drugs [1].

We characterized the following strains of lactobacilli and bifidobacteria: *Lactobacillus casei* IMV B-7280, *L. acidophilus* IMV B-7279, *Bifidobacterium animalis* VK1 and *B. animalis* VK2. It was found that these strains had *in vitro* antagonistic effects in relation to a wide range of pathogenic and opportunistic pathogenic microorganisms, including causative agents of infectious diseases of the urogenital tract. Furthermore, on the model of intact and *Staphylococcus aureus* infected mice, it was shown, that *in vivo* they significantly reduced the number of *S. aureus* colonies plated from the vagina of infected mice, effectively induced production of endogenous interferon and activated cells of the phagocytic system, without affecting the production of the proinflammatory cytokine tumor necrosis factor-α.

Thus, *L. casei* IMV B-7280, *L. acidophilus* IMV B-7279, *B. animalis* VK1 or *B. animalis* VK2 can be used for creating probiotic drugs effective in treating staphylococcosis and for immunity correction.

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T.BELIKOVA [1], V.SKOBTSOV [2], Yu.SKOBTSOV [3]

Evolutionary approach to medical ultrasound image processing

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It is considered the problem of ultrasound medical images processing using genetic algorithms. Ultrasound images of the internal carotid artery at B-mode are used as the training set. The set of filters and their optimal sequences are designed. We performed an analysis to determine if there is an association between filters sequences and images texture parameters. The results of this analysis will help to improve image quality and detection of pathologies [1].

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N. BONO [1], M. PIOLA [2], M. SONCINI [3], F. PRANDI [4], E. PENZA [5], M. AGRIFOGLIO [6], G. POLVANI [7], M. PESCE [8], G. B. FIORE [9]

Pulsatile pressure conditioning of saphenous veins in a compact and automated *ex vivo* vessel culture system

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The design of a novel ex vivo vessel culture system (EVCS), able to replicate the pulsatile pressure pattern experienced by the saphenous vein (SV) after coronary artery by-pass grafting (CABG), is presented. The EVCS consists of a culture chamber, which integrates the medium reservoir, and hydraulic circuit and actuators. The hydraulic actuators are managed by a programmable monitoring and control system (M/C). The pulsatile pressure stimulation cycle consists of: a loading step (the luminal pressure reaches 80 mmHg); a pulsatile stimulation step (pressure oscillates between 80-120 mmHg at a desired pressure rate); an unloading step (pressure is lowered to zero); and a recirculation phase. Preliminary functional tests were performed using SV samples, in order to validate the robustness and the reliability over time of the M/C system, and to verify the sterility maintenance. Afterwards, surplus SV segments were subjected to venous perfusion (3 ml/min steady flow), or CABG-like pressure (80-120 mmHg) conditioning for a preliminary biological validation. The outcomes of the tests indicated a good reliability of the M/C system. The EVCS provided a sterile environment suitable for stimulation experiments and ensured the survival of SVs. Hematoxylin/Eosin staining of transversally-cut sections showed a good integrity of the vessel structure; in all conditions the endothelial and smooth muscle cells and even the adventitia layers appeared well preserved without signs of tissue degeneration nor swelling.

In conclusion, the EVCS is a suitable system for elucidating the mechanisms involved in the SV graft disease, within a controlled and strictly reproducible mechanical environment.

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Gastrointestinal oncology diagnosis based on imaging fractal analysis. Preliminary results

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Paper describes novel mathematical algorithms that can expand the information content of medical images, providing an objective measurement to reduce subjectivity in the perception and interpretation [1, 2]. Fractal Dimension (FD) is a statistical quantity that gives an indication of how completely a fractal appears to fill space, zooming down to more finer scales. We proposed a method of medical images analysis obtained from a wide range of sources — radiology imaging, ultrasound, endoscopy. We calculated the FD for 5 patients with colorectal cancer for ultrasound, CT images (metastases evaluation) and vector models generated from endoscopy data (processing of colon tumor). Mean FD was 1.68 for liver lesions; 1.65–1.72 for complex colon tumors; and 1.15–1.32 for polipiod lesions. Thus fractal analysis of medical images is a promising non-invasive sophisticated approach, it should become highly informative indicator of pathological formations using nonlinear mathematical parameters of structure, gives insights into tumor morphology and can become a useful tool for analyzing tumor growth patterns for diagnosis, staging and treatment follow up. Further studies on large patients cohorts are required assessing different pathological processes to establish scientifically valid standards.

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B. BULAKH [1], M. STEVANELLA [2], E. VOTTA [3], A. REDAELLI [4]

Improving computational performance in heart valve modeling for surgical planning

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An accurate computer simulation can provide crucial information during surgical intervention planning in case of heart valve disease. At

the same time, such prediction is needed as soon as possible, thus forcing to avoid relatively slow FEM simulation of the heart valves and focus on quasi real-time mass-spring models (MSM).

The Biomechanics group at Politecnico di Milano recently developed a MSM in-house code in MATLAB environment; however, in order to be useful in the clinical practice, its computational performance should be further improved to become almost real-time. In the present work, a single-process code optimization into a more effective compiled programming language (C++) was performed, with a particular focus on the improvement of the collision detection technique based on hierarchical bounding volumes. Preliminary results showed a significant speed-up ($4x$ without collision detection and more than $100x$ when also simulating collisions) with closely comparable results. To further improve the time-efficiency of these simulations, the following strategies can be proposed: parallelization of the computing algorithm (on multiple CPUs or GPUs); use of distributed computing technologies e. g. grid or cloud computing to overcome resource limitations (allowing simultaneous execution of multiple experiments on available or reserved resources).

