



Final AMMODIT Conference

**“Mathematics for Life Sciences”**

March 18 – 22, 2019

Kyiv, Ukraine

Book of Abstracts

**Information on the projects:**

The goal of the AMMODIT project is joint research in six research tasks concerning the study of mathematical methods for Magnetic Particle Imaging; entropy-like measures and quantification of system complexity; coarse-grain modelling for (bio)polymers; diagnostic tools for cardiac surgery; regularization methods for causality detection; meta-learning approach to Nocturnal Hypoglycemia prediction. This project brings together research teams from the EU (Germany, Italy, and Austria) and the Ukraine (Kyiv, Donetsk) in the area of applied mathematics with emphasis on medical and life science applications.

August 2015 — July 2019

Marie Skłodowska-Curie Research and Innovation Staff Exchange  
H2020-MSCA-RISE-2014 Project number 645672

**Acknowledgements:** The AMMODIT project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 645672.

**Information on the conference:** This is the final conference in the series of events to be organized in the framework of the Marie Curie RISE project “Approximation Methods for Molecular Modelling and Diagnosis Tools” (AMMODIT). The previous conferences were in Rivne (September 2015), Hasenwinkel (March 2016), Kyiv (January 2017) and Lviv (March 2018).

The conference is devoted to recent research in life sciences based on applications of mathematics to biological and medical studies. It is a multidisciplinary meeting forum for researchers who develop and apply mathematical and computational tools to the study of phenomena in the broad fields of biology, ecology, medicine, bioengineering, environmental science, etc.

**Organizers and Partners:**

- Institute of Applied Mathematics and Mechanics of the National Academy of Sciences of Ukraine
- Institute of Mathematics of the National Academy of Sciences of Ukraine
- National Technical University of Ukraine “Kyiv Polytechnic Institute”, Faculty of Applied Mathematics
- Österreichische Akademie der Wissenschaften, Johann Radon Institute for Computational and Applied Mathematics
- Politecnico di Milano, Biomechanics Research Group
- Universität zu Lübeck, Institut für Mathematik
- Humboldt Club Ukraine

**Organizing Committee:**

Alexandra Antoniouk (Ukraine)  
 Oleg Chertov (Ukraine)  
 Sergei Pereverzyev (Austria)  
 Jürgen Prestin (Germany)  
 Alberto Redaelli (Italy)  
 Nataliya Vasylyeva (Ukraine)

**Local Organizing Committee:**

Alexandra Antoniouk (IM NASU)  
 Nadiia Derevianko (IM NASU)  
 Vitalii Overko (IAMM NASU)  
 Kateryna Pozharska (IM NASU)  
 Evgeniya Semenova (IM NASU)  
 Andrii Shydlich (IM NASU)

**Dates:** March 18 – 22, 2019.

**Location:** Institute of Mathematics NAS Ukraine, Kyiv, Ukraine.

Time	Monday 18.03	Tuesday 19.03	Wednesday 20.03	Thursday 21.03	Friday 22.03
09:00 10:00	Registration	Nesteruk	Perepelytsya	Redaelli	Prestin
10:00 10:30		Tkachenko	Zagumennyi	Passoni	Schober
10:30 11:00	Opening	Coffee break			
11:00 11:30	Pereverzyev	Protsakh	Gautieri	Dzumabaev	Malchykov Chertov
11:30 12:00		Gorban	Piatnytskyi	Assanova	Ivanko
12:00 12:30	Kmit	Pleis	Zdorevskyi	Zhumatov Aliev	Nikolov
12:30 14:00	Lunch break				
14:00 14:30	Semenov	Langemann	Excursion	Kriukova	Voskoboinick
14:30 15:00	Pokutnyi			Siryk	Tereshchenko
15:00 15:30	Verbytskyi	Stepaniuk		Hulianytskyi	Overko
15:30 16:00	Coffee break			Coffee break	
16:00 16:30	Pozharska	Shydlich		Pilipenko	Solodun
16:30 17:00	Veselovska	Savchuk		Vasylyk	Sokolenko
17:00 17:30	Derevianko	Meeting of Coordinators		Stasyuk	Dzyubenko
18:00	Welcome Dinner			Conference Dinner	

## Monday morning

09.00 - 10.00    **Registration of participants**

10.00 - 10.30    **Coffee break**

10.30 - 11.00    **Opening of the Conference**

*Chair: Alexandra Antoniouk*

11.00 - 12.00    **Sergei Pereverzyev**  
*Distance function and effective dimension  
in a kernel analysis of deep networks*

12.00 - 12.30    Iryna Kmit  
*Global classical solutions to boundary value problems  
for quasilinear hyperbolic systems*

12.30 - 14.00    **Lunch break**

## Monday afternoon

*Chair: Nataliya Vasylyeva*

14.00 - 14.30 Vasyl Semenov  
*A strategy for identifying informative variables: case study –  
a prediction of motor and cognitive outcomes of preterm  
neonates from metabolites ratios at MR spectroscopy*

14.30 - 15.00 Oleksandr Pokutnyi  
*Haar polinomials as a basis for numerical differentiation  
with applications in medicine*

15.00 - 15.30 Ievgen Verbytskyi  
*Optimization of resonances in layered cavities*

15.30 - 16.00 **Coffee break**

*Chair: Dirk Langemann*

16.00-16.30 Kateryna Pozharska  
*Best approximations and entropy numbers of the classes  
of periodic functions*

16.30-17.00 Hanna Veselovska  
*On Stability of the Method of Prony-Type Polynomials*

17.00-17.30 Nadiia Derevianko  
*Mathematical description of protein-ligand docking problem*

18.00 **Welcome Diner at café “Moments”  
(Khreshchatyk str., 13)**

## Tuesday morning

*Chair: Emiliano Votta*

- 09.00 - 10.00 **Igor Nesteruk**  
*On the criteria for stenosis detection in arteria vertebralis (AV) and arteria carotis interna (ACI) with the use of artery diameters estimated from MRI data*
- 10.00 - 10.30 Pavlo Tkachenko  
*Identification of T2D patient typologies susceptible to artificial pancreas usage*
- 10.30 - 11.00 **Coffee Break**
- Chair: Iryna Kmit*
- 11.00 - 11.30 Nataliya Protsakh  
*Ultraparabolic Equations in modeling of biological processes*
- 11.30 - 12.00 Yuliya Gorban  
*Equations with  $L^1$ -right-hand sides in mechanics of fluids*
- 12.00 - 12.30 Jan Pleis  
*Numerical solution of stochastic delay differential equations*
- 12.30 - 14.00 **Lunch break**

## Tuesday afternoon

*Chair: Igor Nesteruk*

14.00 - 15.00 **Dirk Langemann**  
*Dominance of mechanisms versus parameter sensitivity  
in a population models*

15.00 - 15.30 Tetiana Stepaniuk  
*Hyperuniform point set on flat tori*

15.30 - 16.00 **Coffee break**

*Chair: Hanna Veselovska*

16.00 - 16.30 Andrii Shydlich  
*Approximation theorems for multivariate  
Taylor-Abel-Poisson means*

16.30 - 17.00 Viktor Savchuk  
*An exact estimate for the remainder in the Voronovskaya-type  
theorem for Fejer means of bounded harmonic functions*

17.00 **Meeting of Coordinators**



## Wednesday

*Chair: Alfonso Gautieri*

- 09.00 - 10.00 **Sergiy Perepelytsya**  
*Recognition of DNA sequence motifs by polyamines:  
a modelling study*
- 10.00 - 10.30 Yaroslav Zagumennyi  
*Study of flow patterns past an unsteady moving solid  
for biological and technical applications*
- 10.30 - 11.00 **Coffee Break**
- Chair: Alberto Redaelli*
- 11.00 - 11.30 Alfonso Gautieri  
*Molecular dynamics investigation of self-assembling peptides*
- 11.30 - 12.00 Dmytro Piatnytskyi  
*Binding of hydrogen peroxide with DNA phosphate group*
- 12.00 - 12.30 Oleksii Zdorevskyi  
*Competitive interaction of hydrogen peroxide and  
water molecules with specific DNA recognition sites*
- 12.30 - 14.00 **Lunch break**
- 14.00 - 16.00 **Excursion to St. Sophia's Cathedral**  
**(Volodymyrs'ka str., 24)**

## Thursday morning

*Chair: Sergiy Perepelytsya*

09.00 - 10.00 **Alberto Redaelli**  
*Computational biomechanics: limits,  
challenges and opportunities*

10.00 - 10.30 Giuseppe Passoni  
*Platelet activation at bi-leaflet MHV:  
the effect of turbulence modelling*

10.30 - 11.00 **Coffee Break**

*Chair: Carsten Trunk*

11.00 - 11.30 Dulat Dzhumabaev  
*A method of solving the nonlinear boundary value problems  
for ordinary differential equations*

11.30 - 12.00 Anar Assanova  
*On the solvability of nonlocal problem for impulsive  
partial differential equation of higher order*

12.00 - 12.30 Sailaubay Zhumatov  
*On a stability of a program manifold of control systems  
with variable coefficients*

12.30 - 14.00 **Lunch break**

## Thursday afternoon

*Chair: Andrey Pilipenko*

14.00 - 15.00 Galyna Kriukova  
*On approximation of local solution for infinite stationary system of difference equations*

14.00 - 15.00 Sergii Siryk  
*Regularized reconstruction of the memory order in semilinear subdiffusion*

15.00 - 15.30 Andrii Hulianytskyi  
*On weak solvability and convergence of a finite-difference approximation for a variable-order reaction-subdiffusion equation*

15.30 - 16.00 **Coffee break**

*Chair: Sergiy Solodkyi*

16.00 - 16.30 Andrey Pilipenko  
*General regularization scheme for functional linear regression model*

16.30 - 17.00 Vitalii Vasylyk  
*Regularized collocation method in electrochemical impedance spectroscopy*

17.00 - 17.30 Serhii Stasyuk  
*Estimates of efficiency for two approaches to stable numerical summation of smooth functions of two variables*

18.00 **Conference Dinner at café “Ruta”**  
**(Volodymyrs’ka str., 54)**

## Friday morning

*Chair: Sergei Pereverzyev*

09.00 - 10.00 **Jürgen Prestin**  
*Multivariate directional uncertainty products*

10.00 - 10.30 Kevin Schober  
*Detection of directional singularities by  
multivariate periodic wavelets*

10.30 - 11.00 **Coffee Break**

*Chair: Oleg Chertov*

11.00 - 11.30 Volodymyr Malchykov, Oleg Chertov  
*Automatic wavelet-based stenosis detection in internal carotid  
and vertebral arteries from lumen diameters*

11.30 - 12.00 Kateryna Ivanko  
*Action potential pattern recognition in cardiomyocytes*

12.00 - 12.30 Nikolay Nikolov  
*Technique automated segmentation of CT bone images*

12.30 - 14.00 **Lunch break**

## Friday afternoon

*Chair: Giuseppe Passoni*

- 14.00 - 14.30 Vladimir Voskoboinick  
*Diagnostic Criteria of Bileaflet Mechanical Heart Valve Operation*
- 14.30 - 15.00 Lidiia Tereshchenko  
*Statistical Analysis of Jet Flow Noise across Bileaflet Heart Valve*
- 15.00 - 15.30 Vitalii Overko  
*The influence of left ventricle's torsion motion  
on the reology of blood flow*
- 15.30 - 16.00 **Coffee break**

*Chair: Jürgen Prestin*

- 16.00 - 16.30 Oleksandr Solodun  
*On sloshing in conical containers*
- 16.30 - 17.00 Igor Sokolenko  
*Approximation by Fourier sums in metrics of the spaces  $L_p$   
on the classes of periodic differentiable functions*
- 17.00 - 17.30 German Dzyubenko  
*One estimate of three-monotone spline approximation*

## Plenary Talks

Monday, 11.00 – 12.00

### **Distance function and effective dimension in a kernel analysis of deep networks**

S. PEREVERZYEYEV

*Radon Institute for Computational and Applied Mathematics,  
Linz, Austria*

Training of deep networks is interpreted sometimes as a data-driven determination of the kernel function in supervised kernel learning. In this model the kernel representation changes iteratively from one hidden layer to another. Then it is natural to assume that the target of the learning process does not belong to reproducing kernel Hilbert spaces generated by intermediate kernels (otherwise no further iterations are needed) that corresponds to the so-called misspecified kernel setting, which has attracted attention again in recent times. In the talk we are going to discuss how recent results in the above setting can be used to estimate the effectiveness of the network architecture.