J. CARTWRIGHT

On the case for an icy origin of life

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A great deal of work is being carried out on the hot origin of life at hydrothermal vents, because the physics, chemistry, and geology all point to this being a very promising hypothesis. Yet at the same time the possibilities of a cold origin of life, either on Earth or elsewhere in the Solar System or beyond, ought not to be dismissed. Here I discuss work that I and others have been doing related to the role of ice along with liquid water in cold prebiotic environments in which life might emerge. Such environments might have been present on the early Earth, but also might be found on other Solar System bodies, in the icy moons of other planets, and in Kuiper-belt objects.

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An adaptive scheme for a general class of semiiteretive methods

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The presentation is devoted to a new wide class of methods for solving ill-posed problems. The proposed approach combines a general class of semiiterative methods that includes both standard ν-methods as well as modified ones (see [1]), adaptive discretization schemes (see [2]) for the input data and the discrepency principle as a stopping rule. The constructed approach has an optimal rate of convergence for solutions with a finite Sobolev-type smoothness. Due to an appropriate adaptive discretization scheme our methods use discrete information more efficiently in comparison with previous approaches and have no restriction on the smoothness of the exact solution.

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On kinetic evolution of interacting cells modeling systems in mathematical biology

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We develop a new approach to the description of the collective behavior of many-cell (many-entity) systems within the framework of the evolution of marginal observables. The developed approach is based on the methods of the kinetic theory of active particles, which shows the ability to retain various complexity features.

The obtained results are applied to the problem of the description of the typical macroscopic (hemokinetic) properties of the blood flows.

One of the advantage of the developed approach is the possibility to construct nonlinear kinetic equations in scaling limits, involving correlations of cells at initial time which characterize the condensed states of interacting cells modeling systems in mathematical biology.

We note also that a such approach is also related to the problem of a rigorous derivation of the non-Markovian kinetic-type equations from underlaying many-cell dynamics which make it possible to describe the memory effects of the kinetic evolution of cells.

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A. PAVESI [1], M. SONCINI [2], A. ZAMPERONE [3],
S. PIETRONAVE [4], M. PRAT [5], G. B. FIORE [6]

Design of a Petri-like culture platform for controlled electrical cell conditioning *in vitro*

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In vitro cardiac tissue engineering often involves the use of bioreactors where multivariate combinations of stimuli are applied, in an attempt to mimic the physiological environment. In a context where bioreactors of increasing complexity are being developed, understanding the role of each biophysical cue is still at the core of basic studies on stem cell differentiation. There is hence a need for simple, reliable and user-friendly laboratory devices designed for cell culture studies under strictly controlled biophysical conditions. We have developed an easy-to-use, cost-effective cell culture platform, able to provide controlled electrical

stimulation, to permit investigating the influence of the electric field in stem cell differentiation process. The bioreactor consists of an electrical stimulator driving twelve petri-like culture chambers. Chambers are completely independent thanks to a module-on-board layout, with a simple *plug-in* conception. A 3-D computational FEM model was used to characterize the distribution and intensity of the electric field generated in the cell culture volume in electroquasistatic conditions, as a function of the culture medium volume filling the chamber. The time course of the voltage inside the culture medium was characterized experimentally for monophasic (8V, 2ms, 1Hz) and biphasic (+4V, 1ms and -4V, 1ms; 1Hz) square pulse stimulation waveforms.

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In silico design and experimental validation of peptidic Self-Assembled Monolayers

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Self-Assembled Monolayers (SAMs) are constituted by small molecules that chemisorb on specific surfaces and spontaneously assemble as an ordered layer. In particular, the recently developed peptide-based SAMs can be exploited in biological applications thanks to their intrinsic biocompatibility. In this study we use atomistic simulations to characterize peptidic SAMs on gold surface to design the best amino acid sequence for biological application. The investigated peptides feature a head-group (Cysteine, for thiolate bond formation with gold), a linker formed by a sequence of 1 to 4 amino acids (chosen between A, F, G, P, S, Y), a zwitterionic layer formed by an alternation of opposite charged residues (KEn), and an integrin binding end group (GRGDSP). In the first screening we test the formation of secondary structures in isolated peptides using Replica Exchange simulations and validating the results

by Circular Dichroism. The most promising peptides are then simulated in SAM configuration on gold surface and analyzed in terms of secondary structure, tilt angle, lateral interactions formation, hydrophilicity, height and RGD exposure to solvent. The results show that the optimal peptide needs a linker of 3 residues of Proline or Phenilanaline and a layer of at least 4 KE pairs.

Ya. I. GRUSHKA

Generalized Lorentz Transforms and Application of Changeable Sets for Mathematically Strict Foundation of Tachyon Kinematics

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We investigate the generalized Lorents transforms in Minkowski space time $\mathcal{M}(\mathfrak{H})$ over any real Hilbert space $\mathfrak{H}$, which in the particular case $\mathfrak{H} = \mathbb{R}^3$ have been introduced in the papers of M. Hill, Barry J. Cox and E. Recami. The set of generalized Lorents transforms $\mathfrak{OT}(\mathfrak{H})$ include the classical Lorents group $\mathfrak{O}(\mathfrak{H})$ over $\mathcal{M}(\mathfrak{H})$, and these transforms may be considered as generalization of classical Lorents transforms for the case, where the velocity of reference frame exceeds the speed of light [1]. We can prove, that, unlike the classical case, the set $\mathfrak{OT}(\mathfrak{H})$ do not form a group of operators in the space $\mathcal{M}(\mathfrak{H})$ [2]. Nevertheless, using the theory of changeable sets [3], we can construct mathematically strict model of kinematics, which include the classical kinematics of special relativity, and allows superlight motion of inertial reference frames. But, since $\mathfrak{OT}(\mathfrak{H})$ is not a group, the last kinematics do not satisfy the relativity principle in the superlight diapason.

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V. KALMYKOV

Variable resolution in biological and computer vision

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The investigations of vision physiology and creation of computer vision objectively are the interconnected areas of human activity. One of the principal differences between the biological vision and the computer vision is variability of the receptive fields excitation zones. The systemological analysis of the neuro-physiology sources let to offer the new model of the neuron functioning.

If the variables resolution will be used in computer vision, the complexity of the tasks to be solved and the quality of visual information processing and can be improved.

I. KARABASH

Optimization of optical resonators for Biological Imaging

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Contemporary biological and medical imaging uses multi-layer optical systems (photonic crystals) to gain smaller X-ray focal spots and to enhance spatial resolution. Further development of imaging techniques requires improvement of resonant properties of multi-layer structures.

In the simplest 1-D case, resonances of an optical multi-layer structure can be defined as eigenvalues ω of the problem $c^2E''(x) =$

$\omega^2\varepsilon(x)E(x)$ with the radiation boundary conditions imposed on the electric field $E(x)$ at $\pm\infty$. The dielectric permittivity function $\varepsilon(x)$ represents the electromagnetic structure of the devise. The following resonance optimization problem has recently attracted considerable interest among specialists in Optical Engineering and Numerical Analysis: find a function ε that create a resonance ω with a very small decay rate $|\mathrm{Im}\,\omega|$. The aim of the talk is to present a new analytic approach to this problem. The method is based on a specially developed two-parameter perturbation technique and on convex analysis of leading terms of perturbed resonances.

In the case when the side constraints $\varepsilon_1 \le \varepsilon(x) \le \varepsilon_2$ are imposed on ε, the main result states that optimal structures consist of alternating layers of two materials with extreme allowed dielectric permittivities ε_1 and ε_2, and that coordinates of the interface planes between the layers can be calculated via a nonlinear eigenvalue problem of the form $c^2E'' = \omega^2 f(E)E$. An explicit expression for the function f allows us to exclude the unknown optimal function ε from the process of calculation of optimal resonances. This reduces the resonance optimization problem to the zeroes-finding problem for a function of three real variables.

K. KELLER, A. UNAKAFOV, V. UNAKAFOVA

Determining and estimating the Kolmogorov-Sinai entropy

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Recent results show that there is a close relation of the Kolmogorov-Sinai entropy and the relatively new concept of Permutation entropy. We discuss why this is interesting for applications in the life sciences and give some overview on the newest results and on open problems concerning the relation of both entropies. Moreover, we demonstrate that some modifications of the permutation entropy could be interesting for estimating the Kolmogorov-Sinai entropy.

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Mathematical modelling of cerebral arteriovenous malformations

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Vascular deceases of the brain are one the main causes of human death and disabling. Arteriovenous malformations (AVM) are widespread cerebrovascular anomalies. AVM is an abnormal connection between arteries and veins — a direct connection in the form of chaotic vessel tangle bypassing capillaries. These anomalies degrade normal blood circulation of the brain areas, change blood flow regimes and very often lead to cerebral haemorrhage.

During recent years medical equipment and technologies were greatly advanced. Endovascular embolization procedure was developed to treat AVMs. At the same time, preoperative mathematical modelling of haemodynamic changes within the anomaly and its surrounding brain area during the embolization is a topical problem.

In this work a mathematical model of the AVM is constructed. It is based on 1D hyperbolic system of differential equations on an unordered graph with edges of different lengths and diameters. The embolization process is simulated via variation of the vessel resistance parameters.

To estimate postoperative complications we introduce a haemodynamic parameter — a specific hydrodynamic load on the AVM nidus. It is shown that this parameter is in conformity with neurosurgical approach to embolization amount in staged treatment of the AVMs.

Our research is based on the clinical data obtained during examinations and endovascular surgery in Novosibirsk Research Institute of Circulation Pathology.

A. G. KYSELOVA

Context-aware approach for processing heterogeneous data

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Multi-parameters system is an information system that support or organization decision-making activities. The problem in multi-parameters system is estimation multiple heterogeneous data in dynamic environment. For this using context model, that can be used to characterize the situation of entities. We performed an analysis to determine a set of algorithms for context-processing tasks and to estimate their capability to fulfill the requirements typical for computing environments with different heterogeneous parameters that are using Multi-parameters system services. The results of context analysis can provide speeding up process of decision making.

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O. G. KYSELOVA [1], Ie. A. NASTENKO [1,2]

Estimation of human cardiovascular circulatory system

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This work is devoted to the research and development of methods and tools for the analysis of human cardiovascular circulatory system, early prediction of the probability of sudden cardiac arrest, as well as

analysis of various cardiac arrhythmias based on the dynamics of the 24h heart rate.