Joint research with Shuai Lu (Fudan University, Shanghai) and Peter Mathe (WIAS-Berlin)

Tuesday, 9.00 – 10.00

### **On the criteria for stenosis detection in arteria vertebralis (AV) and arteria carotis interna (ACI) with the use of artery diameters estimated from MRI data**

I. NESTERUK<sup>1</sup>, S. PEREVERZYEY JR.<sup>2,5</sup>, L. MAYER<sup>3</sup> R. STEIGER<sup>2,5</sup>,  
L. KUSSTATSCHER<sup>2</sup>, K. FRITSCHER<sup>4</sup>, M. KNOFLACH<sup>3</sup>, E. GIZEWSKI<sup>2,5</sup>

<sup>1</sup>*Igor Sikorsky Kyiv Polytechnic Institute, Kyiv, Ukraine*

<sup>2</sup>*Department of Neuroradiology, Medical University of Innsbruck*

<sup>3</sup>*Department of Neurology, Medical University of Innsbruck*

<sup>4</sup>*Department of Medical Image Analysis, University for Health Sciences, Medical Informatics and Technology, Hall in Tirol*

<sup>5</sup>*Neuroimaging Research Core Facility, Medical University of Innsbruck, Innsbruck, Austria*

Different statistical and receiver operating characteristic have been applied to detect stenosis in arteria vertebralis (AV) and arteria carotis

interna (ACI). Real diameter data of 10 patients (80 data sets) provided by the clinical partners from the Department of Neuroradiology and Department of Neurology at the Medical University Innsbruck have been used in the detection tests. Three different criteria have been proposed for stenosis detection. The criteria are applicable to both AV and ACI. Only one False Positive case has been detected for each class of arteries. For ACI it is possible to use initial raw data, while for AV a data presmoothing seems to be necessary. To minimise the number of False Negative cases we recommend to use special combinations of the proposed criteria. The corresponding MATLAB codes have been developed and tested. A user-friendly interface is planned for the future. This research is an example of a cooperation with the health professionals established in the course of AMMODIT.

Tuesday, 14.00 – 15.00

**Dominance of mechanisms versus parameter sensitivity in a population models**

D. LANGEMANN

*Institute of Computational Mathematics, Technische Universität Braunschweig, Braunschweig, Germany*

In recent years, life-science applications came into the focus of mathematical modeling, and mathematical modeling came into the focus of biology, medicine and other life sciences.

The problem of choosing a suitable model to describe a certain application balances between the accuracy of the description and the compactness of the mathematical model. Compact models allow some insight in the interaction of the mechanisms under regard, whereas large and detailed models may provide accurate simulations and reproduce observations also quantitatively.

Since the hierarchy of possible mechanisms is less accepted and less quantified in life-science applications than in most applications in physics and engineering, researchers deal with model families to select appropriate models for the different purposes.

We present a model family in population dynamics which gives a framework to describe the development of resistant sub-populations with respect to environmental changes. The model family is formed by different combinations of growth, interaction between the sub-populations and mutation.

We will see that differently dominant mechanisms lead to models with qualitatively different behavior and that the dominance of certain mechanisms is closely related to the identifiability and the sensitivity of parameters by given measurement data.

Wednesday, 9.00 – 10.00

**Dominance of mechanisms versus parameter sensitivity in a population models**

S. M. PEREPELYTSYA<sup>1,2</sup>, J. ULIČNÝ<sup>3</sup>, A. LAAKSONEN<sup>4,6</sup>, F. MOCCHI<sup>5,6</sup>

<sup>1</sup>*Bogolyubov Institute for Theoretical Physics, Kyiv, Ukraine*

<sup>2</sup>*Kyiv Academic University, Kyiv, Ukraine*

<sup>3</sup>*Institute of Physics, P. J. Šafárik University, Košice, Slovakia*

<sup>4</sup>*Stockholm University, Stockholm, Sweden*

<sup>5</sup>*University of Cagliari, Italy*

<sup>6</sup>*Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania*

DNA is macromolecule with a canonical structure shaped as a double helix, stabilized by water molecules and positively charged counterions (metal ions or organic molecules). In the present work the interactions of natural polyamines (putrescine<sup>2+</sup>, spermidine<sup>3+</sup>, and spermine<sup>4+</sup>) with DNA double helix have been studied using atomistic molecular dynamics simulation. The results show that polyamine molecules are localized with recognizable patterns along the double helix with different residence times. The longest residence time (ca 100ns) is in the minor groove. The analysis of the sequence dependence shows that polyamine molecules prefer the A-tract regions of the minor groove – in its narrowest part. The preferable localization of putrescine<sup>2+</sup>, spermidine<sup>3+</sup>, and spermine<sup>4+</sup> in the minor groove with A-tract motifs is correlated with modulation of the groove width by a specific nucleotide sequences. The developed toy model of DNA-polyamine interaction supports the electrostatic interactions as the most important driving force in this phenomenon, making it even more prominent for polyamines with higher charges. The results of the study explain the specificity of polyamine interactions with A-tract region of the DNA double helix which is observed in experiments.



Thursday, 9.00 – 10.00

**Computational biomechanics: limits, challenges and opportunities**

A. REDAELLI

*Politecnico di Milano, Milan, Italy*

The computation capacities and the tools nowadays available allow for very sophisticated analyses, which can be translated into the clinical practice if not even into routinely patient management. Starting from augmented reality experiences attainable from 3D models built from 3D imaging techniques, to computational simulations of morphological modifications for the prediction of surgical outcomes, the possibility of managing Giga of data in almost real time makes models extremely powerful, realistic and versatile. In this scenario the main challenge is becoming the handling of the physio-pathological uncertainties and variability, inherent to the real patient. As pointed out by Albert Einstein at the Prussian Academy of Science almost one century ago (1921) “so far as laws of mathematics refer to reality, they are not certain, and so far they are certain they do not refer to reality”; indeed, math has to be able to account for the complexity of the real world, sacrificing the pureness of theory; even in a highly controlled status not all the model features are available or stable and not all the boundary conditions are known or predictable. In my talk I will briefly describe the main challenges for realistic modeling, what sources of uncertainties are critical and how they can be handled, and I will illustrate what the scientific community is doing in order to define a shared and robust approach to a verified and validated (V&V) modeling.

Friday, 9.00 – 10.00

### **Multivariate directional uncertainty products**

J. PRESTIN

*Institute of Mathematics, University of Lübeck, Lübeck, Germany*

In this talk we give an overview on general construction principles for uncertainty measures. In particular, a directional time-frequency localization measure for functions defined on the  $d$ -dimensional Euclidean space and on the  $d$ -dimensional torus is introduced. A connection between these measures is established. For a class of functions, an optimization problem for finding the optimal direction, along which a function is best or worst localized, is solved. Moreover, we study the uncertainty product for certain well localized multivariate periodic Parseval wavelet frames. This is joint work with E. Lebedeva and A. Krivoshein both from St. Petersburg State University and E. Neiman from Donetsk National University (see [1, 2]).

- [1] E. Lebedeva, A. Krivoshein, J. Prestin, *Multidimensional Syst. Signal Process.* (2018).
- [2] E. Lebedeva, A. Krivoshein, E. Neiman, J. Prestin, *Math. Inequal. Appl.* **22** (1), (2019), p. 377-399.

## Contributed Talks

### Monday

12.00 – 12.30

#### **Global classical solutions to boundary value problems for quasilinear hyperbolic systems**

I. KMIT

*Institute of Mathematics, Humboldt University of Berlin, Germany*

We consider boundary value problems for quasilinear first-order one-dimensional hyperbolic systems in a strip. The boundary conditions are supposed to be of a smoothing type, in the sense that the  $L^2$ -generalized solutions to the initial-boundary value problems become eventually  $C^2$ -smooth for any initial  $L^2$ -data. We investigate small global classical solutions and obtain the existence and uniqueness result under the condition that the evolution family generated by the linearized problem has exponential dichotomy. We prove that the dichotomy survives under small perturbations in the leading coefficients of the hyperbolic system. This is joint work with L. Recke and V. Tkachenko.

- [1] I. Kmit, L. Recke, V. Tkachenko. Classical Bounded and Almost Periodic Solutions to Quasilinear First-Order Hyperbolic Systems in a Strip. Submitted, 46 pages (2018). E-print: <https://arxiv.org/abs/1812.08006>

14.00 – 14.30

**A strategy for identifying informative variables: case study  
– a prediction of motor and cognitive outcomes of preterm  
neonates from metabolites ratios at MR spectriscopy**

T. DJURDJEVIC<sup>1</sup>, V. YU. SEMENOV<sup>2</sup>, S. PEREVERZYEY JR.<sup>3</sup>,  
L. LAMPLMAYR<sup>4</sup>, V. WALLNER<sup>5</sup>, V. NEUBAUER<sup>6</sup>, R. STEIGER<sup>7</sup>,  
U. KIECHL-KOHLENDORFER<sup>8</sup>, A. E. GRAMS<sup>9</sup>, E. R. GIZEWSKI<sup>10</sup>

<sup>1,3,7,9,10</sup> *Department of Neuroradiology, Neuroimaging Research Core  
Facility, Medical University of Innsbruck, Innsbruck, Austria*

<sup>2</sup> *Department of Algorithms, Delta SPE LLC, Kyiv, Ukraine*

<sup>4,5</sup> *Department of Neuroradiology, Medical University of Innsbruck*

<sup>6,8</sup> *Department of Child and Adolescent Health, Pediatrics II,  
Medical University of Innsbruck, Innsbruck, Austria*