The approach is applied to 24h — 48h Holter recording of heart period variability obtained by examination of patients with normal state of cardio-vascular system and patients with the pathologies such as ischemic heart dilatation with circulatory deficiency, paroxysmal tachycardia, subaortic stenosis with circulatory deficiency.

The software for processing and analyzing output of 24h HR and generating diagnostic conclusion about existing pathologies of the circulatory system and the status of the regulatory reserves of the human body was developed.

Clinical studies using the elaborated computer-aided diagnostic system showed a high predictive value of the developed methods for identifying patients with various stages of hypertension.

D. LANGEMANN

Robust mathematical models for metabolic supply chains

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In recent years, mathematical modeling became more and more important for life science applications. The models differ from models in physics or engineering, and an increasing variety of models are built of mechanisms which are not completely quantified. Often, only a selection of qualitative properties of these mechanisms are known. Nevertheless, mathematical models present a conceptual frame, and observations are discussed and understood within this frame.

We present typical examples of mathematical models using uncertain mechanisms like models for the human energy metabolism, appetite regulation and metabolic supply chains in general. We show that some robust implications can be found anyway, which are independent on the particular specification of the uncertain mechanisms.

In particular, aspects of the Selfish-brain-theory will be addressed. This theory, founded by Achim Peters, discusses the human energy

metabolism and the development of metabolic diseases with an supply-chain-approach where the brain is the final energy consumer in competition with other energy consumers in the human metabolic system. Consequently, mathematical models concerning the Selfish-brain-theory deal with integrated and uncertain mechanisms on an abstracted individual level, and it is necessary to discuss the validity of their implications.

S. MAKSYMENKO

Vector fields and their applications

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Vector fields are models for speed and direction of moving fluid, force fields like electro-magnetic or gravitational, gradients of scalar quantities like temperature, pressure, density, colors in the picture (represented as numbers), etc.

The aim of this talk is to explain what is a *vector field* and disscuss their applications in physics, biology, chemistry, medicine, meteorology, and other life sciences.

I will also discuss Poincaré-Hopf theorem describing probably the most general and important property of topological structure of vector fields.

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Impact of Classical and Berkson Multiplicative errors in Radiation Doses on Dose-Response Analysis

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Widely used nowadays methods of risk estimation presume the presence of fluctuations only along the axis of effects, while as an actual factor (dose) certain its point estimate is used. Meanwhile practically

there is no situation where the individual or simulated dose estimate has no statistical distribution. And though in the last decades reiterated attempts were made to develop mathematical tools which take into account two-dimensional distribution of not only the effect but the dose as well, the problem has not been solved yet neither in purely mathematical nor in procedure aspect. One of the main reasons for such situation is the fact that the dose measurements are inevitably accompanied by errors of either classical or Berkson type, or by certain its mixture. In this connection there is no final decision concerning the influence of the classical and Berkson error in the measured dose on the final result of the risk-analysis, which is usually expressed in terms of relative (ERR) or absolute (EAR) risk.

The most striking example of actualization of this problem is the risk-analysis of results based on yearly radio-epidemiological investigations of the cohort of children with thyroid dose as a result of Chernobyl accident. It is important to note that in these studies the absolute and relative frequencies of thyroid cancer cases in this cohort are found with quite high accuracy. Not only point dose estimates but also interval estimates (in statistical sense) are obtained. But interpretation of results of this thyroid radio-epidemiological study was based on risk estimation methods which do not take into account the presence of significant uncertainties in doses. One of the consequences of the assumption about the absence of errors in doses can be that the risk estimates are biased and the curve "dose – effect" is distorted. The aim of present work is to study the influence of multiplicative classical and Berkson errors in thyroid dose on the estimate of the radiation risk.

I. MAZUR

Donnan Potential as a Tool for Stable Transmembrane Polarization in System Membrane Vesicle Incubation Medium

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Transmembrane potential (V_{mem}) refers to the voltage difference across a cells bilayer membrane that is established by the balance of intracellular and extracellular ionic concentrations. Specificity has been

uncovered in the relationship between changes in V_{mem} levels and alteration of cell function [1, 2] and different membrane proteins [3, 4].

Donnan potential emerges when a semipermeable membrane between two compartments is used and there is different concentration of non-permeable ion inside it. But its value in cells is not high, in range 3-8 mV [5]. Earlier, prof. Kosterin assumed [6] that the value of Donnan potential might be higher if volume of compartments is slightly different. So, using principles of particle conservation, equality of electrochemical potential, and electrical neutrality the general formula of Donnan potential was derived. This formula uses concentration of all salts inside and outside of vesicle and ratio of compartments volume. It was shown that the lower ratio (inside:outside) the higher Donnan potential could be up to 75 mV. Thus, Donnan potential may be used as a tool for creating stable membrane potential of vesicle, which can have practical and methodological implications for investigation the influence of the transmembrane potential on the function of membrane protein.

We are thankful to member of NASU S.O., prof. Kosterin (O.V. Palladin Institute of Biochemistry, NASU) for valued advices during discussion of investigation results.

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R. MAZUR

On Human Mobility Prediction and Opportunistic Networks Routing

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Opportunistic networks can be defined as a one type of challenged networks that should implement integration of diverse computation resources. These networks are based on spontaneous connectivity between

nodes with a goal to enable communication in disconnected environments, where an end-to-end path between the sender and the receiver is often absent.

In such conditions routing becomes a rather interesting and difficult task since networks are based on temporary random connections between devices. Nodes of mobile opportunistic networks are people carrying phones or other gadgets capable to make connections between each other. Thus prediction of human mobility can become a strong basis for efficient routing protocols implementation.

It is reviewed what applications demand on our ability to foresee mobility of individuals, what approaches are currently being used to build human mobility models, and how some of existing opportunistic routing algorithms are designed with application of mobility models.

T. A. MELNYK

Homogenization of Semi-linear Parabolic Problems in Thick Fractal Junctions

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A thick junction of type $m : k : d$ is the union of some domain, which is called the junction's body, and a lot of joined thin domains situated ε-periodically along some manifold, which is called the joint zone, on the boundary of the junction's body. The type $m : k : d$ refers to the limiting dimensions (as $\varepsilon \to 0$) of the junction's body, the joint zone and each of the attached thin domains. The small parameter ε characterizes distance between neighboring thin domains and their thickness. The aim of investigation of boundary-value problems in thick junctions is the asymptotic behavior of solutions as $\varepsilon \to 0$, i.e. when the number of joined thin domains infinitely increases and their thickness goes to zero.

Since various constructions of the thick junction type are successfully used in nanotechnologies and microtechnique, the extensive study of boundary-value problems in thick junctions with more complicated configurations are appeared in the last time (see for instance [1] - [4] and references therein).

In my report I am going to present new results for boundary-value problems in thick junctions that have fractal structure.

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Swimming efficiency estimations for animals

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We show that the best swimmers have a streamlined shape that ensures an attached flow pattern and a laminar boundary layer at rather large values of the Reynolds number. We obtain simple expressions for the volumetric drag coefficient for an ideal laminar unseparated body of revolution and for a capacity-efficiency factor together with estimations of a critical value of the Reynolds number. The capacity-efficiency factor, calculated for different organisms and underwater vehicles, demonstrates that information about animal shapes and locomotion, as well as being of biological interest, should be of great use to improve robot fish and underwater vehicles.

O. V. OGLOBLYA, G. M. KUZNETSOVA, A. V. ZHOLOS

Analysis of correlation effects in the activity of the TRPM8 cold and menthol receptor

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Transient receptor potential (TRP) channels play significant roles in cell signaling by responding to various environmental physical and chemical factors and translating them into cell membrane potential changes

that modulate calcium influx. The TRPM8 cation channel has been extensively studied as a major neuronal cold sensor. TRPM8 is also activated by membrane depolarisation, calcium store depletion, and some lipids as well as by compounds that produce cooling sensations, such as menthol or icilin. Despite a large progress has been made in understanding the molecular mechanisms of its activation, the underlying TRP channel kinetics at the single channel level are still incompletely understood.

In this study, we propose a general mathematical approach for fast express analysis of the existence of correlation effects (possibly of non Markov type of behavior) in the activity of single TRP channels. The novelty of our approach consists in statistical evaluation of distribution function for difference of duration of two subsequent pairs of adjacent open and close states with the distribution function for the chain of open-close-open-close events. Experimental observations are then compared to the theoretical predictions for non-correlation behavior. In the framework of our approach we found pronounced correlation effects present in the activity of the TRPM8 cation channel.

V .S. OVERKO

Features of the blood flow in the helical-like curved vessels

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Mathematical simulation of the blood flow in the pathologically planar curved and non-planar curved blood vessels was performed. Influence of degrees of the curvature by the intensity and the features of the secondary and the reverse blood flow in the vessels at different times cardiac cycle was determined. The most significant secondary flow features comprise the generation of non-plane Dean vortices in braking phase of period of the pulsating, as consequent, forming difficult 3D structure of vorticity. The study has indicated that the dominant geometric effects on secondary flow arise in models with uniform number of Dean. Hence, this model has minimal loss of power that is evidence of the stabilizing role Dean's vortex for flow in the curved pipes. Investigation demonstrated that non-planar geometry of the curved channel modifies

the features of the flow. This phenomenon has as negative as positive influence on the flow in the blood vessels. Positive influence consists in creating uniform profile velocity. The formation of the swirling flow for some geometry types of 3D curved channel is negative part of this effect. In conclusion note that Dean's number is not completely describing flow in tightly curved channel with altered curvature. For example, value Dean's number that were calculated for inner radius, central radius and outer radius have wide range of alteration.

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Two-Dimensional Frequency Detection

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We consider the problem of detecting periodicities in two-dimensional exponential sums from sampled values. For this purpose we extend a method for the one dimensional case, which uses orthogonal polynomials on the unit circle.