We discuss the problem of detecting the most informative coordinates / variables of input vectors that allow an accurate reconstruction of the corresponding outputs from previously unseen inputs. In our study we are motivated by predicting neurodevelopmental outcomes of preterm neonates from the ratios of the amplitudes of the peaks of metabolite spectra provided by magnetic resonance spectroscopy (MRS). One of the difficulties of the above prediction problem is that the available clinical data contain only a few input-output pairs associated with neurodevelopmental impairments such as delayed Motor development or Cognitive deficits. As a result, from the available data set one can extract only a small number of examples to train and to test the prediction algorithms, while a number the coordinates of prediction inputs is comparatively large. From the view point of the Approximation Theory, the informative variables and their number can be detected by finding the maximum value of the best prediction accuracy observed for predictors from all considered input combinations. Of course, the best prediction accuracy is not observed in practice, because the ideal prediction function is unknown. In our study we use the area under a receiver operating characteristic curve (AUC) as a surrogate for the prediction accuracy. Note that in the context of the prediction of neurodevelopmental outcomes the AUC has been already used by G.S. Kendal et al. (2013). The predictors considered in our study are obtained by kernel ridge regression (KRR) with various input variables as regressors. In KRR we employ universal Gaussian kernels and the kernels constructed from

the data according to the recently proposed approach [1]. In this way we try to cover a variety of predictors exhibiting universality or specificity. From the results [2] we know that by aggregating a given family of predictors we can construct a new predictor that performs at least at the level of the best predictor from the aggregated family. Therefore, in each random simulation we take into account only the largest AUC-value achieved by the constructed predictors. Then for each combination of the input variables, the average value of the largest AUC over 10 simulations is considered as a surrogate for the best prediction accuracy corresponding to the considered combination. In our study the maximal value of the above mentioned surrogate has been observed for the following combinations of input variables: for the case of prediction of delayed Motor development - Left Parietal White Matter NAA/Cho Ratio, Right Parietal White Matter Cho/Cr Ratio, Right and Left Parietal White Matter Average Values of Apparent Diffusion Coefficient; for the case of prediction of Cognitive deficit - Right and Left Frontal White Matter NAA/Cho Ratios, Left Frontal White Matter In/Cr Ratio, Left Frontal White Matter NAA/Cr Ratio. Note that in medical literature some of the above mentioned variables have been already reported to be predictive of neurodevelopmental outcomes of preterm neonates, that can be seen as an evidence of reliability of the proposed approach.

- [1] H. Mhaskar, S. Pereverzyev, V. Yu. Semenov, E. V. Semenova, *RICAM-Report 2018-25*.
- [2] J. Chen, S. Pereverzyev Jr., J. Xu, *Inverse Problems Journal* **31**, (2015), 075005.

14.30 – 15.00

# **Haar polynomials as a basis for numerical differentiation with applications in medicine**

S. PEREVERZYEY<sup>1</sup>, O. POKUTNYI<sup>2</sup>

<sup>1</sup>*Radon Institute for Computational and Applied Mathematics,  
Linz, Austria*

<sup>2</sup>*Institute of Mathematics of NAS of Ukraine, Kyiv, Ukraine*

We consider the problem of reconstruction of the derivative of a function  $f$  from its noisy pointwise evaluations  $f_\delta(x_i) = f(x_i) + \delta\xi$  at dyadic rational points  $x_i = i/2^n, i = 0, 1, 2, \dots, 2^n - 1$ , with the goal to detect the points of the discontinuity of  $f$ .

To this end we extend the analysis of [1] to the case of Haar polynomials. In our analysis we use the relation between Haar and Faber-Schauder systems, as well as the concept of strong generalized invertible operators [2].

Theoretical results are illustrated by an application in stenosis direction problem.

- [1] Shuai Lu, Valeriya Naumova, Sergei Pereverzyev, *J. Inverse Ill-posed Probl.*, **21**, (2013), p. 193-216.
- [2] Boichuk A.A., Pokutnyi A.A. *Ukrainian Math. Journ.*, **67** (9), (2016), p. 1327-1335.

15.00 – 15.30

## **Optimization of resonances in layered cavities**

I. V. VERBYTSKYI

*Igor Sikorsky Kyiv Polytechnic Institute, Kyiv, Ukraine*

Multilayered cavities are widely used in optics, photonics and radio technics as high quality dielectric reflectors or optical cavities. Often the multilayer cavities have quarter wave stack structure, known as Bragg mirror [1]. Such structures is easily to design and fabricate, but their volume are redundant. During the last two decades variation problems for transmission and resonance effects attracted considerable attention in connection with active studies of photonic crystals and high quality-factor (high-Q) optical cavities. However presently available analytic and numerical methods do not give clear answers about optimal cavity designs. On one side, the design, which was suggested in [2] introduces defects in the alternating periodic structure. The width of each of these defects is small in comparison with the period of the original structure without defects. On the other side, resonances of periodic structures with a defect in the center were considered in [3]. This defect is not necessarily small in comparison with the period.

In the paper [4] new theoretical tools and more accurate numerical approaches are proposed. The numerical experiments of suggested that optimal resonators may involve combination of the both types of defects mentioned above.

- [1] M. Born, E. Wolf. *Principles of optics*, Pergamon Press, New York, 1968.
- [2] S. Burger, J. Pomplun, F. Schmidt, L. Zschiedrich, *Proc. SPIE 79330T (Physics and Simulation of Optoelectronic Devices XIX)* **7933**, (2011).
- [3] Y. Akahane, T. Asano, B. Song, S. Noda, *Nature* **425**, (2003), p. 944-947.

- [4] I. M. Karabash, H. Koch, Ie. V. Verbytskyi, Pareto optimization of resonance-sand minimum-time control. *arXiv:1808.09186*, (2018).

16.00 – 15.30

### **Best approximations and entropy numbers of the classes of periodic functions**

K. V. POZHARSKA

*Institute of Mathematics of NAS of Ukraine, Kyiv, Ukraine*

The talk is devoted to the estimates obtained for certain characteristics of the classes of periodic multivariate functions, namely, the best orthogonal and  $M$ -term trigonometric approximations of the classes of functions with bounded generalized derivatives, and the entropy numbers of Nikol'skii–Besov type classes of functions.

Approximative characteristics that are connected with nonlinear approximation are being actively studied for more than forty years. The great interest in such approximations is mainly caused by advantages of nonlinear methods over a linear one in many situations. Comparing the estimates obtained with the known results for the approximations of corresponding functional classes by the step hyperbolic Fourier sums and by trigonometric polynomials with the “numbers” of harmonics from the step hyperbolic crosses, one can observe an improvement of these estimates caused by the use of nonlinear methods.

16.30 – 17.00

### **On Stability of the Method of Prony-Type Polynomials**

H. VESELOVSKA

*Institute of Computational Mathematics, Technical University of Braunschweig, Braunschweig, Germany; Institute of Mathematics of NAS of Ukraine, Kyiv, Ukraine*

The general problem of parameter estimation of an exponential sum  $f(\mathbf{k}) = \sum_{j=1}^N a_j \exp(-i\langle \boldsymbol{\omega}_j, \mathbf{k} \rangle)$ , where  $a_1, \dots, a_N \in \mathbb{C} \setminus \{0\}$  and  $\mathbf{k} \in \mathbb{Z}_+^2$ , is to recover elements  $\boldsymbol{\omega}_1, \dots, \boldsymbol{\omega}_N \in (0, 2\pi]^2$  using some samples of  $f$ . Recently, a number of research has been carried on this issue, e.g. [2, 3]. However, stability of solutions in the case of noise corruption still has a lot of questions opened, especially when the number of parameters increases.

We propose to use the method of Prony-type polynomials, when the parameters  $\omega_1, \dots, \omega_N$  can be recovered as a set of common zeros of the monic bivariate polynomial of an appropriate multi-degree. Numerical computations show that the PTP method is more resistant to the noise than other methods, even when  $N$  rises. Moreover, combining the PTP method and an autocorrelation sequence allows to improve the stability of the method in general.

This is joint work with Jürgen Prestin (Institute of Mathematics, University of Lübeck).

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17.00 – 17.30

### **Mathematical description of protein-ligand docking problem**

N. DEREVIANKO

*Institute of Mathematics of NAS of Ukraine, Kyiv, Ukraine*

The talk is based on joint research with Alfonso Gautieri and Alberto Redaelli (Politecnico di Milano) and Jürgen Prestin (Universität zu Lübeck).

Molecular docking is a kind of bioinformatic modelling which involves the interaction of two or more molecules to give the stable adduct. We consider a case when one small molecule that is called ligand bonds to macromolecule that is called protein.

To choose a suitable scoring function is the crucial in all docking approaches. On the one hand, we consider an approach based on the force-field-based scoring function and develop fast algorithm for finding the best matching between two molecules. Docking in the solution is of special interest to us. For evaluation of Coulombic potential we use the so called NFFT based fast Ewald summation technique [2] the main idea of which is to use the following simple identity  $\frac{1}{r} = \frac{\text{erf}(\alpha r)}{r} + \frac{\text{erfc}(\alpha r)}{r}$ . Choice of optimal splitting parameter  $\alpha$  is very important for the accuracy of the computation of the score and was suggested in the paper [1]. Some practical results will be presented.

On the other hand, we consider the scoring function based on Van der Waals clashes. The affinity functions for both protein and ligand are



defined via Gaussians that are used to describe the electron density distribution of atoms. We consider the question of approximation of Gaussians in the weighted Hilbert space  $L_2(\mathbb{R}^3, \exp(-|\cdot|^2/\lambda))$  by the spherical Gauss-Laguerre basis  $\mathcal{H}^\lambda$  (see [3, 4]). Our goal was to investigate the behaviour of the error of approximation of Gaussians by basis  $\mathcal{H}^\lambda$  with respect to parameter  $\lambda$  in the space  $L_2(\mathbb{R}^3, \exp(-|\cdot|^2/\lambda))$  and find optimal parameters  $\lambda$  suitable for docking approach based on this scoring function.

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## Tuesday

10.00 – 10.30

### Identification of T2D patient typologies susceptible to artificial pancreas usage

P. TKACHENKO, F. REITERER, L. DEL RE

*Institute for Design and Control of Mechatronic Systems, Johannes Kepler University Linz, Austria*

In this work we are intended to explore which subgroup of patients is expected to benefit substantially from a potential artificial pancreas (AP) system and whether this subgroup can be identified using patient information that is a priori available (i.e. before the implementation of the AP on a patient). The key fact behind it is that AP is not expected to be necessary or even beneficial for every type 2 diabetes (T2D) patient, but only for a subgroup of insulin treated T2D patients that does not succeed in accomplishing the therapy goals with simpler insulin dosing approaches.

Against this background, a sample of insulin treated T2D patients was used to estimate the possible benefit of automated insulin dosing via an AP and compare it to the achievable performance with continuous subcutaneous insulin infusion (CSII) therapy. The analysis was done using state-of-the-art deviation analysis in an in silico testing environment.

The key result is that a simple hybrid AP approach would be beneficial for the vast majority of analyzed patients. However, for 60% of the analyzed patients improved settings of basal insulin dosing via CSII together with fixed bolus quantities is sufficient for a good glycemic control as well. Most of the remaining patients exhibit significantly higher glycemic variability and diurnal variations in insulin needs and therefore require a more complex therapy scheme. For those patients AP seems to be the therapy of choice.

This subgroup could be identified a priori using only a limited number of features. Additionally, a continuous score that estimates the therapeutic outcomes of the different treatment options has been proposed and a regression analysis can be used to estimate the potential benefits a priori as well.

11.00 – 11.30

### **Ultraparabolic equations in modeling of biological processes**

N. P. PROTSAKH

*Ukrainian National Forestry University, L'viv, Ukraine*

Mathematical modeling of age structured population dynamics often leads to the initial-boundary value problems for linear and nonlinear ultraparabolic equations.