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The role of pulsatile pressure in the arterialization of human saphenous vein after coronary artery bypass grafting surgery

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Saphenous vein (SV) graft disease represents an unsolved problem in coronary artery bypass grafting (CABG). After CABG, progressive

structural modifications of the SV wall lead to the occlusion of the graft lumen. In the present contribution, we investigated in vitro the effects of physiological pressure patterns of the coronary circulation on human SV samples. This is indicated as one of the major causes of stress for SV segments after implantation. To this aim, we used an ex vivo vessel culture system (EVCS), developed in our Laboratories, able to apply the desired pressure patterns to SV segments and to maintain the vessels viability. The EVCS consists of a culture chamber, which integrates the medium reservoir, and hydraulic circuit and actuators. The hydraulic actuators are managed by a programmable monitoring and control system (M/C). The pulsatile pressure stimulation cycle consists of: a loading step (the luminal pressure reaches 80 mmHg); a pulsatile stimulation step (pressure oscillates between 80-120 mmHg at a desired pressure rate); an unloading step (pressure is lowered to zero); and a recirculation phase. Afterwards, we used 24 human SV segments: 12 samples were subjected to CABG-like pressure stimulation (CABG-PS, 80-120 mmHg), while 12 samples were cultured under venous perfusion conditions (3 ml/min steady flow, and 5 mmHg). Native SV segments served as control. After 7-days CABG-PS, the main findings were: i) distension and reorganization of the vessel wall components with partial endothelial denudation, smooth muscle cells rearrangement and disarrangement of the vasa vasorum; ii) decrease of SVs wall thickness; iii) enlargement of the SVs luminal perimeter; iv) increased proliferation rate; v) increased up-regulation of MMP-2; and vi) basal level of TIMP-1 expression. These results suggested that the CABG-like pressure has an important role in the early events associated with the remodelling of the SV wall. Studies are currently performed in our Laboratories to correlate each of these changes to the establishment of cellular and molecular pro-pathologic pathways involved in the SV graft disease.

O.A.POKUTNYI

Operator Differential Equations in Frechet space

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The report is devoted to obtaining necessary and sufficient conditions for existence of generalized solutions of boundary value problem

$$\dot{x}(t) = A(t)x(t) + f(t), \tag{1}$$

$$lx(\cdot) = \alpha, \tag{2}$$

in Frechet space $(F, \|\cdot\|_n)_{n\in\mathbb{N}}$. Unbounded operator-function $A(t)$ with dense in F domain D is infinitisemal operator of evolution semigroup $\{U(t,\tau)|\ t,\tau \in \mathbb{R}\}$, extended by continuity on space F. Operator-functional l is bounded and maps vector-function $x(t)$ into another Frechet space F_1, $\alpha \in D$.

Condition of solvability of (1), (2) is given. Generalized solutions of (1), (2) built with using generalized-inverse operators [1] and generalized Greens operator [2,3].

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J. PRESTIN

Periodic Multiresolution

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It is the aim of this lecture to present some ideas of multiscale analysis and time-frequency-localization for spaces of periodic functions.

In particular, we consider finite dimensional nested spaces of trigonometric polynomials constructed from de la Vallée Poussin means of the Dirichlet kernel. Following an approach of C.K. Chui and H.N. Mhaskar we investigate the corresponding Multiresolution Analysis. The scaling functions and wavelets are given explicitly as trigonometric fundamental interpolants and decomposition and reconstruction algorithms can be described in simple matrix notation. The circulant structure of all relevant matrices allows the use of Fast-Fourier-Transform techniques for the actual implementation. Thus we achieve almost optimal complexity

compared to other wavelet approaches derived from implicit two-scale relations, while dealing with a fully computable trigonometric multiresolution analysis with explicit algebraic formulas.

Furthermore we describe the multivaraite setting and discuss different approaches including tensor products and Boolean sums.

The special structure of the underlying de la Vallée Poussin means allows to transform most of these results to the algebraic case. In particular we obtain algebraic polynomial wavelet bases for $C[-1,1]$, where certain interpolation conditions for the wavelets are satisfied.

M. V. PRIVALOV

Methods and tools of 3D reconstruction and visualization of a brain from the image series

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At present time image datasets composed from image series are applied in lots of medical and scientific tasks, such as CT and MRI studies, 4D and 5D medical imaging, neural, vascular and brain research projects. Most common task is visualization of datasets that could be handled in several ways. More advanced projects requires registration, segmentation and recognition tasks and integration with other software [1, 2].

Proposed approach, methods and tools that could be used as basis of 3D image reconstruction, visualization and processing framework. It allows to create heterogeneous systems being built on different software platforms. It is shown how can be solved task of reconstruction and visualization of 3D models built from abdominal CT studies and brain image series using proposed approach. Described an easy way for adding advanced processing plugins to already developed pipeline.

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Local nearrings of order at most 31

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Nearrings are a generalization of rings in the sense that the addition in nearrings need not be commutative and only one distributive law holds. A nearring R is called local, if the set L of all non-invertible elements of R forms a subgroup of its additive group R^+.

The nearring library of the package "SONATA" [1] of the computer algebra system GAP 4.6.4 [2] contains all nearrings up to order 15 and all nearrings with identity up to order 31.

Recall that an abelian group is a group of type $(p^k, p^l, \ldots, p^m)$ if it is isomorphic to a direct sum of cyclic p-groups of orders p^k, p^l,..., p^m, respectively, with prime p and integers $k, l, \ldots, m$. Let C_n denote a cyclic group of order n.