We shall show examples of such problems and present the results of the unique solvability of the inverse coefficient problems for the equation

$$u_t + \lambda(x, y, t)u_y - \sum_{i,j=1}^n (a_{ij}(x, y, t)u_{x_i})_{x_j} + c(t)u + g(x, y, t, u) = f_1(x, y, t)q(t) + f_2(x, y, t),$$

where  $g$  is Lipschitz continuous function on  $u$ . As a sequence, we obtain the conditions of the existence and the uniqueness of the solution from Sobolev spaces for the initial-boundary value problem for the ultraparabolic equation with the integral term.

11.30 – 12.00

### Equations with $L^1$ -right-hand sides in mechanics of fluids

YU. S. GORBAN

*Vasyl' Stus Donetsk National University, Vinnytsia, Ukraine*

We consider the Dirichlet problem for nonlinear second-order elliptic equations with anisotropic and degenerate (with respect to the independent variables) coefficients and  $L^1$ -right-hand sides.

One of the applications of  $L^1$ -theory is to simulate two stationary turbulent fluids coupled by boundary conditions on the interface. The mathematical model is a nonlinear system of partial differential equations with unknown velocities of fluids, their pressures, and their turbulent kinetic energies. This system is motivated by the coupling of two turbulent fluids, such as in the framework ocean/atmosphere or in the case of two layers of a stratified fluid (see [1]). Equation for turbulent kinetic energy has right-hand sides only belong to  $L^1$ . In this case, it is taken in the entropy concept (see [2]).

In [3, 4] we proved the theorems of existence a unique entropy solution for nonlinear elliptic degenerate anisotropic equations.

- [1] C. Bernardi, T. Chacón Rebollo, R. Lewandowski, F. Murat *Studies in Mathematics and its Applications* **31**, (2002), p. 69–102.
- [2] Ph. Bénilan, L. Boccardo, T. Gallouët, R. Gariepy, M. Pierre, J.L. Vazquez *Ann. Scuola Norm. Sup. Pisa Cl. Sci. (4)* **22**, (1995), No. 2, p. 241–273.
- [3] Yu. Gorban *Open Math.* **15**, (2017), p. 768–786.
- [4] Yu. Gorban, *Mat. Stud.* **47**, (2017), No. 1, p. 59–70.

12.00 – 12.30

### Numerical solution of stochastic delay differential equations

J. PLEIS

*Institute of Mathematics, University of Lübeck, Lübeck, Germany*

Let  $(\Omega, \mathcal{F}, P)$  be a complete probability space and  $(W_t)_{t \geq 0}$  be an  $m$ -dimensional Wiener process on  $(\Omega, \mathcal{F}, P)$  with respect to the filtration  $(\mathcal{F}_t)_{t \geq 0}$  that satisfies the usual conditions. Consider the Itô stochastic delay differential equation with a delay  $\tau > 0$  given by

$$X_t = \begin{cases} \xi_t, & t \in [-\tau, 0], \\ \xi_0 + \int_0^t a(X_s, X_{s-\tau}) ds + \sum_{j=1}^m \int_0^t b^j(X_s, X_{s-\tau}) dW_s^j, & t > 0, \end{cases}$$

where the initial condition  $\xi$  belongs to  $C([-\tau, 0]; \mathbb{R})$  and the coefficients  $a, b^j: \mathbb{R}^2 \rightarrow \mathbb{R}$ ,  $j \in \{1, \dots, m\}$ , satisfy a global Lipschitz and a linear growth condition, cf. [4, 5]. In this talk, we focus on numerical approximations  $Y: \mathbb{R}_+ \times \Omega \rightarrow \mathbb{R}$  that converge in the strong sense to the solution  $X$  of the stochastic delay differential equation [1, 2, 3].

- [1] C. T. H. Baker and E. Buckwar, *LMS J. Comput. Math.* **3**, (2000), p. 315–335
- [2] Y. Hu, S.-E. A. Mohammed and F. Yan, *Ann. Probab.* **32**, (2004), p. 265–314
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- [4] X. Mao, *Stochastic Differential Equations and Applications*, Horwood Publishing Limited, Chichester, 2007.
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15.00 – 15.30

### Hyperuniform point set on flat tori

T. A. STEPANIUK

*Radon Institute for Computational and Applied Mathematics, Linz, Austria; Institute of Mathematics of NAS of Ukraine, Kyiv, Ukraine*

In the talk we study hyperuniformity on flat tori. Hyperuniform point sets on the unit sphere have been studied by J. Brauchart, P. Grabner, W. Kusner and J. Ziefle. It is shown that point sets which are hyperuniform for large balls, small balls or balls of threshold order on the flat tori are uniformly distributed. We also show that QMC–designs sequences for Sobolev classes and probabilistic point sets (with respect to jittered samplings) are hyperuniform.

16.00 – 16.30

### An exact estimate for the remainder in the Voronovskaya-type theorem for Fejér means of bounded harmonic functions

V. V. SAVCHUK

*Institute of Mathematics of NAS of Ukraine, Kyiv, Ukraine*

Let  $f(z) = \sum_{k \in \mathbb{Z}} c_k \rho^{|k|} e^{ikx}$ , where  $c_k \in \mathbb{C}$ ,  $c_{-k} = \overline{c_k}$ ,  $z = \rho e^{ix}$ , be a bounded real-valued harmonic function in the unit disk  $\mathbb{D} := \{z \in \mathbb{C} : |z| < 1\}$  and let  $\sigma_n(f)(z) = n^{-1} \sum_{|k| \leq n-1} (n - |k|) c_k \rho^{|k|} e^{ikx}$ ,  $n \in \mathbb{N}$ ,  $z = \rho e^{ix}$  be its Fejér means.

The Voronovskaya-type theorem for the Fejér means  $\sigma_n(f)$  state that under the assumption  $\|\tilde{f}'\| < \infty$ ,  $\lim_{n \rightarrow \infty} \|n(f - \sigma_n(f)) - \tilde{f}'\| = 0$ , where  $\tilde{f}'(z) := \sum_{k \in \mathbb{Z} \setminus \{0\}} |k| c_k \rho^{|k|} e^{ikx}$  and  $\|f\| := \sup_{z \in \mathbb{D}} |f(z)|$ .

Set  $hB := \{f : \text{harmonic in } \mathbb{D} \text{ and } \|f\| \leq 1\}$  and  $\widetilde{hB} := \{f : \tilde{f} \in hB\}$ . Our main result is the following.

**Theorem 1.** *Suppose that  $n \in \mathbb{Z}_+$  and  $z \in \mathbb{D}$  and let  $\mathfrak{H}$  be one of the classes  $hB$  or  $\widetilde{hB}$ . Then*

$$\max_{f \in \mathfrak{H}} \left| n(f(z) - \sigma_n(f)(z)) - \tilde{f}'(z) \right| = \frac{4|z|^{n+1}}{\pi(1 - |z|^2)}.$$

For given  $z \neq 0$  this maximum is attained only for the function

$$f(t) = e^{i\alpha} \begin{cases} \frac{2}{\pi} \arg \frac{1 + ib_n(t)e^{-i(n+1)\arg z}}{1 - ib_n(t)e^{-i(n+1)\arg z}}, & \text{if } \mathfrak{H} = hB, \\ \frac{2}{\pi} \ln \left| \frac{1 + b_n(t)e^{-i(n+1)\arg z}}{1 - b_n(t)e^{-i(n+1)\arg z}} \right|, & \text{if } \mathfrak{H} = \widetilde{hB}, \end{cases}$$

where  $\alpha \in \mathbb{R}$  and  $b_n(t) := t^n(t - z)/(1 - t\bar{z})$ .

16.30 – 17.00

#### Approximation theorems for multivariate Taylor-Abel-Poisson means

J. PRESTIN<sup>1</sup>, V. SAVCHUK<sup>2</sup>, A. SHYDLICH<sup>3</sup>

<sup>1</sup>*Institute of Mathematics, University of Lübeck, Lübeck, Germany*

<sup>2,3</sup>*Institute of Mathematics of NAS of Ukraine, Kyiv, Ukraine*

Let  $L_p = L_p(\mathbb{T}^d)$ ,  $1 \leq p \leq \infty$ , be the space of all functions  $f$  defined on  $\mathbb{R}^d$ ,  $2\pi$ -periodic in each variable, with the usual norm  $\|f\|_p$ . For  $f \in L_1$ ,  $\varrho \in [0, 1)$  and  $r \in \mathbb{N}$ , we set

$$A_{\varrho, r}(f)(x) := \sum_{\nu=0}^{\infty} \lambda_{\nu, r}(\varrho) \sum_{|k|_1=\nu} \widehat{f}_k e^{i(k, x)},$$

where  $\widehat{f}_k$  are Fourier coefficients of  $f$ ,  $|k|_1 = \sum_{j=1}^d |k_j|$ ,  $\lambda_{\nu, r}(\varrho) \equiv 1$  when  $0 \leq \nu \leq r-1$  and  $\lambda_{\nu, r}(\varrho) = \sum_{j=0}^{r-1} \binom{\nu}{j} (1-\varrho)^j \varrho^{k-j}$  when  $\nu = r, r+1, \dots$

If for  $f \in L_1$  and  $n \in \mathbb{N}$ , there exists the function  $g \in L_1$  such that  $\widehat{g}_k = 0$  when  $|k|_1 < n$  and  $\widehat{g}_k = \widehat{f}_k \nu! / (\nu - n)!$  when  $|k|_1 = \nu \geq n$ ,  $k \in \mathbb{Z}^d$ , then  $g$  is called the  $n$ th radial derivative of the function  $f$  and denoted as  $g =: f^{[n]}$ . Let also

$$K_n(\delta, f)_p := \inf\{\|f - h\|_p + \delta^n \|h^{[n]}\|_p : h^{[n]} \in L_p\}, \quad \delta > 0,$$

denote  $K$ -functional of  $f \in L_p$ , generated by the  $n$ th radial derivative.

**Theorem.** Assume that  $f \in L_p$ ,  $1 \leq p \leq \infty$ , such that  $\widehat{f}(k) = 0$  for  $k \in \mathbb{Z}^d \setminus \{\mathbb{Z}_+^d \cup \mathbb{Z}_-^d\}$ . Let also  $n, r \in \mathbb{N}$ ,  $n \leq r$  and  $\omega$  be an increasing continuous on  $[0, 1]$  function,  $\int_0^\delta \frac{\omega(t)}{t} dt + \delta^n \int_\delta^1 \frac{\omega(t)}{t^{n+1}} dt = \mathcal{O}(\omega(\delta))$ ,  $\delta \rightarrow 0+$  and  $\omega(0) = 0$ . Then

$$\|f - A_{\varrho, r}(f)\|_p = \mathcal{O}\left((1 - \varrho)^{r-n} \omega(1 - \varrho)\right), \quad \varrho \rightarrow 1-,$$

iff there exists the derivative  $f^{[r-n]} \in L_p$  and

$$K_n(\delta, f^{[r-n]})_p = \mathcal{O}(\omega(\delta)), \quad \delta \rightarrow 0+.$$

## Wednesday

10.00 – 10.30

### Study of flow patterns past an unsteady moving solid for biological and technical applications

G. A. VOROPAIEV, YA. V. ZAGUMENNYI

*Institute of Hydromechanics of NAS of Ukraine, Kyiv, Ukraine*

A lot of problems in biophysics and hydrodynamics are associated with an unsteady motion of certain elements of a system, which can be mathematically modelled by specifying unsteady varying boundary conditions. Among such problems are simulation of blood flow and valve operation in circulatory systems, flapping wings, wind and water turbines, various drag reduction methods implemented by utilizing different kinds of deformable surfaces, etc. [1-3]. Due to complexity of such problems, they are practically impossible to be analysed analytically in the full mathematical formulation and, therefore, have to be studied numerically. Such problems are of a great practical interest and serve as an

incentive for constructing high-accuracy and high-resolution numerical simulations with implementation of various dynamic mesh techniques [2].

In the present talk, some results are presented on 3D numerical simulation of unsteady flows around bodies performing periodic oscillations in the uniform free stream based on a high-accuracy and high-resolution direct numerical simulation of the non-stationary Navier-Stokes equations at transitional Reynolds numbers. The numerical simulation of the problem is implemented using dynamic mesh libraries, utilities and program codes of own development within the open source computational tools OpenFOAM in parallel regime on multicore personal computers and cluster systems.

The present study is based on the idea originating from the ability of aero- and hydro-bionts to provide the most rational ways of swim and flight which have been developed during their long biological evolution stimulated by the fight for survival. Based on studying the physical mechanisms involved in the generation of lift force and propulsion by flying and swimming animals, it is possible to develop new approaches to creating vehicles and devices with a deformable surface or an oscillating wing as working elements. The numerical approach developed can be applied, as well, to a wide range of biophysical and hemodynamical problems which involve unsteady motions of separate elements of a biological system taking into account the feedback influence, as well.

The calculations demonstrate the perturbed 3D flow field on the flat surface under action of the oncoming steady free stream can be controlled downstream by varying both wave and amplitude characteristics of a deformable area on the surface [1, 2]. The results also show possibility of degeneration of the 3D growing perturbations in the boundary layer on the surface of a wing profile performing rotating-oscillating motion, and formation of coherent vortex structures in the wake flow with a finite amplitude at transitional Reynolds numbers,  $Re > 20000$ , and Strouhal ones varying in the range,  $0.5 < St < 1.2$  [3].

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- [2] G. A. Voropaev, Ia. V. Zagumennyi, *Proc. 5th Int. Conf. HPC-UA 2018, Kyiv, Ukraine*, P. 179–182.
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11.00 – 11.30

**Molecular dynamics investigation of self-assembling peptides**

A. REDAELLI, A. GAUTIERI

*Politecnico di Milano, Milan, Italy*

Besides their biomolecular relevance, amyloids, generated by the self-assembly of peptides and proteins, are highly organized structures useful for nanotechnology applications. The introduction of halogen atoms in these peptides, and thus the possible formation of halogen bonds, allows further possibilities to finely tune the amyloid nanostructure. In this work, we performed molecular dynamics simulations on different halogenated derivatives of the  $\beta$ -amyloid peptide core-sequence KLVFF, by using a modified AMBER force field in which the  $\sigma$ -hole located on the halogen atom is modeled with a positively charged extra particle. The analysis of equilibrated structures shows good agreement with crystallographic data and experimental results, in particular concerning the formation of halogen bonds and the stability of the supramolecular structures. The modified force field described here allows describing the atomistic details contributing to peptides aggregation, with particular focus on the role of halogen bonds. This framework can potentially help the design of novel halogenated peptides with desired aggregation propensity.

11.30 – 12.00

**Binding of hydrogen peroxide with DNA phosphate group**

D. V. PIATNYTSKYI, O. O. ZDOREVSKYI, S. N. VOLKOV

*Bogolyubov Institute for Theoretical Physics NAS Ukraine, Kyiv, Ukraine*

The effect of DNA deactivation during particle irradiation of living cells is widely used in cancer therapy. But the mechanism of DNA damage is still being discussed [1]. There are some theories, which include damage by secondary electrons, oxidative stress by OH-radicals, shock-wave damage etc. It was proposed in [2] that DNA deactivation can be a result of intracellular medium change after irradiation. During irradiation of water medium by high-energy ions the hydrogen peroxide molecules  $H_2O_2$  are formed. As the most long-living product [3] of water radiolysis they can diffuse on considerable distances in the cell after irradiation and reach the active sites of DNA macromolecule.



The analysis of interaction of solvent molecules with non-specific DNA recognition sites (phosphate groups  $\text{PO}_4$  of backbone) is performed. Geometry optimizations and energy calculations are carried out for complexes, which consist of hydrogen peroxide and water molecules, phosphate group and sodium counterion using atom-atom potential functions and quantum chemistry methods in the framework of Gaussian program taking into account model of water solution (PCM). It is shown, that phosphate group can form a complex with hydrogen peroxide molecule which is as stable as the same complex with water molecule, especially when sodium counterion is present.  $\text{H}_2\text{O}_2$  molecule can stay near DNA double helix longer than water molecule, because it is nearly twice as heavy as  $\text{H}_2\text{O}$ . Situated in a close proximity to DNA backbone the hydrogen peroxide molecule can decay into OH-radical and induce double strand breaks or directly block genetic activity.

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- [2] D. V. Piatnytskyi, O. O. Zdorevskyi, S. M. Perepelytsya, S. N. Volkov, *Eur. Phys. J. D* **69**, (2015), p. 255.
- [3] M. S. Kreipl, W. Friedland, H. G. Paretzke, *Radiat. Environ. Biophys.* **48**, (2009), p. 11.

12.00 – 12.30

### **Competitive interaction of hydrogen peroxide and water molecules with specific DNA recognition sites**

O. O. ZDOREVSKYI, D. V. PIATNYTSKYI, S. N. VOLKOV

*Bogolyubov Institute for Theoretical Physics NAS Ukraine, Kyiv, Ukraine*

One of the most progressive methods of cancer treatment is ion beam therapy. But the current mechanism of the DNA deactivation of cancer cells has not been determined yet. Monte-Carlo simulations [1] show that among many different species occurring in the cell medium under water radiolysis, the most long-living are hydrogen peroxide ( $\text{H}_2\text{O}_2$ ) molecules. In the present work interaction of  $\text{H}_2\text{O}_2$  and  $\text{H}_2\text{O}$  molecules with specific DNA recognition sites (nucleic bases and base pairs) is studied. Atom-atomic potential functions method and density functional theory are used for the calculations. Complexes consisting of nucleic bases Adenine (A), Thymine (T), Guanine (G) and Cytosine (C) [2] and base pairs A·T and G·C with  $\text{H}_2\text{O}_2$  and  $\text{H}_2\text{O}$  molecules are considered. Results obtained by both methods show that there are definite atomic groups

of nucleic bases that are much more favorable to be bound by hydrogen peroxide than by water molecule. Also it is shown that there are non-Watson-Crick configurations of A·T and G·C base pairs (‘preopened’ and ‘stretched’ states) that are stabilized much better by  $H_2O_2$  molecule compared to water molecule. As it was shown in the work [3], such states can be observed in unzipping experiments performed by single-molecule manipulation technique. Therefore, these technique can be used to detect interaction of hydrogen peroxide with nucleic base pairs. Formation of such interaction complexes can block the processes of DNA recognition by enzymes and consequently block genetic information transfer processes in cancer cell during ion beam therapy treatment.

- [1] M. S. Kreipl, W. Friedland, H. G. Paretzke, *Radiation and Environmental Biophysics*, **48**(1), (2008), p. 11.
- [2] O. O. Zdorevskyi, D. V. Piatnytskyi, S. N. Volkov, submitted to *Journal of Bioinformatics and Computational Biology*, (2019).
- [3] O. O. Zdorevskyi, S. N. Volkov, *European Biophysics Journal*, **47**(8), (2018), p. 917.

## Thursday

10.00 – 10.30

### **Platelet activation at bi-leaflet MHV: the effect of turbulence modelling**

G. PASSONI, D. DOMINISSINI, S. BOZZI, A. REDAELLI  
*Politecnico di Milano, Milan, Italy*

The assessment of platelet activation, as indicator of blood damage in cardiovascular devices, has been long debated within the scientific community. Most of the research efforts have been directed in identifying the relevant physical quantities to improve the predictability of the Platelet Activation State (PAS). The stress accumulation (SA) model [1] has later been improved by taking into account the Stress Rate (SR) [2]. A more recent modal analysis [3] also revealed the crucial role of high frequency components in platelet activation. Numerical issues have also been investigated for lagrangian damage models [4] and their sensitivity in terms of stress accumulation, as well. However, the effects of turbulence modelling for the eulerian flow and the consequences on the lagrangian statistics has not yet been ascertained.

In this contest we'll compare three different turbulent closure schemes (k- $\omega$ , SST, LES) with DNS (no turbulence model) in terms of both eulerian variables and lagrangian indicators (SA, PAS), using the predictive models for platelet activation/sensitization quoted before.

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- [2] J.S. Soares et al, *Biomech Model Mechanobiol*, **12**, (2013), p. 1127-1141.
- [3] F. Consolo et al, *Scientific Reports*, **7-1**, (2017), p. 4994.
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11.00 – 11.30

### **A method of solving the nonlinear boundary value problems for ordinary differential equations**

D. S. DZHUMABAEV

*Institute of Mathematics and Mathematical Modeling,  
Almaty, Kazakhstan*

In the communication we consider the boundary value problem for the ordinary differential equation (ODE)

$$\frac{dx}{dt} = f(t, x), \quad t \in (0, T), \quad x \in R^n, \quad (1)$$

$$g[x(0), x(T)] = 0, \quad (2)$$

where  $f : [0, T] \times R^n \rightarrow R^n$  and  $g : R^n \times R^n \rightarrow R^n$  are continuous functions.

The interval  $[0, T]$  is divided into  $N$  parts according to the partition  $\Delta_N$ :  $t_0 = 0 < t_1 < t_2 < \dots < t_N = T$ , and the  $\Delta_N$  general solution to a nonlinear ODE introduced.

The  $\Delta_N$  general solution, denoted by  $x(\Delta_N, t, \lambda)$ , contains an arbitrary vector  $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_N) \in R^{nN}$ . Using  $x(\Delta_N, t, \lambda)$ , boundary condition (2) and continuity conditions at the interior points of the partition  $\Delta_N$ , we construct the system of nonlinear algebraic equations

$$Q_*(\Delta_N, \lambda) = 0, \quad \lambda \in R^{nN}. \quad (3)$$

It is established that the solvability of problem (1), (2) is equivalent to the solvability of the system (3).

Proposed method is based on solving system (3).

The value of  $Q_*(\Delta_N, \lambda)$  at the given  $\lambda = \tilde{\lambda}$  is defined by solving the Cauchy problems for nonlinear ODE on subintervals. Elements of the Jacoby matrix  $\frac{\partial Q_*(\Delta_N, \lambda)}{\partial \lambda}$  at  $\lambda = \tilde{\lambda}$  is computed by solving the Cauchy problem for the linear matrix ODE on subinterval. Solution to the system of nonlinear algebraic equations (3) is determined by the iterative method.