Proposition 1 *Let R be a local nearring of order at most 31, which is not a nearfield. Let $n(G)$ be the number of all non-isomorphic local nearrings whose multiplicative group is isomrphic to G. The following statements are hold: 1) G is isomorphic to group C_4 and $n(G) = 4$. 2) G is isomorphic to group $(2, 2)$ and $n(G) = 7$. 3) G is isomorphic to group C_6 and $n(G) = 1$. 4) G is isomorphic to group $(4, 2)$ and $n(G) = 227$. 5) G is isomorphic to group $(2, 2, 2)$ and $n(G) = 114$. 6) G is isomorphic to group $(6, 2)$ and $n(G) = 4$. 7) G is isomorphic to group $(6, 3)$ and $n(G) = 14$. 8) G is isomorphic to group C_{20} and $n(G) = 1$. 9) G is isomorphic to symmetric group S_3 and $n(G) = 2$. 10) G is isomorphic to group $C_3 \times S_3$ and $n(G) = 15$. 11) G is isomorphic to quaternion group Q_8 and $n(G) = 48$. 12) G is isomorphic to dihedral group D_8 and $n(G) = 236$. 13) G is isomorphic to alternative group A_4 and $n(G) = 9$. 14) G is isomorphic to Miller-Moreno group $(C_3 \times C_3) \rtimes C_2$ and $n(G) = 4$. 15) G is isomorphic to Miller-Moreno group $C_5 \rtimes C_4$ and $n(G) = 1$. 16) G is isomorphic to group $C_5 \rtimes C_4$ with nontrivial center and $n(G) = 3$.*

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A biomechanical insight into aortic root pathophysiology: Fluid-Structure Interaction (FSI) simulations based on MRI-derived geometries

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Background: the aortic root (AR) is the anatomic and functional unit that constitutes the proximal portion of the outflow tract of the left ventricle, including the aortic valve (AV). AR pathologies have high incidence and mortality and require surgical intervention; to this purpose, surgical techniques and devices are continuously developed. Bicuspid aortic valve (BAV) is the most common congenital cardiac anomaly affecting the AR and it usually results from the fusion of two out of the three AV leaflets. BAV alters AR hemodynamics and tissue stresses and, in more advanced pathological scenarios, it can be lethal, in that it is often associated with ascending aorta (AA) dissection.

Objective: numerical modeling can provide detailed and quantitative information on AR biomechanics, improving the understanding of AR physiology and allowing the analysis of clinically relevant problems. In particular, the quantification of the biomechanical alterations induced by BAVs may contribute elucidating the processes underlying the advancement of the pathological condition and the relation between BAV and AA dissection.

Methods: Fluid-structure interaction (FSI) modeling was used to characterize AR biomechanics through the cardiac cycle. Magnetic resonance imaging (MRI) was performed on 10 healthy subjects and 8 BAV-affected patients. Multiple long-axis and short axis cut-planes were acquired for the upper ventricular chamber, the AR and the AA. Geometrical parameters were manually measured, including AV commissures mutual position, Valsalva sinuses position and extent, sino-tubular junction (STJ) dimensions, and AA dimensions and spatial orientation. Averaged

measurements values were used to define the corresponding 3-D geometrical models of AR and AA. The same constitutive models and boundary conditions were assumed for both models. AV tissues stress-strain response was described as non-linear, elastic and transversely isotropic, aortic wall response was modeled as linear, elastic and isotropic, and blood was assumed as a Newtonian, inviscid and nearly incompressible fluid. Both ends of the solid model were constrained with respect to translations. Physiological time-dependent blood pressures were applied at the inlet, i.e. the aorto-ventricular junction, and at the outlet, 25 mm distally from the STJ, of the fluid domain. FSI was simulated through a combined Lagrangian-Eulerian approach within the commercial software LS-DYNA.

Results: simulations highlighted the potential of the FSI modeling approach as a suitable tool both to assess AR physiological dynamics and to study fluid-dynamic abnormalities and structural alterations associated to BAV. As concerns the BAV model, in diastole the AV was continent, but leaflets coaptation line was shifted from the valvular orifice centerline, and a minor prolapse of the fused leaflets was observed. In systole, the valvular orifice was elliptic, 50

Conclusions: the adoption of an FSI approach allowed to capture the fast transient phenomena characterizing AV function and provided, with respect to a purely structural AR model, additional quantitative information regarding blood fluid dynamics. The BAV-affected model closely reproduced the asymmetric flow pattern found in vivo by MRI and the computed hemodynamic alterations were consistent with the AA region where the typical BAV-related complications preferentially develop.

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A New Method for Evaluation of the Coefficient Vectors in Protein Docking

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We present a new computational method for computing the coefficient vectors in docking problems by using orthonormal spherical polar radial

basis functions. This computational technique arises from the modeling of the molecule. Representing the molecules as three-dimensional functions in terms of orthonormal spherical polar radial expansion provides a straightforward way of computing the correlation between pairs of these functions. After rotating and translating the original functions, the correlation has the form of scalar products of suitably rotated and translated coefficient vectors. In this work we explain our algorithem for computing these coefficients.

Keywords: shape complementarity; electrostatics complementarity; Laguerre polynomials; spherical harmonics; spherical polar radial Fourier coefficients, I-coefficients

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M. Yu. SAVKINA

Statistical tests for comparing two probabilities and their application to cancerous tumour diagnosis

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Statistical tests for comparing two probabilities in the case of dependent trials are proposed. One of them is constructed on confidence intervals, another test is based on the 2s-rule. It is shown [1] that the asymptotic significance levels of these tests do not exceed 0.05. The proposed tests are developed and applied to cancer risk analysis among persons who participated in the clearing of the Chernobyl zone in 1986–87.