11.30 – 12.00

### **On the solvability of nonlocal problem for impulsive partial differential equation of higher order**

A. T. ASSANOVA

*Institute of Mathematics and Mathematical Modeling,  
Almaty, Kazakhstan*

At the domain  $\Omega = [0, T] \times [0, \omega]$  we consider the nonlocal problem for impulsive partial differential equations of higher order in the form

$$\begin{aligned} \frac{\partial^{m+1}u}{\partial x^m \partial t} = \sum_{i=0}^{m-1} A_i(t, x) \frac{\partial^{m-i}u}{\partial x^{m-i}} + \sum_{i=1}^{m-1} B_i(t, x) \frac{\partial^{m-i+1}u}{\partial x^{m-i} \partial t} \\ + C(t, x)u + f(t, x), \end{aligned} \quad (1)$$

$$P(x) \frac{\partial^m u(t, x)}{\partial x^{m-1} \partial t} \Big|_{t=0} + S(x) \frac{\partial^m u(t, x)}{\partial x^{m-1} \partial t} \Big|_{t=T} = \varphi_0(x), \quad x \in [0, \omega], \quad (2)$$

$$\lim_{t \rightarrow t_i+0} \frac{\partial^m u(t, x)}{\partial x^{m-1} \partial t} - \lim_{t \rightarrow t_i-0} \frac{\partial^m u(t, x)}{\partial x^{m-1} \partial t} = \varphi_i(x), \quad x \in [0, \omega], \quad i = \overline{1, k}, \quad (3)$$

$$u(t, 0) = \psi_0(t), \quad \frac{\partial u(t, x)}{\partial x} \Big|_{x=0} = \psi_1(t), \dots, \quad \frac{\partial^{m-1} u(t, x)}{\partial x^{m-1}} \Big|_{x=0} = \psi_{m-1}(t), \quad (4)$$

$t \in [0, T]$  and  $m = 2, 3$ .

Problem (1)–(4) is the nonlocal problem for non-classical impulsive system of partial differential equations with two variables. This system is a mathematical model of various processes arising in biology, physics, information technologies and life sciences.

We investigate questions of the solvability and uniqueness of solution to problem (1)–(4). We also construct an algorithm for finding approximate solution to problem (1)–(4). To solve problem (1)–(4) we use the methods and results in [1–5].

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- [3] A. T. Assanova *J. Discontinuity, Nonlinearity and Complexity* **5:2**, (2016), p. 153-165.
- [4] A. T. Asanova, Z. M. Kadirbaeva, E. A. Bakirova *Ukrainian Math. J.* **69:8**, (2018), p. 1175-1195.
- [5] A. T. Assanova, Z. M. Kadirbayeva *Electronic J. Differ. Equ.* **2018:72**, (2018), p. 1-8.

12.00 – 12.15

### **On a stability of a program manifold of control systems with variable coefficients**

S. S. ZHUMATOV

*Institute of Mathematics and Mathematical Modeling,  
Almaty, Kazakhstan*

Consider the system of equations arising in the construction of stable automatic control systems for a given program manifold

$\Omega(t) \equiv \omega(t, x) = 0$ :

$$\dot{\omega} = -A(t)\omega - H(t)b(t)\xi, \quad \xi = \varphi(\sigma), \quad \sigma = p^T(t)\omega, \quad (1)$$

where  $H = \frac{\partial \omega}{\partial x}$ ,  $t \in I = [0, \infty)$ .

A given program is carried out exactly only when, if  $\omega(t_0, x_0) = 0$  holds. But these conditions are not always fulfilled, since there are initial and permanent disturbances.

Therefore, it is advisable to investigate for stability the program manifold itself with respect to some given function.

The sufficient conditions of absolute stability of program manifold are received by means of construction Lyapunov function.

14.00 – 14.30

**On approximation of local solution for infinite stationary system of difference equations**

O. I. KASHPIROVSKII, G. V. KRIUKOVA

*National University of Kyiv-Mohyla Academy, Kyiv, Ukraine*

In the paper, we consider an infinite system of difference equations

$$U_{k+1} - 2AU_k + U_{k-1} = f_k, \quad (1)$$

where  $k \in \mathbb{Z}$ ,  $(f_k)_{k \in \mathbb{Z}}$  is some sequence of vectors within  $\mathbb{R}^n$ ,  $U_k$  – unknown system of vectors,  $A$  – square matrix.

We study cubic splines approximation by means of spline collocation method for bounded on real axes solutions for linear differential equations with unbounded operator coefficients. Pros and cons of the proposed method are discussed, as well as some applications.

Classes of uniqueness of solutions for the system (1) are described, and formula for local approximation is constructed. These results are obtained by means of unification creation method for local splines for minimal defect under certain conditions on matrix  $A$  and vector sequence  $f_k$ .

- [1] U. Zavjalov, B. Kvasov, V. Miroshnychenko. *Spline function methods.*, M. Nauka, 1980.
- [2] M. Androsenko, O. Kashpirovskii, *Scientific Bulletin of Taras Shevchenko University of Kyiv. Series: Mathematics and Mechanics* **25**, (2011), p. 7-11.
- [3] O. Kashpirovskii, O. Semeniv, V. Yatsenko, *Scientific Notes of National University of Kyiv-Mohyla Academy. Series: Physics and Mathematics* **61**, (2007), p. 17-22.

14.30 – 15.00

**Regularized reconstruction of the memory order in semilinear subdiffusion**

M. KRASNOSCHOK<sup>1</sup>, S. PEREVERZHEV<sup>2</sup>, S. SIRYK<sup>3</sup>, N. VASYLYEVA<sup>4</sup>

<sup>1,4</sup>*Institute of Applied Mathematics and Mechanics, Sloviansk, Ukraine*

<sup>2</sup>*Radon Institute for Computational and Applied Mathematics, Linz, Austria*

<sup>3</sup>*Igor Sikorsky Kyiv Polytechnic Institute, Kyiv, Ukraine*

In the last two decades, fractional partial differential equations play a key role in the description of the so-called anomalous phenomena. The

signature of an anomalous diffusion is that the mean square displacement of the diffusing species  $\langle(\Delta \mathbf{x})^2\rangle$  scales as a nonlinear power law in time, i.e.  $\langle(\Delta \mathbf{x})^2\rangle \sim t^\nu$ ,  $\nu > 0$ . For a subdiffusive process, the value of  $\nu$  is such that  $0 < \nu < 1$ , while for normal diffusion  $\nu = 1$ , and for a superdiffusive process, we have  $\nu > 1$ .

However, sometimes a value of the subdiffusion order is not given a priori. Here we discuss an approach to the reconstruction of a subdiffusion order  $\nu$  from the state measurements for small time. To this end, for  $\nu \in (0, 1)$ , we analyze initial boundary value problems for semilinear integro-differential equations on the multidimensional space domain  $\Omega \subset R^n$  with the unknown  $v = v(x, t)$ :

$$\mathbf{D}_t^\nu v - \mathcal{L}_1 v - \int_0^t \mathcal{K}(t-s) \mathcal{L}_2 v(\cdot, s) ds = f(x, t, v) + g(x, t),$$

where  $\mathbf{D}_t^\nu$  is the Caputo fractional derivative and  $\mathcal{L}_1, \mathcal{L}_2$  are certain uniform elliptic operators of the second order with time-dependent smooth coefficients. It is worth mentioning, these equations play significant role in theory of materials with memory.

Based on the observation data  $\psi(t) = v(x_0, t)$  for small time  $t \leq t^*$ , we obtain the explicit reconstruction formula for order  $\nu$ :

$$\nu = \lim_{t \rightarrow 0} \frac{\ln |\psi(t) - v(x_0, 0)|}{\ln t},$$

where the only requirement for  $x_0 \in \bar{\Omega}$  is

$$\mathcal{L}_1 v(x_0, t)|_{t=0} + f(x_0, 0, v(x_0, 0)) + g(x_0, 0) \neq 0.$$

The main difficulty with the use of this formula is that only noisy observations  $\psi_\delta(t_k) \approx v(x_0, t_k)$  at a finite number  $N$  of time moments  $t = t_k$ ,  $k = 1, 2, \dots, N$ , are available in practice. To overcome this difficulty, we at first propose to reconstruct  $\psi(t) = \psi_{\delta, \lambda}(t)$  by means of the regularized regression from the given noisy data  $\psi_\delta$ , where the regularization is performed in the finite-dimensional space

$$\text{span}\{t^{\nu_i}, P_j^{(-\gamma, 0)}, \quad i = 1, 2, 3, \quad j = 1, 2, \dots, m(N)\}$$

according to the Tikhonov scheme with the penalty term  $\lambda \|\cdot\|_{L_{t-\gamma}^2(0, t_N)}$ . Here  $\lambda$  is the regularization parameter;  $\nu_i$  are our initial guesses about

$\nu$  (in particular,  $\nu_i = 0$ ),  $L_{t^{-\gamma}}^2(0, t_N)$  is a weighted space  $L^2$  with the weight  $t^{-\gamma}$ ,  $\gamma \in (0, 1)$ ;  $P_j^{(0, -\gamma)}$  are Jacobi polynomial shifted to  $[0, t_N]$ . Then, according to our formula, we consider the quantities

$$\nu(\lambda, t) = \frac{\ln |\psi_{\delta, \lambda}(t) - v(x_0, 0)|}{\ln t}$$

calculated for the sequences of (regularization) parameters:

$\lambda := \lambda_p = \lambda_0 \beta_1^p$ ,  $t := t_q = t_0 \beta_2^q$ ,  $0 < \beta_1, \beta_2 < 1$ ,  $\lambda_0, t_0 > 0$ ,  $p, q = 0, 1, \dots$

Finally, the regularized reconstructor

$$\nu := \nu_{reg} = \nu(\tilde{\lambda}, \tilde{t})$$

is chosen from the set of approximate values  $\{\nu(\lambda_p, t_q)\}$  by applying two-parameter quasi-optimality criterion [1] selecting  $\tilde{\lambda} \in \{\lambda_p\}$ ,  $\tilde{t} \in \{t_q\}$ . The proposed method is illustrated by numerical examples and compared with the known approaches.

- [1] M. Fornasier, V. Naumova, S.V. Pereverzyev, *SIAM J. Numer. Anal.*, **52**(4) (2014) 1770–1794.

15.00 – 15.30

### **On weak solvability and convergence of a finite-difference approximation for a variable-order reaction-subdiffusion equation**

A. L. HULIANYTSKYI, K. S. TOKAR

*Taras Shevchenko National University of Kyiv, Ukraine*

During early development of an embryo, functional differentiation of cells is mediated by the concentration of signalling molecules called morphogens. Hence the study of morphogen transport in extracellular environment is an important problem of developmental biology. We consider the following time-fractional equation in a bounded domain  $\Omega$  as a possible mathematical model of this process:

$$\frac{\partial u(x, t)}{\partial t} = \Delta \left( e^{-\theta(x)t} K(x) D_0^{1-\alpha(x)} \left( e^{\theta(x)t} u(x, t) \right) \right) - \theta(x) u(x, t) + f(x, t), \quad (1)$$

$$u|_{t=0} = u_0(x), u|_{\partial\Omega} = 0, \quad (2)$$

where  $u$  is the unknown concentration,  $D_0^{1-\alpha(x)}$  is the Riemann-Liouville time derivative,  $\theta$  is the reaction rate,  $\alpha$  is the position-dependent diffusion exponent, and  $f$  is the source term.



In the talk, we discuss the weak solvability of (1)–(2) and give a convergence theorem for the  $L1$  discretization of this problem with respect to time. Additionally, we discuss the numerical solutions for some model examples.

16.00 – 16.30

**General regularization scheme for functional linear regression model**

S. V. PEREVERZHEV<sup>1</sup>, A. Y. PILIPENKO<sup>2</sup>

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Igor Sikorsky Kyiv Polytechnic Institute, Kyiv, Ukraine*

The infinite-dimensional linear model

$$Y = \langle X, f_0 \rangle + \varepsilon,$$

is considered, where  $X$  is a random element with values in a separable Hilbert space  $H$ ,  $f_0 \in H$  is unknown,  $\varepsilon$  is a noise.

Given a training sample  $(X_1, Y_1), \dots, (X_n, Y_n)$  we construct an estimate  $\hat{f}_n$  for  $f_0$ , and find upper bounds for prediction errors

$$\|\hat{f}_n - f_0\|_H \text{ and } E^* \langle X^*, \hat{f}_n - f_0 \rangle_H^2,$$

where  $X^*$  is independent of the training sample,  $E^*$  is the expectation over  $X^*$ .

We consider the problem from the point of view of the general theory of ill-posed problems. Obtained error bounds are formulated in terms of a covariance operator of  $X$  and an effective dimension of a covariance-type operator.

This abstract setting covers, for example, the problem of prediction for functional linear regression

$$Y = \int_0^T X(t) f_0(t) dt + \varepsilon.$$

16.30 – 17.00

**Regularized collocation method in electrochemical impedance spectroscopy**

S. PEREVERZYEY<sup>1</sup>, S. SOLODKYI<sup>2</sup>, V. VASYLYK<sup>3</sup>, M. ZIK<sup>4</sup>

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<sup>2,3</sup>*Institute of Mathematics of NAS of Ukraine, Kyiv, Ukraine*

<sup>4</sup>*Ruder Boskovic Institute, Zagreb, Croatia*

One of the main areas of research is the study of electrochemical impedance spectra (EIS). Mathematical models for analysis of EIS were recently built in using terms of a distribution of diffusion times (DDT) [1]. Such models lead to Fredholm integral equations of the first kind with singular kernel that are ill-posed problems. That is why the development of mathematical methods for analysis that equations is very important. In the present work we develop a method to analyze electrochemical impedance spectra in terms of DDT for a parallel array of circuit elements. We consider a Fredholm integral equation of the first kind with singular kernel that describes the diffusion processes in nanostructured electrochemical energy systems. For analysis we construct a method based on Tikhonov regularization and efficient collocation schemes. The optimality of the accuracy of the given approach is established in the case of a priori choice of the regularization parameter. The effectiveness of proposed strategy is demonstrated in numerical examples. Our research is a continuation of the investigation of regularized collocation in the context of electrochemical impedance spectroscopy [2].

[1] Juhyun Song and Martin Z. Bazant, *Phys. Rev. Lett.*, 120(11):116001, 7, 2018.

[2] S. Jr. Pereverzyev, M. Zic, *RICAM-Report*, (16), 2018.

17.00 – 17.30

**Estimates of efficiency for two approaches to stable numerical summation of smooth functions of two variables**

S. G. SOLODKY, S. A. STASYUK

*Institute of Mathematics of NAS of Ukraine, Kyiv, Ukraine*

We study ill-posed problem of summation for finite smooth functions of two variables. In order to achieve stable approximation we propose two

different approaches to summation. One of them is a standard approach connected with rectangles and the other one is an alternative approach connected with hyperbolic crosses. For both of these approaches we obtain error bounds and estimate their efficiency in the sense of computational resources. An unexpected fact follows these results, that the recommendations of approximation theory with regard to the choice of the optimal method for summation of functions does not work in the case of perturbed input data. Namely, the alternative approach is more effective in comparing with the standard approach in the sense of accuracy and volume of computational resources.

## Friday

10.00 – 10.30

### **Detection of directional singularities by multivariate periodic wavelets**

K. SCHÖBER

*Institute of Mathematics, University of Lübeck, Lübeck, Germany*

Multivariate wavelet systems based on the decomposition of finite dimensional shift-invariant spaces were developed for example in [1, 2]. In these papers, the corresponding wavelet functions are trigonometric polynomials of de la Vallée Poussin-type, which can be well localized in time and frequency domain. In addition, the construction includes many different dilation matrices on each level, especially shearing matrices, which allow for directional decompositions of the frequency domain. This talk gives an overview on the construction of de la Vallée Poussin-type wavelets  $\psi_{j,\ell,\mathbf{y}_\ell}$  on the torus and their properties with respect to the detection of directional singularities of multivariate functions.

In particular, for characteristic functions  $\mathcal{T}_{2\pi} = \chi_T, T \subset [-\pi, \pi)^2$  and large scales  $j$ , there exists  $\mathbf{y}_\ell \in \mathcal{P}(\mathbf{N}_{j,\ell})$  close to the boundary  $\partial T$ , such that

$$|\langle \mathcal{T}_{2\pi}, \psi_{j,\ell,\mathbf{y}_\ell} \rangle| \geq C 2^{-3j/4}.$$

Together with the corresponding upper bound, this result implies that the location of the singularity curve is related to peaks in the magnitude of the wavelet coefficients. A similar result has been proved in [3] for discrete shearlet systems on the real line.

This is a joint work with Jürgen Prestin, UzL, and Serhii Stasyuk, IM NASU, Kyiv.

- [1] R. Bergmann, J. Prestin, *Journal of Fourier Analysis and Applications*, **21**, (2014), p. 342-369.
- [2] D. Langemann, J. Prestin, *Applied and Computational Harmonic Analysis*, **28**, (2010), p. 46-66.
- [3] K. Guo, D. Labate, *Journal of Geometric Analysis*, **28**, (2017), p. 2102-2128.

11.00 – 11.30

**Automatic wavelet-based stenosis detection in internal carotid and vertebral arteries from lumen diameters**

O. CHERTOV<sup>1</sup>, V. MALCHYKOV<sup>2</sup>, S. PEREVERZYEV JR.<sup>3</sup>, L. MAYER<sup>4</sup>,  
L. LAMPLMAYR<sup>5</sup>, R. STEIGER<sup>6</sup>, L. KUSSTATSCHER<sup>7</sup>, K. FRITSCHER<sup>8</sup>,  
M. KNOFLACH<sup>9</sup>, E. R. GIZEWSKI<sup>10</sup>

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<sup>4,9</sup>*Department of Neurology, Medical University of Innsbruck, Austria*

<sup>8</sup>*Department of Medical Image Analysis, University for Health Sciences, Medical Informatics and Technology, Hall in Tirol*

<sup>3,6,10</sup>*Neuroimaging Research Core Facility, Medical University of Innsbruck, Innsbruck, Austria*

The problem of automatic detection of stenosis usually appears in MRI angiography after performing of vessel lumen segmentation and centre-lines extraction. The main idea of the most common approach is to compare measured vessel diameters with the corresponding diameters of healthy vessel.

In this paper, authors propose to use for stenosis detection in internal carotid and vertebral arteries method based on wavelet transform technique. It includes the next steps.

First, from the evaluated diameters for internal carotid artery, it is necessary to exclude the beginning part that corresponds to the ostium. Then source data are smoothed with the help of wavelet de-noising. Authors use thresholding on three levels of wavelet transform with the Daubechies-4 wavelet and Heuristic SURE method for selection of the threshold.

As a model of a healthy vessel for carotid artery, an approximation component of the last (but no more the eight) level of wavelet decomposition is taken. For the vertebral artery, an approximation component from the penultimate level is used.

Possible stenosis is detected by computing the relative change between the expected and estimated vessel diameter and comparing it with the threshold. In order to increase the quality of detection according to [1] the length of the stenosis zone is also taken into account.

Input dataset contains records for 10 patients with two measurements of right and left carotid and vertebral arteries for each one. Performance of the proposed method was estimated using proposed in [2] three metrics – the sensitivity, the specificity, and the positive predictive value. Our method shows better results than the most powerful (according to [2]) algorithm [3].

[1] G.-M. von Reutern, *Stroke*, 43, (2012), p. 916.

[2] H. Kirişli, *Medical Image Analysis*, 17, (2013), p. 859

[3] R. Shahzad, *Stroke*, 25, (2012), p.17.

11.30 – 12.00

### **Action potential pattern recognition in cardiomyocytes**

N. IVANUSHKINA<sup>1</sup>, K. IVANKO<sup>2</sup>, Y. PROKOPENKO<sup>3</sup>, A. REDAELLI<sup>4</sup>,  
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<sup>4</sup>*Politecnico di Milano, Milan, Italy*

Generation and propagation of action potentials (AP) reflect electrical activity of the cardiac cells. According to the shape of AP it is possible to estimate functionality and electrophysiological properties of the cardiac cells. Whereas, genesis and formation of AP is determined by main ionic currents of cardiomyocytes for  $K^+$ ,  $Na^+$ ,  $Ca^{2+}$  ions, which are characterized by passing through channels with noise.

The AP morphology is key moment in determining of normal or pathological processes of cardiac cells and in the diagnosis of heart diseases in personalized medicine. Methods of drug screening are performed on the base of AP changes in cardiac cells. Also different morphologies of cardiac AP allow for evaluating the degree of maturation of human-induced pluripotent stem cells differentiated into cardiomyocytes (hiPSC-CMs) and their transformation to the main types cardiac cells.

The present study is devoted to the improvement of AP pattern recognition methods, which allow for obtaining the useful information about AP morphology without the noise. The complex method to detect and evaluate action potentials of cardiomyocytes is proposed. Signal processing

of cardiac AP is performed by means of wavelet transform and decomposition in eigenvectors basis of cardiac cycles. The parallel conductance model is used to simulate the cardiac AP with noise. Numerical experiments demonstrate the opportunity of the AP detection for various signal-to-noise ratio (SNR) and the AP features extraction.

Obtained results of simulated AP pattern recognition confirm that the new method allows us to investigate cardiomyocytes' electrical activity without masking mechanisms and to perform the feature extraction for classification of heart cells. Proposed method for cardiac AP pattern recognition is useful to test the influence of different factors on cardiac cells, evaluate the functionality of cardiomyocytes based on the change of AP morphologies and to interpret experimental results with hiPSC-CMs on the lab-on-chip platform.

12.00 – 12.30

### **Technique automated segmentation of CT bone images**

A. S. KOZEI<sup>1</sup>, N. A. NIKOLOV<sup>2</sup>, S. V. BURBURSKA<sup>3</sup>,  
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Segmentation of medical images by the existing application software does not adequately separate the background area qualitatively and the allocation of anatomical structures is partial with a significant number of artifacts. Thus, the aim of this work is to develop a technique for the automated segmentation of computed tomography of skeletal bones. Developed image segmentation algorithm has based on threshold segmentation, morphological transformations and comparison segmentation results of adjacent slices. The developed algorithm for automatized segmentation shows 22% more qualitative results bone selection compared to usual threshold method.

The obtained results significantly are reducing the time of CT images processing by a specialist in the area of radiation diagnostics and 3D printing of biological tissues and their models. Future prospects for the proposed methodology development are: its integration into specialized software tools with a user interface with a wide range of tools; improvement of machine code, reducing of computer time calculations;

improvement of the segmentation algorithm, reducing of the segmentation artifacts.