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S. A. STASYUK

The best multivariate approximation of Nikol'skii-Besov classes (mixed smoothness) of periodic functions

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The approximation of Nikol'skii-Besov classes (with mixed smoothness) of periodic multivariate functions is considered. Namely, the estimation of these classes by trigonometric polynomials with the spectrum from the step hyperbolic crosses is obtained. These investigations complete the results obtained in [1], [2]. It is shown that the exact order estimates of the Kolmogorov widths are achieved in some cases of considered subspaces of the trigonometric polynomials.

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K. V. STIEPANOVA

Weakened Localization for Quasilinear Parabolic Equations

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The poster is devoted to propagation of solutions' supports of initial–boundary problem with arbitrary boundary regimes $f(t,x)$ (strongly or weakly degenerate or nondegenerate as $t \to 0$) for a wide class quasilinear parabolic equations with a potential $g(t,x)$. We establish a weakened localization of solutions for an arbitrary $g(t,x)$ which degenerates only on the initial plane. Our approach uses appropriate local integral a priori estimates for solutions in a neighbourhood of the initial plane $t = 0$ and is related to combining ideas and constructions from the method of local energy estimates (this method was developed and used in [1], [2], [3], [4],

[5]) and a priori estimates of Saint–Venant's principle type (this second approach was offered by G.A. Iosif'jan and O.A. Oleinik [6]).

The talk is based on a joint project with A. E. Shishkov.

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Structural analysis and ion translocation mechanisms of the muscle-type acetylcholine receptor channel

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The aim of this work is to analyze the conformational changes in the acetylcholine receptor caused by channel opening and to investigate the electrostatic profile during ion translocation through the channel. A computational model of the human muscle-type acetylcholine receptor (AChR) was built and used to analyze channel structure and its interactions with different ions. Using the Torpedo AChR crystal structure as a homologous template, the 3D structure of the human muscle-type AChR was reconstructed. This first model was optimized and an open structure of the channel was generated using Normal Mode Analysis in order to assess morphologic and energetic differences between open and closed structures. In addition, the issue of ion translocation was investigated in further detail. Results elucidate different aspects of the channel: channel gate structure, channel interactions with translocating ions, differences between muscle-type AChR and previous neuronal-type AChR models. The model here reconstructed is ideal for further computational studies on muscle-type AChR and its pathologic mutations.

N. V. VASYLYEVA

On a Moving Boundary Problem in the Case of Anomalous Diffusion

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Some problems in solid and fluid mechanics, heat conduction, molecular diffusion are typical moving boundary problems (free boundary problems). In a free boundary problem one or more of the domain boundaries is an unknown function of time.

One of an important application of the free boundary problem is to describe the diffusional release of a solute from a polymeric matrix in which the initial drug loading is greater then the solubility limit which is a problem of interest in controlled release drug delivery. Liu and Xu [2] were the first who introduced the time-fractional diffusion equation to the drug release process in the case of 1-dimensional space. As was shown [2], [3], the mathematical model of this process is the fractional Stefan problem (free boundary problem for subdiffusion equation). This problem was studied in [1], [3], [2] and some exact solutions were constructed.

In the case of slow diffusion, the fractional Stefan problem tends to the fractional Hele-Shaw problem (see [4]) which has been studied numerical by Voller [4] only in the one dimensional case.

We prove the classical solvability locally in time of the fractional Hele-Shaw problem for enough smooth initial data in the case of the 2-dimensional fluid domain.

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Design of a mechano responsive molecular brush with tuned biomimetic architectures

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At a fundamental level, cartilage consists of extracellular matrix, cells, and signalling factors. The mutual interaction among all these components assures the proper functionality. In case of injury this functionality is never recovered and the therapeutic modality for the treatment of osteoarticular disorders are still far from being able to generate a tissue that is comparable to native cartilage with respect to quality, stability, and integration. Based on this observation Tissue Engineering tries to reproduce in analogy with Nature this complexity: the scaffold provides cells with an in vivo-like microarchitecture; the cells settle this matrix; and the biological, chemical and physical factors direct the cells to express or maintain the desired tissue phenotype. Concerning scaffold production, Nanoscience and Nanotechnology are driving the revolution of Materials Science and Engineering and are enabling to design and fabricate novel scaffolds incorporating biomimetic characteristics at the cellular and molecular scales. A bottom-up strategy for the design and the synthesis of a biometic and mechano-responsive molecule is shown. In particular it will be shown the molecular features to be reproduced with particular enphasis on the design process.

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Inversion of Initial Conditions for Temperature-Driven Stokes Flow

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Simulations of dynamical natural processes relies on initial conditions which are usually poorly constrained, while the current state of system is

well-known. Thus, inversion of initial conditions is considered as a PDE-constrained optimization problem with the goal functional representing mismatch between numerical results and observations. We consider an incompressible Stokes flow driven by the temperature changes. The system of equations consists of momentum equation, incompressibility condition and energy equation. This flow type describes motion of fluids with very slow velocities and large viscosities, and it is used in simulation of convection in the Earth's mantle [1]. Optimization problem is solved by the adjoint approach [2].

[1] G. F. Davies, *Dynamic Earth*, Cambridge University Press, 1999.

[2] M. D. Gunzburger, *Perspectives in Flow Control and Optimization*, SIAM, Philadelphia, 2003.

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