14.00 – 14.30

#### **Diagnostic criteria of bileaflet mechanical heart valve operation**

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The results of determining the diagnostic criteria for the operation of a bileaflet mechanical heart valve based on measurements of the pressure fluctuation field inside the left ventricular model, noise and vibrations outside this model are presented. The experiments were carried out in-vitro in Politecnico di Milano with a prosthetic heart valve of Sorin Biomedica Cardio (Italy). Physical simulations were performed for flow conditions of pure water and glycerine solution through an open and semi-closed mitral valve. The flow rate of the steady flow varied from 5 l/min to 20 l/min and the pulsating flow was unsteady with a frequency of 60 beats per minute. The average pressure and pressure fluctuations near the side and central jet were measured by a group of miniature total pressure and pressure fluctuation sensors [1]. The noise of the open and semi-closed valve was measured by piezoceramic heart noise sensors. The vibrations of the models of the left ventricle and atrium were measured with miniature piezoceramic accelerometers. To obtain cross correlation and spectral dependencies, measurements of pressure and acceleration fields were carried out simultaneously by a group of sensors [2]. During the measurements, the integral, spectral and correlation characteristics of the research parameters were obtained. The mean and rms values of the velocity, pressure, and acceleration fluctuations and their probability density functions were determined [3]. The coefficients of skewness and kurtosis were calculated, and the differences of hydroacoustic noise and vibrations were determined depending on the operating conditions of the bileaflet mechanical valve and the hydrodynamic characteristics of fluid flow through mitral valve [4]. It has been established that measurements of hydroacoustic noise and vibrations are an effective means of diagnostics of the operating conditions of a bileaflet mechanical heart

valve.

- [1] V. A. Voskoboinick, A. Redaelli, G.B. Fiore, ets., *Proc. Acoustical Symposium "Consonans-2015"*, (2016), p. 59-65.
- [2] V. A. Voskoboinick, A. Redaelli, O. R. Chertov, ets., *Naukovi visti NTUU KPI*, **5**, (2017), p. 41-50.
- [3] V. Voskoboinick, A. Redaelli, O. Chertov, ets., *Abstr. 6-th Inter. Conf. "Computer hydromechanics"*, (2018), p. 76-77.
- [4] V. A. Voskoboinick, A. A. Voskoboinick, A. V. Voskoboinick, ets., *Hydrodynamics and Acoustics*, **1** (91), (2018), p. 7-32.

14.30 – 15.00

### **Statistical analysis of jet flow noise across bileaflet heart valve**

L. TERESHCHENKO, V. VOSKOBOINICK, I. KUDYBYN,  
A. VOSKOBOINICK, O. RUDNYSKYI

*Igor Sikorsky Kyiv Polytechnic Institute, Kyiv, Ukraine*

The vortex and jet flow behind an open and semi-closed bileaflet mechanical heart valve is a non-linear, random process. Such processes are analyzed using the methods of mathematical statistics and probability theory. Processing and analysis of the experimental results of measuring the field of pressure fluctuations, hydrodynamic noise near the mitral valve and vibrations of the left ventricle and atrium models were carried out with the determination of statistical moments of various orders. The probability density functions of pressure fluctuations and accelerations showed differences for the operation of an open and semi-closed valve. The average values of the measured parameters, their dispersions and standard deviations increase when one valve leaflet closes and the flow and viscosity of the fluid increase [1]. In the spectral power densities of the pressure and acceleration fluctuations, as well as in their first moments, significant deviations are observed at different frequencies for the operating conditions of an open and semi-closed valve [2]. Auto and cross-correlation functions, coherence functions and phase spectra [3] undergo changes with changes in valve operating conditions, fluid viscosity and flow rate. The statistical moments of the third and fourth orders, namely, the coefficients of skewness and kurtosis of the field of pressure and acceleration fluctuations also react to changes in the conditions of the experiments. Analysis of the space-time characteristics of the pressure and acceleration fluctuation fields, which were measured by a group



of sensors, made it possible to determine the scales of the vortex structures, the direction and velocity of their transfer [4]. Statistical analysis has shown that measurements of hydroacoustic parameters and vibrations are an effective means of diagnosing the operation of a bileaflet mechanical heart valve.

- [1] V. A. Voskoboinick, A. Redaelli, O. R. Chertov, ets., *Naukovi visti NTUU KPI*, **5**, (2017), p. 41-50.
- [2] V. A. Voskoboinick, A. A. Voskoboinick, A. V. Voskoboinick, ets., *Hydrodynamics and Acoustics*, **1** (91), (2018), p. 7-32.
- [3] V. A. Voskoboinick, *Applied hydromechanics*, **14**, (2012), p. 49-62.
- [4] V. A. Voskoboinick, V. T. Grinchenko, A. P. Makarenkov, *Acoustic bulletin*, **3**, (2000), p. 21-29.

15.00 – 15.30

### **The influence of left ventricle's torsion motion on the reology of blood flow**

V. OVERKO

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The Newtonian assumption of the blood is almost the common approximation in the numerical study of the cardiovascular systems. In most published research the effect of the blood non-Newtonian characteristic has been neglected and most researchers have assumed a constant viscosity during the whole cardiac cycle. This assumption could affect the prediction of the hemodynamics of the cardiovascular system in the whole or in a part of the cardiac cycle, especially in a period with low shear rate [1]. Moreover, it has been argued that the blood significantly exhibits the non-Newtonian behavior in disease conditions such as the myocardial infarction, cerebrovascular diseases, and hypertension [2] and [3]; consequently, the rheological parameter of the blood must be employed in numerical simulation of patient-subject cardiovascular systems. In addition, due to the recent advancement of CFD modeling, it is now much more feasible to implement the complex non-Newtonian constitutive assumptions in Navier-Stokes equations.

The left ventricular (LV) torsion motion plays an important role for LV ejection and forming the complex structure of flow in the aorta. Non-Newtonian effects were seen to be important in aortic regions presenting high velocity gradients.

The results of our simulation displays that the difference in the reological properties increases significantly in the phase of the negative acceleration of cardiac circle. It represents more brightly for zones of backward flow. We can note than Non-Newton properties of blood suppress the backward flow at the aorta.

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16.00 – 16.30

### **On sloshing in conical containers**

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Linear and nonlinear liquid sloshing in a circular truncated coaxial conical tank due to horizontal excitation is studied by using the multimodal method which involves the analytically approximate sloshing modes [4]. The forcing frequency is close to the lowest natural sloshing frequency and there are no secondary resonances in the forcing frequency range. General fully and weakly nonlinear modal equations are derived by using the non-conformal mapping technique and the Moiseev-type asymptotics [1, 3]. This modal system is a generalization of the parers [2, 3]. The Moiseev-Narimanov modal system is used to construct an asymptotic time-periodic solution and, thereby, classify the corresponding steady-state wave regimes appearing as stable and unstable planar waves and swirling. The Lukovsky formula [1] is utilized to evaluate liquid force response when tank is under external harmonic excitation.

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- [3] O. V. Solodun, *Rep. Institute of mathematics, NASU* **14**, 2, (2017), p. 33-149.
- [4] O. V. Solodun, *Rep. Institute of mathematics, NASU* **15**, 1, (2018), p. 233-259.

**Approximation by Fourier sums in metrics of the spaces  $L_p$  on the classes of periodic differentiable functions**

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Let  $L_p$ ,  $1 \leq p \leq \infty$ , be the space of  $2\pi$ -periodic functions with the standard norm  $\|\cdot\|_p$ . Let  $r > 1$  and  $\bar{\beta} = \{\beta_k\}_{k=1}^\infty$  be an arbitrary sequence of real numbers. Further, let  $W_{\bar{\beta},1}^r$  be the set of all  $2\pi$ -periodic functions  $f$ , representable as convolutions of the form

$$f(x) = \frac{a_0}{2} + \frac{1}{\pi} \int_{-\pi}^{\pi} \varphi(x-t) B_{r,\bar{\beta}}(t) dt, \quad a_0 \in \mathbb{R}, \quad \|\varphi\|_1 \leq 1, \quad \varphi \perp 1,$$

with the kernel  $B_{r,\bar{\beta}}(t) = \sum_{k=1}^{\infty} k^{-r} \cos\left(kt - \frac{\beta_k \pi}{2}\right)$ ,  $r > 1$ ,  $\beta_k \in \mathbb{R}$ .

If  $\beta_k \equiv \beta$ , then  $W_{\bar{\beta},1}^r$  is the Weyl-Nagy class  $W_{\beta,1}^r$ .

We investigate the quantity  $\mathcal{E}_n(W_{\bar{\beta},1}^r)_{L_p} = \sup_{f \in W_{\bar{\beta},1}^r} \|f - S_{n-1}(f)\|_p$ , where

$S_{n-1}(f)$  is the partial Fourier sum of order  $n-1$  of  $f$ .

**Theorem 1.** *Let  $r > 1$ ,  $1 \leq p \leq \infty$ ,  $n \in \mathbb{N}$  and  $\bar{\beta} = \{\beta_k\}_{k=1}^\infty$  be an arbitrary sequence of real numbers. Then for  $r \geq n+1$  the following estimate holds*

$$\mathcal{E}_n(W_{\bar{\beta},1}^r)_{L_p} = n^{-r} \left( \frac{\|\cos t\|_p}{\pi} + O(1) \left(1 + \frac{1}{n}\right)^{-r} \right), \quad (1)$$

where  $O(1)$  is a quantity uniformly bounded with respect to the all considered parameters. If  $r/n \rightarrow \infty$ ,  $n \rightarrow \infty$ , then the estimate (1) becomes the asymptotic equality.

For  $p = 1$  and  $\beta_k = \beta$ ,  $\beta \in \mathbb{R}$ , the estimate (1) was established by S. B. Stechkin [1, Theorem 4].

[1] S. B. Stechkin, *Proc. Steklov Inst. Math.*, **145** (1981), 139-166.

17.00 – 17.30

### One estimate of three-monotone spline approximation

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For any 3-monotone on  $[0, 1]$  function  $f$  (i.e. its third divided differences are nonnegative for all choices of four distinct points, or equivalently,  $f$  has a convex derivative on  $(0, 1)$ ) in [1] a cubic 3-monotone (like  $f$ ) spline  $s$  with  $n \in \mathbb{N}$  "almost" equidistant knots  $a_j$  is constructed such that locally

$$\|f - s\|_{[a_j, a_{j+1}]} \leq c \omega_4(f, 1/n, [a_{j-3}, a_{j+4}]), \quad j = 1, \dots, n,$$

and so

$$\|f - s\|_{[0, 1]} \leq c \omega_4(f, 1/n, [0, 1]),$$

where  $c$  is an absolute constant,  $\omega_4(f, t, [\cdot, \cdot])$  is the 4-th modulus of smoothness of  $f$ , and  $\|\cdot\|_{[\cdot, \cdot]}$  is the max-norm over  $[\cdot, \cdot]$ . Remark that  $\omega_4$  here cannot be replaced by  $\omega_k$  with  $k > 4$ .

- [1] G. A. Dzyubenko, *Collection of works of the Inst. of Math. of NAS of Ukraine* **13**, (2016), No. 2, p. 1–14 (Ukrainian).

## Participants

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